

Review of Australian access to ISIS

- The World's Most Intense Spallation Neutron Source

9 March 2006



January 2006 ISIS and Diamond (showing 2nd ISIS target station - building now complete)

**Submission by the
Australian Institute of Science and Engineering (AINSE)
to the review committee**

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Introduction

This document responds to the request by Professor Erich Weigold, Executive Director, Physics Chemistry and Earth Sciences, Australian Research Council of the 14th December 2005 for the review of funding provided by the Australian Research Council's Linkage Infrastructure Equipment and Facilities (LIEF) scheme "Access for Australian Researchers to Advanced Neutron Beam Techniques". Included with this document, as requested, are:

- A strategic plan for the next three years and beyond;
- The publication record (including joint publications) with other participants since the last review;
- The numbers of participating postgraduate students, including completion rates and postdoctoral fellows since the last review; and
- List of user grants including collaborative grants with other participating institutions since the last review.

This submission is based upon the growth of new areas of science and the training of a new generation of students and postdoctoral fellows in those areas. The areas of growth accessed through ISIS map upon areas of scientific and technological strength in Australia, using facilities not available in Australia. The submission notes the complementarity between some of the expected nuclear facilities in Australia through the OPAL reactor and those presently at the ISIS spallation neutron source and at the ISIS Second Target Station in 2007-8 of which there will be no equivalent in Australia.

This submission has been prepared by a group of the principal users of the ISIS facility - Professor Stewart Campbell (University of New South Wales (ADFA)), A/Professor Evan Gray (Griffith University), A/Professor Ian Gentle (University of Queensland), A/Professor Brendan Kennedy (University of Sydney), A/Professor Erich Kisi (University of Newcastle), A/Professor Jim Low (Curtin University), Professor John White (Australian National University) and Dr Allan Pring (University of Adelaide). This submission and the associated proposal for 2007 have the support of the AINSE Council of ANSTO, and, for specific contributions towards the project, of the University partners in the previous and proposed Linkage arrangements.

The issues to be addressed in the submission to the Australian Research Council, set out in Professor Weigold's letter, are reproduced in Appendix 1. The structure of this report addresses those issues sequentially. Access to ISIS has allowed Australian research in "soft matter" science to develop, as well as areas of "hard matter" science including muons and inelastic scattering, for which there is no provision in Australia.

At present Australia pays for about 1% of the available instrument time at the ISIS source. The list of Australian users since 1998 (including postdoctoral fellows and students) is given in Appendix 2, and the geographical distribution shown in Figure 1. The scientific and geographical breadth of interest in ISIS access, places the process squarely within the remit of the Australian Institute for Nuclear Science and Engineering (AINSE).

A mark of Australia's scientific contribution to using neutrons, was the decision to award to Australia the 2005 International Conference on Neutron Scattering (ICNS2005), held in Sydney in November. Figure 2 shows a photograph of the ca. 700 participants from all parts of the world.

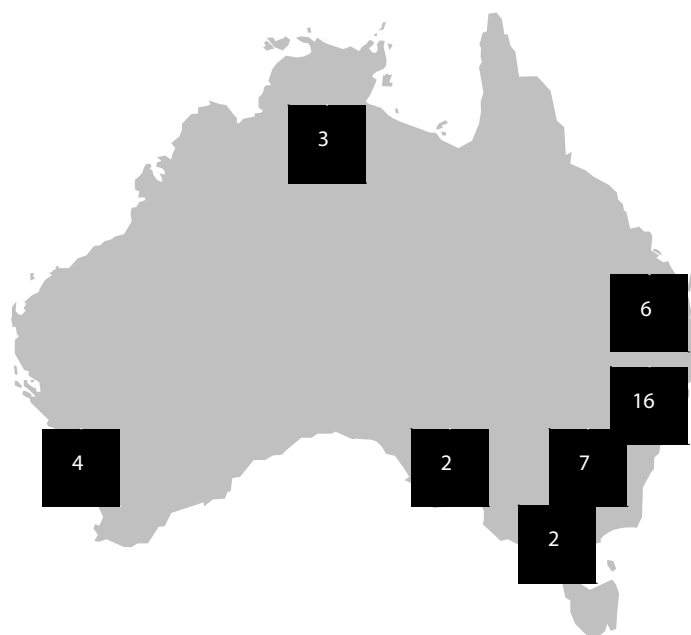


Figure 1. Geographical (and number) distribution of Australian Users from 2001 - 2005 inclusive



Figure 2. Group photograph of attendees at the International Conference on Neutron Scattering, Sydney Convention Centre 27 November – 2 December 2005

Chapter 1

Evidence of significant benefits to Australia resulting from access to a major facility not otherwise available to Australians

An Australian Strategy

An overall strategy for Australia to participate in essential “cutting edge” science beyond our national resources was elaborated in 1990:

‘...It is therefore imperative that Australian scientists be permitted to increase their overseas access if the existing momentum of Australian neutron scattering research is to be maintained and if Australian scientists are to remain abreast of their overseas colleagues’

Small Country – Big Science, ASTEC report to the Prime Minister, 1990.

The need for Australia to base strong scientific infrastructure at home, as well as to be involved with international links, has been reiterated in the recent National Competitive Infrastructure Scheme (NCRIS) roadmap “Exposure Draft”, which AINSE strongly supports. The AINSE submission to NCRIS says:

- ***AINSE endorses the principles set out (on page 6 of the NCRIS “Exposure Draft” Principles November 2005) associated with integrating capabilities.***

“The Strategy should seek to enable the fuller participation of Australian researchers in the international research system”

- ***AINSE recommends that the NCRIS committee give consideration to the balance of investment in national and international facilities where the idea of “complementarity” can be effectively used. International collaboration is itself a strategic component of the investment in major infrastructure in Australia.***

This submission focuses on three key benefits of access to ISIS for Australian Science and Technology: **Creativity, Contestability and Complementarity**. These themes will reoccur throughout this submission.

Creativity

In the past five years new neutron and synchrotron methods have made the area of “soft matter” research scientifically assessable in new ways. Through the ISIS subscription, Australians have participated, **and in some cases led these advances**. This area, at the interface between physics, chemistry and biology embraces polymer and biological macromolecular research, surfaces and interfaces and the design of new materials of commercial importance. The “cold neutron” (long wavelength) scattering accessed at ISIS is not available in Australia at present, but should be from OPAL in 2007 for some experiments if all goes to plan. At the same time, unique instruments currently at ISIS – such as the high-resolution powder diffractometer GEM, the inelastic scattering instruments and the muon facility have opened new areas of science in “hard matter”.

The new \$AUD295M “second target station” with its own instrument budget will take the “next step” of innovation for cold neutron instrumentation at ISIS. Australians have been involved in the working parties for this facility and the instrumentation will complement that at the OPAL reactor in many respects. This facility is due to open in 2007-2008.

Contestability

Access for both hard and soft matter science has placed Australian researchers in direct competition (through the ISIS proposal review process) with the best international groups. This aspect of “contestability” is of continuing value to test the quality of Australian programs in new areas as well as create new international linkages. Evidence of the quality of the scientific and industrial components of this research is given below.

Complementarity

The OPAL research reactor at Lucas Heights will be a facility of international quality when in operation. All Australian users look forward to the extensive use of this facility, and if international trends are followed, the number of groups using neutrons will grow. AINSE has implemented a “tenure track” Research Fellowship scheme to promote this. The situation with respect to international participation at other neutron sources is very similar to that we will have here. The large investment overseas has produced instruments complementary to what we have in Australia. The best strategy to manage this useful but inevitable phenomenon is to ensure that what is built in Australia is the best of its kind. This with our strong international links, developed through “suitcase science”, should be kept so that we benefit from major investments elsewhere using their complementary instrumentation, possibly in exchange for their access here.

Benefits to Australia Resulting from Access.

Research

Quality of Australian Proposals

The area of “soft matter” science in Australia has grown to produce a significant body of researchers, tested by international competition and now capable of making the best of what will be provided at OPAL - this area will become one of Australia’s strengths from a situation several years ago where Australia had fallen behind Europe and North America in areas of “soft matter” science including polymer and interfacial structure.

Australia’s subscription to ISIS buys entry to the ISIS peer review process, which is openly contested at the highest international level. The quality of Australian proposals measured against international competitors has increased with the level of demand. In the most recent 5-year period, ISIS selection panels awarded Australian proposals 214 beam days out of 452 requested, a ratio of 1:2.11. The most recent data are shown in Table 1.

The over-subscription ratio at instruments at ISIS, measured in the same way, approaches three across the board, and is up to five for the instruments most frequently requested in Australian proposals. Hence the projects of Australian researchers have achieved sustained excellence when measured in international terms at one of the very finest neutron beam facilities in the world.

Another way of expressing Australian performance is that, while the subscription corresponds to about 1% of the ISIS operating budget, Australian science secured 1.75% of the facility on average in 1994-8. The most recent figures indicate that Australian proposals secure nearly 3% of the available ISIS beam time compared to the 1% that we now pay for.

Table 1. Performance of Australian Research Proposals at ISIS

The drop in the number of days allocated in 2004 and 2005 is largely explained by extended scheduled shutdowns in the middle of 2004 and at the end of 2005.

Year	Request	Allocated	Australia Success%
1998	48	35	73%
1999	75	58	77%
2000	49	37	76%
2001	83	74	89%
2002	151	77	51%
2003	140	96	69%
2004	126	54	43%
2005	84	56	67

Research Training

For a new graduate student or for a postdoctoral fellow who has never worked at a top international research facility before, the experience of working at ISIS is an important career step. Work at such a facility can be at the lowest level just making a series of measurements, but at top facilities like ISIS the excellent data acquisition systems allow real time interaction between the experimenters and the experiment. An experiment is done rather than a measurement.

For success in such an enterprise it is essential that the experiments are well prepared, that there is familiarity with the data handling and with first approximation models for online data analysis as the experiment proceeds. Such experimenter – experiment interaction is vitally important in chemical and biological experiments where the initial characterisation of the sample (which might have aggregated or decomposed) is essential. The preliminary use of X-rays and other characterising techniques in Australia and UK before doing the neutron experiments is an integral part of the work. This process is a most important discipline for new researchers.

Another novel aspect of research training given by work at ISIS is the creation of research networks both at the academic and the graduate student levels. As a result of ISIS interactions collaborative programs between Australian, UK and European scientists have developed. Two examples are;

- Australia contributed to the capital cost of the world's best liquid surface reflectometer (SURF). Australian groups are pioneers here. As a result, Dr Michael James from ANSTO was "seconded" to ISIS for six months to act as instrument scientist with UK colleagues for the newly developed instrument. Dr James has subsequently returned to a permanent position at ANSTO and is developing Australia's first neutron reflectometer on the HIFAR reactor. This will be complementary to that at ISIS.
- Dr Stephen Holt who constructed Australia's first X-ray reflectometer in collaboration with Professor J W White and Professor DC Creagh at the Research School of Chemistry, ANU was recruited as a permanent staff member at ISIS to work as officer responsible for the SURF instrument. He is serving as a key "local contact" for Australian and European users and promoting further international collaborations for our users at ISIS.
- Dr Duncan McGillivray, Rhodes scholar from Australia to Oxford University, 2001, and subsequently Post Doctoral Fellow at John Hopkins University, USA, has become a

promising young researcher in the area of biological structures at interfaces using neutron scattering and synchrotron techniques. He will be returning to Australia in August 2006 after extensive work under the supervision of Dr R K Thomas FRS during his PhD at Oxford.

- There are other examples of research students from Australia joining British groups after their theses and vice-versa.

An important aspect of networking at ISIS is the age distribution of the scientists using this facility. This is shown in Figure 3, which peaks at age 30. There is thus a high probability for young researchers meeting up and eventually collaborating with other young researchers from the international scientific community. When this fact is coupled with the wide spread of the science done at the ISIS facility it can be seen that cross fertilisation between physics, chemistry, geology, biology, engineering and materials science readily occurs in the use of this facility. With around 1600 visitors per year a unique quality to the research training is added. The list of Australian users at ISIS since 1998 is given in Appendix 2.

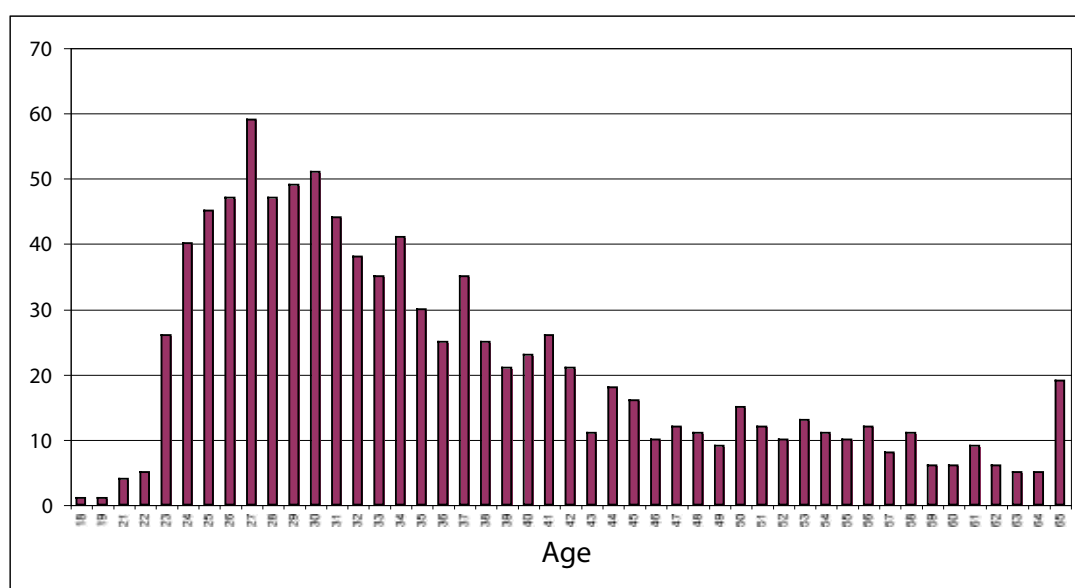


Figure 3. Age distribution of the users of ISIS

The Public Sector and Industry

Through access to ISIS new science – technology linkages have been created. We cite here programs for which access to ISIS has been essential. For these there is a component of underlying research, which could not have been done without this access and which has potential and actual benefits to Australian health science and industry.

The work of Professor Ian Gentle, at the University of Queensland, on “Lung Surfactants” has shed light on the mechanism of operation of a **lung surfactant protein** that is crucial for the breathing process in humans and animals. Neutron reflectivity studies have indicated that the protein changes its shape at the air/water interface as it is compressed, an observation which has important implications for the development of therapies for respiratory distress syndrome, an ailment that afflicts most infants born prematurely. The results of this work were selected by the ISIS Facility as a Research Highlight and featured in the 2003 ISIS Annual Report.

The work of Professor John White and his group at the Research School of Chemistry on the structure and stability of **emulsions** is an area of physical chemistry of industrial interest ranging from food science to explosives technology. Neutron small angle scattering and

reflectometry at ISIS have been of unique value for finding a radically different model of the structure of high internal phase emulsions, detecting for the first time the surfactant distribution in quantitative terms between the phases and at the interfaces. Control of the microstructure in these systems determines their stability and rheology. The work is being done as part of an ARC linkage program, which has been renewed for a further 3 years with the full support of ORICA Australia Ltd. The application of similar techniques to milk and milk products has shown how the interfacial structure in this emulsion changes with temperature mechanical treatment.

The application of similar techniques to **milk and milk products** has shown how the interfacial structure in this emulsion changes with temperature mechanical treatment. Experiments are being undertaken to understand the nanoscale changes induced by processing in the casein micelle and the milk fat membrane. These experiments on emulsions are highly relevant to industrial and food processing technologies.

Related work on **protein structure at interfaces** in the White group has shown for the first time, that the interfacial region of proteins – for example at the air-water interface can be studied up to temperatures of up to 80°C in the absence and the presence of denaturing substances. These studies produced the first evidence of the consequent structural changes and the thermodynamic quantities associated with them for the 100Å thick interfacial region. It appears that the distribution of hydrophobic and hydrophilic components of the protein is put under such tension by the disparity in forces at an air-water interface that proteins with weak internal bonding may be “torn apart” and lose all of their tertiary structure – even in the absence of chemical denaturants. This work is highly relevant to identifying the way in which proteins act in biology as “templates” for biomineralisation of shell and bone. It has now been mimicked in the laboratory and by studies at ISIS producing the first example of a silicate film grown on a protein centering substrate.

As part of an ARC Discovery project, Kennedy (Sydney University) Withers (ANU) and Howard (ANSTO) have examined the details of the **structural phase transitions in complex oxides** using the High Resolution Powder Diffractometer at ISIS. This work has increased our fundamental understanding of the nature of phase transitions in this technologically important class of materials.

A “cluster” of Sydney, Newcastle and ACT scientists have developed an approach to perovskite crystallography (that is studies of the multitudinous variants) based on a combination of high-resolution neutron powder diffraction with group theoretical analysis. Perovskites are of interest for devices, in other materials applications, and to earth sciences. The group includes Harold Stokes (Brigham Young University), Brendan Kennedy (Sydney), Erich Kisi (Newcastle), Withers (ACT) and more recently Zhaoming Zhang.

The work is well recognised as evidenced by

- >100 citations of original group theory paper (Howard & Stokes, Acta Cryst B54, 782, 1998).
- reproduction of work from this paper in monograph published in 2000
- invited talk at European Crystallography Meeting, 2003
- invitation to write review for Acta Crystallographica: Foundations of Crystallography (Howard & Stokes, Acta Cryst A61, 93, 2005).
- invited talk at International Crystallography Congress, Florence, 2005
- invited to talk at General Meeting of the International Mineralogical Association, Kobe, July 2006.

The experimental aspects of this work depend critically on neutron data, and the high resolution

accessible using the **High Resolution Powder Diffractometer (HRPD) located at the ISIS facility**. This is the only diffractometer capable of yielding data of the quality we need, and will remain so into the foreseeable future. This high resolution is maintained across the whole diffraction pattern, whereas reactor based instruments, if they could match it, would do so only over a very limited angle range. We have recently tried an approach of matching the resolution using synchrotron based diffractometer (at SPring-8, Japan), then recording the required neutron data at lower resolution, but this has not really been successful. One reason is that sample preparation for the synchrotron work (none required for an HRPD measurement) has damaged the samples to the extent that the expected resolution has not been obtained. We are therefore not particularly optimistic that even with both new X-ray and neutron sources in Australia that we can complete the work here. The interest of ISIS staff and other U.K. scientists in this work might also be lost.

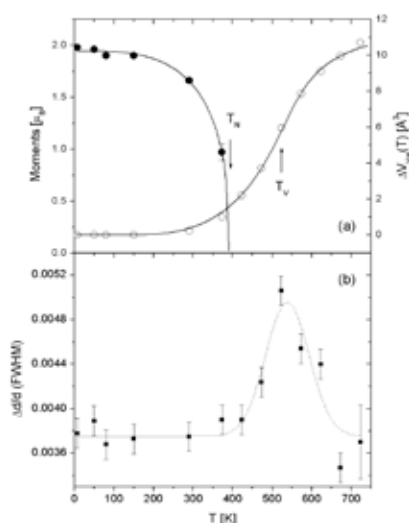


Figure 4. (a) Graphs of the Mn magnetic moment and the valence-induced volume change of EuMn_2Si_2 as a function of temperature. **(b)** The variation of the line-width of the (110) reflection (expressed in terms of the interplanar spacing d) of EuMn_2Si_2 as a function of temperature. The dashed line shows a Gaussian fit to the data.

Australian researchers have made outstanding contributions in experimental and theoretical areas of **condensed matter** and materials physics, particularly **magnetism**, over the past three years. As part of their long-standing research collaboration in the structural and magnetic properties of materials, Professor Stewart Campbell (UNSW@ADFA) and Dr Michael Hofmann (Technische Universität München) have investigated important series of rare-earth intermetallics. Europium-based compounds are of special interest as they exhibit a wide range of unusual physical and magnetic properties as well as intermediate valences associated with the transition from the Eu^{2+} ($4f^6$) configuration to the Eu^{3+} ($4f^7$) configuration.

Another area of excellence is at Curtin University (A/Professor Jim Low and A/Professor Craig Buckley). Their Centre for Sustainable Resource Processing is conducting a major research project into the development of **geopolymer concrete**. This project is a collaborative effort between the Applied Physics, Chemistry and Civil Engineering departments at Curtin University, the Australian Nuclear Science and Technology Organisation (ANSTO), and industry partners. Part of this project is investigating the optimisation of the properties of geopolymers with respect to the Si:Al:Na *molar* ratio of the starting materials. A study of the correlations between compressive strength and Si:Al:Na chemical composition has shown that the compressive strength may be chemically optimised.

Aluminosilicate inorganic polymers, also known as geopolymers, are materials with useful physical properties. Potentially, they are suitable for many applications such as Portland cement replacement, high temperature composites, radioactive waste encapsulation, castable ceramics and others. The aim of the proposed experiment is to determine high resolution Total Correlation Functions $T(r)$ from neutron scattering data. These are to be used for gaining more

information about how the molecular structure in these amorphous materials is influenced by elemental composition.

The research involves collaborations with colleagues in Germany, Canada, Italy, and the United Kingdom, and will contribute to Australia's already high standing in the international field of magnetism research. An ARC research associate will shortly be appointed to work on this project with funds also available for a PhD scholarship.

Research in the group of Cameron Kepert, Federation Fellow in the School of Chemistry at the University of Sydney focuses on the structure and dynamics of a new family of crystalline materials that display negative thermal expansion (NTE; i.e., contraction upon warming). This fascinating and highly useful property has been observed previously only in a small number of oxide-based materials, in which transverse vibrations within the material lattices have the effect of pulling distant atoms closer together as the temperature is increased. A unique feature of the new materials is their molecular rather than atomic connectivity; the structures consist of molecular frameworks bridged by cyanide linkers. The extension of the field of NTE to an entirely new class of materials opens up numerous exciting avenues for exploring the fundamental mechanism of thermal expansion. Further, the potential of the new materials for commercial application, for example as substrates, supports, optical components, composites, etc., is being explored.

A concerted research program is underway both to elucidate the novel mechanism for NTE in these materials and to extend the family to include new members with enhanced properties. A barrage of structural and physical techniques are being employed to characterise these phases. Of principal importance amongst these are neutron methods. Recent neutron diffraction experiments on the HRPD and POLARIS beamlines at ISIS have provided variable temperature data of unprecedented accuracy on the thermal evolution of the structures of $\text{Zn}(\text{CN})_2$, $\text{ZnPt}(\text{CN})_6$ and $\text{MnPt}(\text{CN})_6$. Detailed refinement of these data reveals the thermal excitation of transverse vibrations of the cyanide bridges, a mechanism we believe is principally responsible for the NTE behaviour. Atomic pair distribution functions obtained from total neutron scattering experiments on the GEM beamline at ISIS on $\text{Zn}(\text{CN})_2$ and $\text{ZnPt}(\text{CN})_6$ further support this proposed mechanism, and point to the existence of Rigid Unit Mode (RUM) type behaviour in these phases. Inelastic neutron scattering experiments performed on the PRISMA beamline at ISIS have demonstrated the presence of low energy phonon bands in $\text{Zn}(\text{CN})_2$ and $\text{ZnPt}(\text{CN})_6$, which we believe are associated with concerted transverse displacement of the cyanide units.

Direct application of research results

The wide science applications of neutron scattering have led to actual and potential use in industry-linked research. With the recent improvements in facilities (particularly the ISIS access and ARC RIEF assistance with the upgrading of instruments at HIFAR) such potential will be easier to achieve in the future.

The processes of **ore formation** in nickel deposits and the mineral reactions that occur during their weathering and ore processing have been studied using the high resolutions and high flux offered by the ISIS source. This work has recently been extended to in situ studies under hydrothermal conditions in specially designed hydrothermal cells for in situ neutron powder diffraction. The research has been undertaken as part of a collaboration with scientist at the University of Adelaide, Western Mining Corporation (now BHP Billiton) and the Universities of Münster and Cambridge.

Harsh Environments Characterisation of engineering ceramics by neutron diffraction has

established the existence of previously unsuspected phases in **zirconia ceramics** and subsequently used for quantitative phase analysis (ICI Advanced Ceramics, ANSTO, CSIRO Division of Materials Science and Technology, Sydney University). Neutron residual strain assessments have also been used in the development of processing methods for fracture-resistant zirconia-alumina ceramics (Alcoa of Australia Ltd, Rojan Advanced Ceramics, and Curtin University of Technology).

Surface Chemistry of Minerals

The research project area at Griffith University is concerned with the interaction of leaching and deposition reagents with the surface of various metal sulphides and metals. Specific topics include:

- Flotation reagents
- Chemical bath deposition (CBD) of semiconductors
- Electroless plating (CBD) of copper and gold
- Non-cyanide gold leaching processes
- Quantum confined multi layer semiconductors by CBD

Current ISIS based research work is investigating the mechanism of copper sulphide deposition and the initial stage of the synthetic covellite leaching process (Hope, Holt, Munce and Parker). This investigation utilises the high intensity pulsed neutrons available at ISIS to enable the investigation of changes occurring at the sample surface in real time. It is proposed to combine the neutron scattering experiments with concurrent Surface enhanced Raman scattering spectroscopy to provide chemical bonding information as well as scattering density and thickness data in real time. The time dependence of these experiments is such that OPAL is unlikely to have sufficient flux or sensitivity to be suitable for this research project. High intensity ionizing radiation sources, such as APS in Chicago are useful for investigating leaching processes, but they perturb the deposition / plating reactions by decomposing required intermediates in the reaction. ISIS appears to provide the only suitable non-Raman facility for our research.

The covellite (CuS) deposition process has been used to elucidate the mechanism of film formation in the chemical bath deposition of semiconductors. Ms Buckley is commencing her PhD program and her topic centres on studying the deposition of quantum confined multi layer structures. The semiconductor materials will be chosen to optimise the structure "band gap" properties and will probably utilise cadmium / indium telluride with zinc sulphide coatings. Our research at ISIS involves the deposition of 100 nm thick films onto optically flat solid surfaces, two dimension nano structures. The deposition process is also capable of generating particles with the same size range, but in three dimensions (quantum dots). We will need to investigate these multilayer structures during the next three years.

Electrode-less plating is an important semiconductor processing technology and surface finishing process. The mechanism of the surface deposition process is not characterised. The combination of neutron scattering and Raman spectroscopy offers us the possibility of investigating these surface reactions in real time. We propose to combine our Renishaw 100 fibre optic Raman probe and a neutron scattering deposition cell on SURF at ISIS in 2006. The experiment will require the pulsed neutron source intensity in order to gain good quality scattering data. Demonstration of this combination of techniques will be undertaken using the electroless plating of one of either silver, copper or gold thin film. Successful results will then allow investigation of a range of gold hydrometallurgy leaching processes with Jeffrey from CSIRO.

Chapter 2

The relevance of the facility to national needs and the availability of comparable infrastructure in Australia. In particular, the benefits to Australia of continued access

The National Needs

An access agreement for Australian scientists to ISIS¹ was concluded on the basis of the ASTEC report quoted above and took effect from 1992. The decision to internationalise our neutron scattering effort responded to the decreasing competitiveness of the only Australian facility, HIFAR² at ANSTO and a leap forward in European and US science using neutron methods.

'Progress in condensed-matter and materials physics, as in many other scientific fields, will require continued investment in major facilities for experiments in such areas as neutron scattering and synchrotron radiation. These facilities provide capabilities far beyond those available in individual laboratories. Though they have been developed and supported primarily by the condensed-matter and materials physics community, they also serve thousands of scientists and engineers in other endeavours, such as structural biology and environmental science.'

The Physics of Materials, report by the Committee on Condensed-Matter and Materials Physics of the US National Research Council, 1997.

The quote above remains true today. Neutron scattering continues to occupy a central place in the thinking of major agencies concerned with infrastructure provision. In the United States the US\$1 billion "Spallation Neutron Source" (SNS) is under construction at Oak Ridge and in Japan a US\$1.3 billion accelerator and spallation neutron source project is also being made by the Japanese Atomic Energy Research Institute and KEK. This need will persist after 2006 for certain important techniques for which the replacement reactor instruments will be complementary to those at a spallation neutron source, such as inelastic scattering and muon science.

Fifteen years after the ASTEC report, Australia now has a strong and growing community of internationally tested neutron scattering users across the broad field of biological, chemical, physical and material sciences - through "suitcase science", and the development of facilities using thermal beams at HIFAR. The OPAL reactor will strongly build upon these developments and the intended international participation in it will provide some contestability for Australian work - an essential aspect in AINSE's opinion. The point about future complementarity has been made above in paragraph 13.

The Benefits to Australia of Continued Participation

¹ ISIS is the neutron spallation source operated by the Rutherford Appleton Laboratory in the UK on behalf of the Engineering and Physical Sciences Research Council.

² HIFAR (High-Flux Australian Reactor) was built in the late 1950s. In the modern context it is quite low in neutron flux and is not optimised for neutron beam research.

The three key benefits of continued participation are:

- Access to complementary infrastructure;
- Access to the ISIS contestability processes and international collaborations through participation there; and
- Access to new developments in neutron technology and instrument design through participation.

Relevant points related to the first two benefits have been made above in the discussion of quality, contestability and complementarity.

We add to the complementarity and contestability points the statistics of Australian use of ISIS instruments by type (to illustrate complementarity), the overall statistics of Australian use of ISIS and an update on the high success rate achieved against the strong European and international demand for ISIS over the last two years when both ISIS and ILL (Grenoble) have had shut downs for long periods for refurbishments.

The last dot point above is also significant. The Rutherford-Appleton Laboratory has much broader scope than the ISIS facility. The remit of the Central Laboratory of the Research Councils, UK, (CLRC), is much wider than ISIS and involves development of neutron scattering instrumentation, X-ray instrumentation, laser physics and nanotechnology. Broader collaborations in both technology as well as science will be initiated by keeping this link.

The level of demand for neutron scattering in Australia has grown and diversified since access to ISIS became possible. The percentage of time gained compared to requested in competition with all users of ISIS is shown in Figure 5 below. The high success rate of Australian proposals is noted as is also the percentage of time gained compared to the 1% for which we pay. During 2004-5 there was significant downtime at both ISIS and the ILL Grenoble.

Since the last review the demand has diversified with four new research groups accessing ISIS: Professor Greg Hope, Dr Paul Meredith, Dr Garry Denis and Professor Allan Pring. In addition, people who were students in the previous period have commenced research in their own right: Dr Tomasz Blach and Dr Jenny Forrester. AINSE has awarded two postgraduate top up scholars to doctoral candidates who are conducting research at ISIS: Adam Perriman and Karena Chapman.

With these growth points and AINSE's strategic plan for future developments (see Appendix 6) AINSE undertook a bench marking exercise of all neutron scattering carried out through it (in Australia and overseas) in comparison to the performance of ANSTO-based projects with the same national and international scope. The benchmarking was based on inputs, outputs and outcomes as measured by various parameters and showed an essentially equal quality of performance from the two groups. (AINSE is also carrying out similar benchmarking operations for other parts of its program in connection with development of the next strategic plan.)

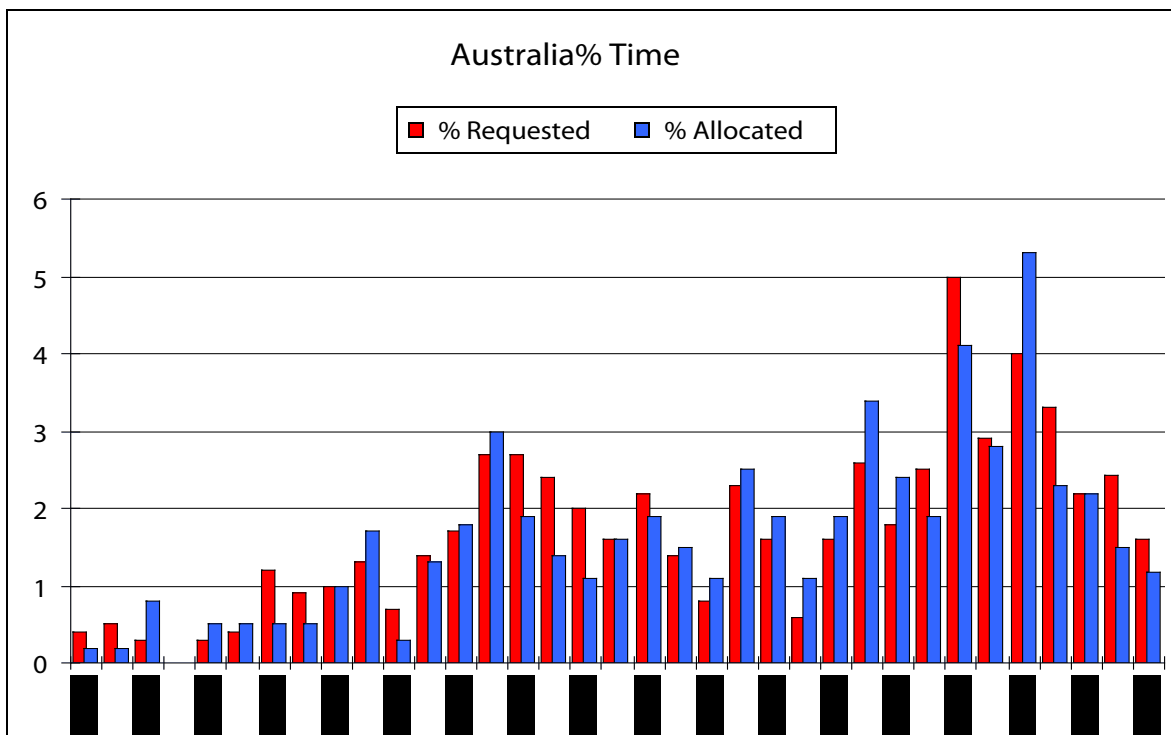


Figure 5. Level of Australian Demand for ISIS access (requested and allocated % time) in half year allocations 1989 to 2005)

At HIFAR about 1000 beam days are used per year by all users (university, ANSTO and collaborative) on all instruments, averaged over the past five years.

ISIS receives between twenty and forty proposals per year (see Table 1, Chapter 2) from Australian university researchers. Chemists and physicists working on materials problems constitute the largest sector. Since the access agreement in 1992, this demand has amounted to requests for some 608 beam days at ISIS, averaging 48 days per year for the past five years, with a cumulative total of about 150 different users in about 20 groups.

The number of groups has risen from about six groups in 1995 to twenty three in 2005. None of this demand could be met within Australia. ISIS instruments are around ten times faster than those at HIFAR, in the few cases where the same kind of instrument exists at each facility, so this demand translated to HIFAR would equate to perhaps 1000 days per year of beam time. Moreover, only experiments which cannot be carried out at HIFAR are supported with travel funds by the DEST Access to Major Research Facilities Program. Even then, these funds do not stretch to meet the demand on them fully.

Hence there has been a *university-based* demand for techniques that are unavailable at HIFAR and experiments that are unfeasible in Australia, of a size comparable to the *total* HIFAR facility capacity. Moreover, these are technically the most demanding experiments and therefore, likely to be closest to the forefront in their research field. Figure 6 summarises Australian beam days requested and awarded at ISIS since 1990. Present Australian users of ISIS and other international facilities have been pioneers in some areas. They represent only the most determined researchers from the potential community, yet they easily oversubscribe Australia's notional beam time entitlement at ISIS with projects that succeed in its internationally contested peer review process.

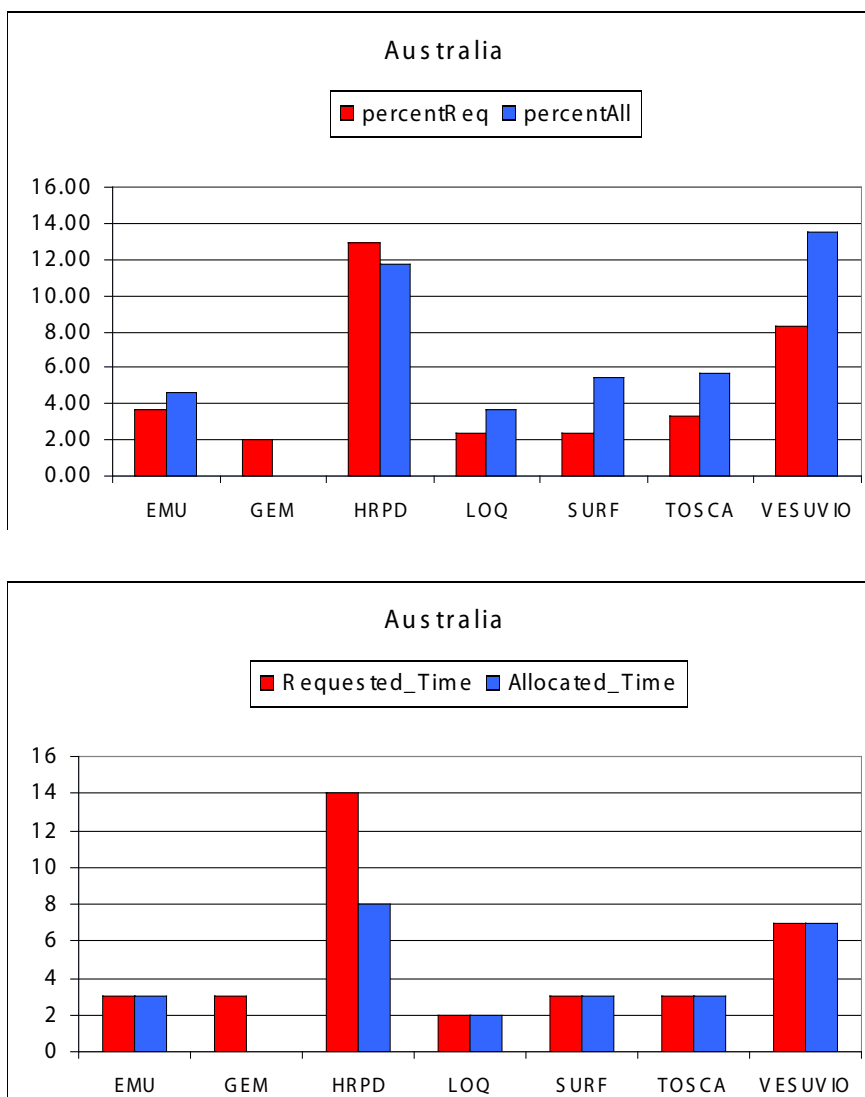


Figure 6. Percentage Time and days requested per instrument in 2005.

Complementarity to Lucas Heights

(a) HIFAR

The complementarity of the work at ISIS and at Lucas Heights until 2007 (likely) is shown by the historical distribution of instruments requested for experiments at ISIS shown above in Figure 6. There is a strong concentration of interest at ISIS on cold neutron instruments for “soft matter” science, LOQ (small angle scattering instrument), SURF & CRISP (the two time of flight neutron reflectometers). For materials, physics and solid state chemistry, the HRPD (High Resolution Powder Diffractometer), with the highest resolution in the world, is of unique value. The inelastic, diffuse scattering and muon facilities have no equivalent in Australia, and will not have in the foreseeable future on OPAL.

(b) OPAL

The cold neutron instruments at OPAL should accommodate most of the work done on LOQ, SURF and the thermal neutron instruments at OPAL (ECHIDNA and WOMBAT), should do much of the work currently undertaken by Australians on HRPD, POLARIS and GEM (at ISIS). A significant proportion (20-30%) of the work currently conducted on HRPD at ISIS

cannot be satisfactorily completed on the high-resolution powder diffractometer (ECHIDNA) because they require very high resolution over the entire diffraction pattern – a condition only available on time-of-flight instruments. One principal Australian ISIS user comments that the High Resolution Instrument at OPAL will not be able to resolve a fair proportion of the problems currently studied on HRPD at ISIS. This is because of inferior resolution (in particular, the resolution distribution across the diffraction pattern).

Examples of complementarity to OPAL

The research done by the group at the **University of Newcastle** has two main foci:

- the $M_{n+1}AX_n$ materials (MAX phases, M – early transition metal, A group IIIA or IVA element, X either C or N) which have an exciting mix of metallic and ceramic properties and
- the giant piezoelectric effect materials $PbZn_{1/3}Nb_{2/3}O_3 - x\%PbTiO_3$ (PZN-PT) which has ten times the piezoelectric strain of conventional piezoelectric materials. Both have benefited from access to ISIS instruments.

i) Synthesis of MAX phases was studied using the instrument POLARIS by simulating the reactive sintering treatment at 1600°C *in-situ* whilst simultaneously recording neutron diffraction patterns every 2.5 minutes. This showed that the solid state reaction of $3Ti + SiC + C$ proceeds via two intermediate phases TiC_x and $Ti_5Si_3C_x$ ($0 < x < 1$) which are the only solid phases in the sample for a period of ~8 minutes before the product phase Ti_3SiC_2 forms. The corresponding time resolution at Lucas Heights is 20 minutes, insufficient to observe these effects properly. In addition to observing the sequence of phases, we have been able to study the kinetics of the final conversion of the intermediate phases to Ti_3SiC_2 and extract the kinetic parameters. These experiments were later augmented by extremely rapid kinetic studies of the same reaction under combustion synthesis conditions at the ILL that resulted in the following recognition:

- Invited to coordinate and chair a micro symposium of the XX International Union of Crystallography Congress and General Assembly, Florence, Italy, September 2005
- Invited talk - XIX International Union of Crystallography Congress and General Assembly, Geneva, Switzerland, August 2002
- Invited talk - IUCr Satellite Meeting – Crystal chemistry of New Materials and Soft Matter, Grenoble France, August 2002
- Plenary lecture - AsCA '03/Crystal 23 – Combined meeting of the Asian Crystallographic Association and the Society of Crystallographers in Australia and New Zealand, Broome WA, August 2003
- Plenary lecture – Australian X-ray Analytical Association/West Australian Society of Electron Microscopists Annual Conference, Rottneest Island, 16-19 September, 2004
- Invited talk – International Conference on Neutron Scattering, Sydney 27 Nov – 2 Dec 2005

The projected capability of the instruments at the new OPAL reactor will, if realised, be able to service this work after 2007/8.

ii) PZN-PT is shrouded in controversy over its crystal structure and the origins of the extraordinary piezoelectric response. The giant piezoelectric response is along a completely different crystal axis than the spontaneous polarisation, causing much speculation. Most previous studies have used X-ray (including synchrotron) radiation and have focussed entirely on the apparent lattice symmetry. To understand the giant piezoelectric effect, it is necessary to obtain precise ion positions so that the electric polarisation can be determined as a function of applied field or stress. To begin clarifying the situation, we have studied PZN-PT ceramics on the instrument HRPD at ISIS at 4 different chemical compositions to determine baseline crystal structures.

The work can only be conducted on HRPD due to its unparalleled resolution as these structures have pseudo-cubic unit cells despite heavily displaced ion positions. The work is topical (e.g. our latest publication was downloaded >250 times in the first fortnight) and has resulted in an invitation to collaborate with scientists from Los Alamos National Laboratory in the USA.

The instruments at the new *OPAL reactor nor any other neutron diffractometer in the world cannot satisfactorily service this work.*

“Hot Neutrons” - Case for ISIS Access (TOSCA & GEM)

At the recent Blue Mountains workshop (2-4 December 2005) on “Future Opportunities in Neutron Scattering” there was strong support for the installation of a hot source at OPAL to support both elastic and inelastic instruments. This is a potential niche area for ANSTO. Other regional and US reactor sources are not planning one. It would be first outside of Europe. In particular, there was support for:

- A liquids and amorphous diffractometer to enable pair distribution function (PDF) analysis.
- An inelastic instrument over the energy range 5 - 250 meV that would for example be useful in the study of hydrogen dynamics.

As can be seen from the above paragraph there is strong support in the Australian community for a “Hot Source” to be built at OPAL. Unfortunately the earliest that this could possibly occur would be in 3 years time (more likely to be 5 years). Hence in the period from 2006 – 2008 Australian scientists will require access to ISIS to use inelastic instruments such as TOSCA and the GEM (General Materials Diffractometer) instrument for PDF analysis. Once the Hot Source is built at OPAL (2008 and beyond) PDF analysis will most likely be limited to momentum transfer vectors $q < 30 \text{ \AA}^{-1}$, whereas GEM can access out to $q = 55 \text{ \AA}^{-1}$ (resolution of 0.1 Å), therefore access to ISIS will still be required.

As far as the Welberry group’s work on diffuse scattering is concerned, although there are some things that they will be able to do on the new reactor this kind of work is more suited to ‘spallation sources’. The very different capabilities of reactor and spallation-based neutron sources allow different science to be done. In Welberry’s case, the time-of-flight (TOF) diffraction technique practiced at ISIS, and on SXD in particular, allows us to collect a large volume of diffraction data in reciprocal space, whereas a reactor-based instrument is limited to collecting data in well-defined but small regions of reciprocal space – usually around the Bragg peaks – because of its monochromaticity. The pulsed nature of spallation source neutrons is inherently suited to the TOF diffraction that allows many multi-pixel detectors to be used to gain images of large regions of reciprocal space. These images contain a vast amount of data about the structure and dynamics of materials, information we are only now learning how to extract and use.

Work done by the Welberry research group at ANU on the diffuse scattering from benzyl was selected as an ISIS scientific highlight for the 2004 Annual Report. The article is titled ‘Diffuse neutron scattering in benzil, $C_{14}D_{10}O_2$ ’ by T.R.Welberry, D.J.Goossens and A.P.Heerdegen (ANU) and W.I.F.David, M.J.Gutmann and M.J.Bull (ISIS). Our images were used on the cover of *The ISIS Facility* section of the 2004 report.

<http://www.isis.rl.ac.uk/isis2004/4highlights/Welberry.htm>

International scientists have noted this work as at the leading edge. One of these is Dr Ray Osborn of the Intense Pulsed neutron Source (Argonne national Laboratory, USA), who is constructing a diffuse scattering neutron spectrometer and is proposing such an instrument for the SNS in the USA. This is an indication that the technique is timely. Our figures are

reproduced in his recent article in *Neutron News* (Vol. 15, No. 3, pages 21-24).

Associate Professor Jim Low and his student from Curtin University of Technology (Z.Oo) went to ISIS to collect research data using the POLARIS and HRPD for the following two projects:

- (1) Effect of Purity and Grain-Size on the Thermal Stability of Titanium Silicon Carbide in Vacuum
- (2) In-Situ Characterisation of Residual Stresses in Model Ceramic Bilayers

Several research papers have been produced from the data collected and a collaborative work with Dr. Ron Smith of ISIS was also established to help with the quantitative analysis of data collected.

In view of the extremely high neutron flux which allows good quality to be collected from small samples and at a much shorter times, they plan to make use of the following instruments at ISIS to study the structural and phase stability of advanced ceramics and complex biological tissues:(a) POLARIS (b) LOQ (c) HRPD

An important caveat relating to full use of OPAL instruments is that if ancillary facilities (such as sample environments, laboratories, access to the ANSTO site and data processing) are not at international standards there will be a lack of productivity and some frustration for Australian users. Every attempt is being made by ANSTO to avoid this. As mentioned above (eg. Paragraph 13) there will remain a need for access to instruments not available at OPAL.

A final point is that a new dimension of complementarity will be opened up in 2007-2008 through the second target station at ISIS. This will have a new range of instruments based on the scientific projections of the whole international ISIS user community. Many instruments will work beyond what is currently available at ISIS or at OPAL. (<http://ts-2.isis.rl.ac.uk/>)

Second target station at ISIS - It's impact

Since the start of the major civil engineering work on the ISIS site to accommodate the Second Target Station in June 2003, there has been an ever-increasing visual impact of the project construction work. The landscape to the south of ISIS has been transformed, and a new support building has been constructed. The construction of the main target station and experimental building is making rapid progress. The detailed design and construction of the target station monolith is making good progress, along with the other major technical components, the moderators and cryogenic systems, the target, and the proton beam line. Most of the major contracts are now placed, and the project is on schedule to meet it's major milestones of, 'first proton beam to target' in June 2007, 'first instrument operation' in November 2007, and 'the start of the experimental programme' in October 2008.

The low frequency (10 Hz) and relatively low operating power (48 kW) of the Second Target Station has provided the opportunity to produce a target / moderator / reflector assembly, using a combination of a coupled and a decoupled moderator, highly optimised for the production of cold neutrons. The significantly enhanced cold neutron flux (compared to the existing 50 hz facility), the simultaneous access to an unprecedentedly broad spectral range, and the potential for high resolution, are all features which are highly tuned for studies in the key strategic areas of Soft Matter, Bio-Materials, Advanced Materials, and Nanotechnology.



Figure 7. Views of recent progress on the new target station and experimental hall building, R80.

The ‘day one’ instrument suite (November 2007), of seven instruments, has been chosen to maximize the impact in these key scientific areas. They comprise of two surface reflectometers / diffractometers, **INTER** and **poIREF**, for the study of chemical and magnetic surfaces and interfaces, the surface diffractometer **offSPEC**, for the study of surface structure, the low scattering vector diffractometer, **SANS2B**, to probe mesoscale structures, and the diffractometer, **NIMROD**, to probe near and intermediate range order, the spectrometer, **LET**, for the characterization of slow dynamics, and the powder diffractometer, **WISH**, to measure larger d spacings, optimised for magnetic structures. They will all offer new capabilities and levels of performance compared to existing instrumentation at ISIS. These instruments are now fully funded from the UK government and the EU FP6 programme, and the detailed engineering design and procurement is now underway.

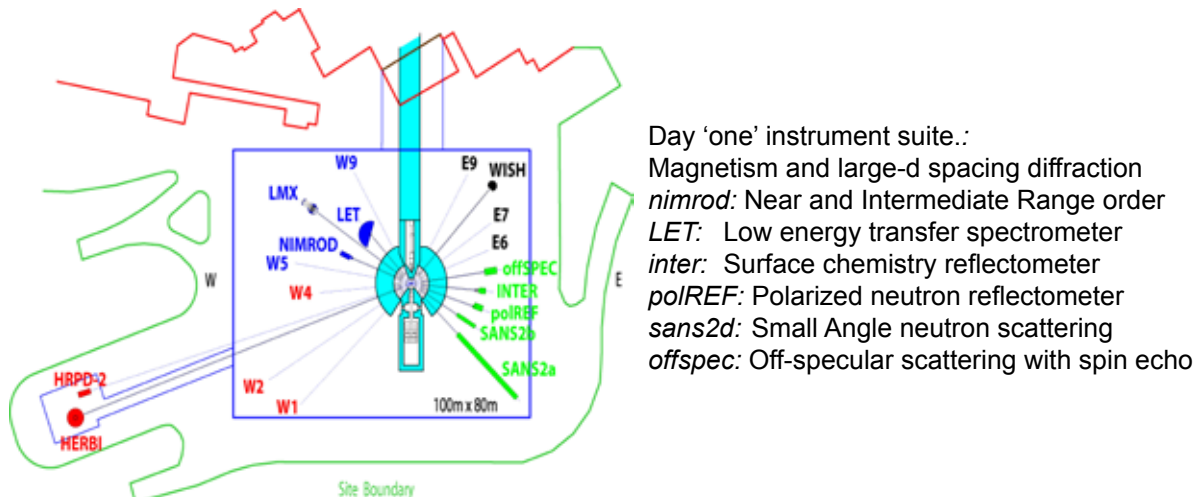


Figure 8. Instrument layout, showing the location of the seven ‘day one’ instruments.

For studies in **Soft Matter**, and **Biomaterials** the key instruments for the study of the bulk structure are **SANS2B** and **NIMROD**, and **INTER**, **poIREF**, and **offSPEC** provide access to interfacial structures. In terms of simultaneously available bandwidth, flux, signal / noise and resolution these instruments will offer world leading capabilities.

At ISIS and more broadly there are discernable trends towards the study of complex multi-phase or multi-component materials, the study of kinetic processes, the use of complex or difficult environments, the requirement for smaller samples, and the need for extensive parametric studies, are all evident. A common feature in many of these emerging areas is a **hierarchy**

of structures and the need to characterize structure over a wide range of length scales, from molecular to mesoscale dimensions. Extensive parametric studies (the need to make measurements over a wide range of conditions, temperature, pH, pressure, concentration, composition etc) will be possible with better resolution, in shorter times and on more dilute systems. More complex multi-component systems (more closely resembling industrially relevant materials) will be accessible, providing the opportunity to investigate the often-critical role of minority components. More complex environments (relevant to the conditions in different processing routes, extruders, electrochemical cells etc) and more complex interfaces will be accessible. Measurements of time dependent processes will open up poorly understood areas such as dynamic surface properties and the molecular origins of complex rheological phenomena.

The reflectometer, **INTER**, optimised for the study of wet chemical interfaces will provide a higher throughput (x 10-20 compared to **SURF**), improved signal / noise (x 2-10 compared to **SURF**), and an increased bandwidth (0.01 to 1.0 Å⁻¹) in a single measurement). This will provide the opportunity to extend surface studies into using significantly smaller samples (<1 cm²), and probe all the important interfaces (air-liquid, liquid-solid, and liquid-liquid) routinely with high precision.

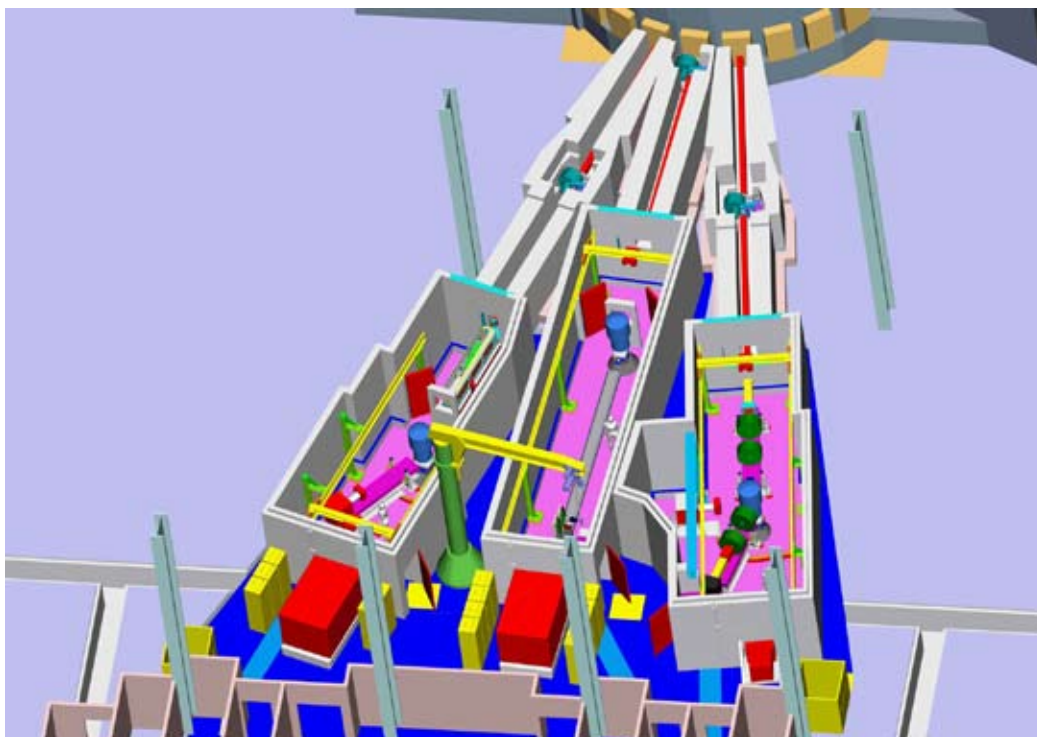


Figure 9. Reflectometer village on TS-2, showing layout of **INTER**, **poIREF**, and **offSPEC**.

poIREF is similar to **INTER** in its enhanced performance, but is optimised for polarized neutron reflection studies on thin magnetic films and multi-layers. It will have vertical and horizontal scattering geometries available, and the ability to measure out of the plane. Full polarization analysis and the ability to have full 3-D spin manipulation will provide an instrument with unique capabilities.

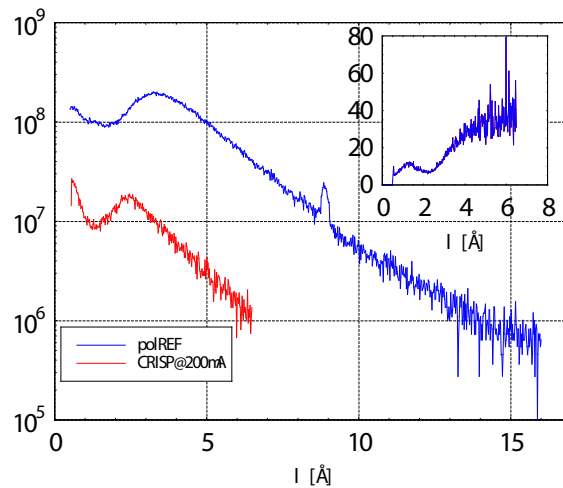


Figure 10. Enhanced flux and q range on **polREF** compared to **CRISP**, a similar enhancement is calculated for **INTER**.

offSPEC is an entirely new concept, and is a surface scattering instrument optimised for off-specular scattering studies. Its design on TS-2 and the incorporation of the SEESANS option will provide access to an in-plane q range that is not accessible elsewhere. It is expected that this will impact significantly on our understanding of in-plane structure in a wide variety of systems.

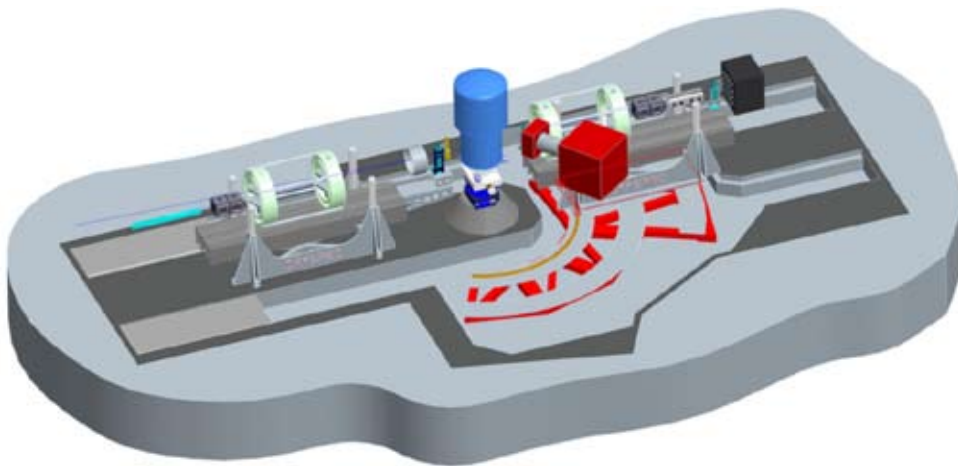


Figure 11. Layout of the offSPEC instrument on TS-2
Shown below is the Q_z , Q_x , Q_y space that will be accessible. Of particular importance is the use of SEESANS to provide an in-plane q range that coincides with the Q_z range

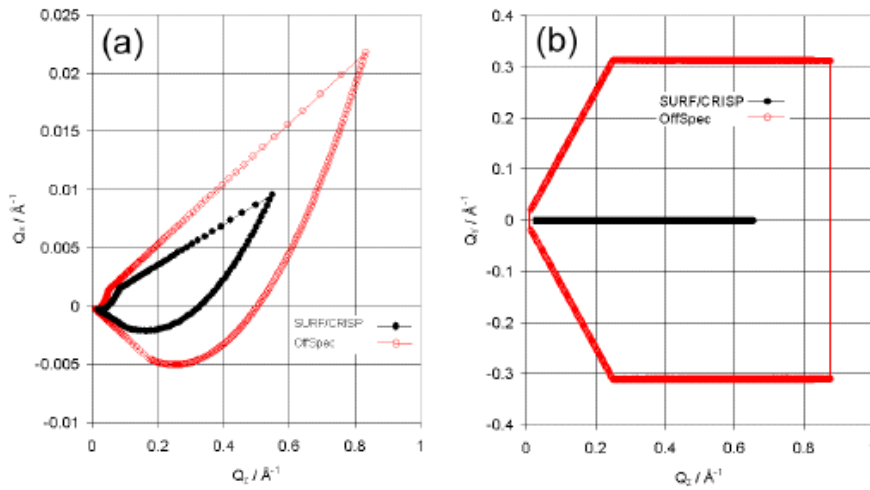


Figure 12. Calculated comparisons of the possible Q_x (a) and Q_y (b) ranges available on Offspec compared to the current ISIS target station instrumentation.

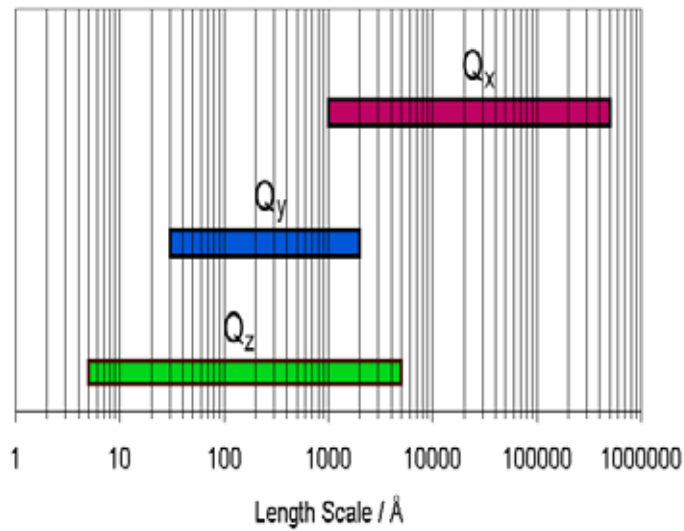


Figure 13. Length Scale / \AA

The SANS instrument, **SANS2D**, will provide an improvement in performance over the existing ISIS instrument **LOQ** by $\sim x 20-40$. Coupled with the extended Q range available in a single simultaneous measurement **SANS2D** will compete with the best in the world for flux, Q range and resolution. Furthermore the two 1m^2 area detectors and the ability to adjust the sample to detector distance will give it a flexibility not normally associated with pulsed source SANS instruments.

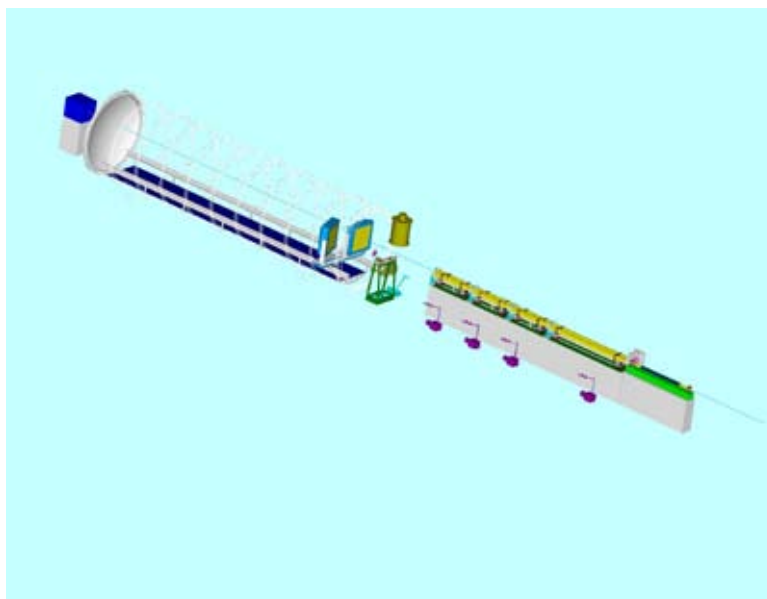


Figure 14. Layout of SANS2D instrument on TS-2

These instruments will all provide capabilities which will allow the development of scientific programmes which can focus on kinetic, non-equilibrium effects, multi-component and multi-phase systems, surface and near surface structures, surface ordering and lateral surface or interfacial ordering and structure, complex and difficult interfaces and environments, and high throughput. They will complement and augment the best available on current and emerging reactor based sources.

Beyond that ‘day one’ instrument suite plans are already emerging for the next phase of instruments, beyond 2008. The proposals for new instruments focus on extending the accessible length scales to longer length scales, access to slower dynamical processes, and the ability to incorporate extreme environments.

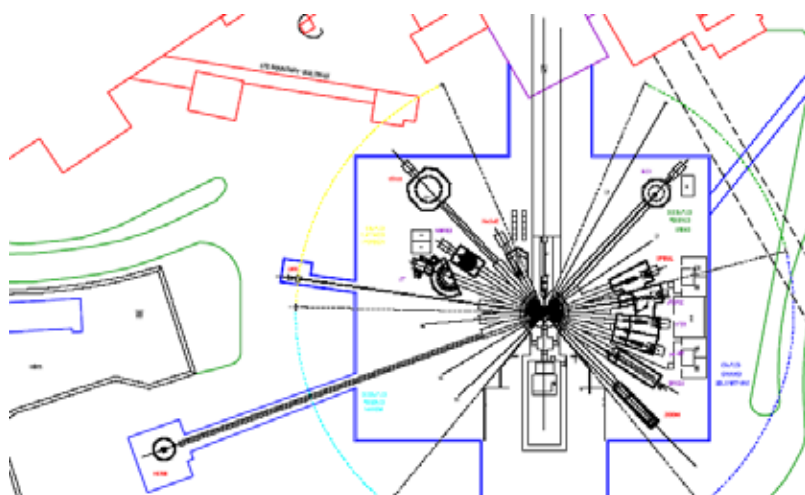


Figure 15. Layout of the instruments at the Second Target Station.

The proposals for this next phase of instruments include **LMX**, for large molecule crystallography, and **EXESS** for diffraction and spectroscopy using extreme environments, very high magnetic fields and high pressure. A high resolution backscattering spectrometer, **HERBI**, and a time of flight spin echo spectrometer, **NESSIE**, will extend the capability to study slow dynamics with high resolution. **BOUNCE**, **SPIRAL**, and **ZOOM** and different small angle scattering designs,

aimed at extending the SANS capability, and particularly the lengths scales accessible to longer length scales. **BOUNCE** is a Bonse- Hart type of USANS instrument, and by measuring in TOF higher order diffraction will extend the q range down to 10^{-5} \AA^{-1} . **SPIRAL** is a novel new concept based on SEESANS, where a direct correlation function in real space is measured, over a length scale from 10's nm to 100's μm . **ZOOM** is a more conventional SANS instrument which would complement **SANS2D** by providing a flexible, high-count rate instrument where focusing could be used to focus onto the detector to access a minimum $Q \sim 10^{-4} \text{ \AA}^{-1}$, or focus onto the sample to provide high spatial resolution.

New opportunities for soft matter science

- Surface, interfacial and bulk properties of complex fluids (polymers, surfactants, colloids)
- Interfacial studies: self-assembly and ordering of complex mixtures of surfactants, polymers and proteins at interfaces, with emphasis on kinetic processes and multi-component systems at technologically relevant interfaces (liquid-liquid and liquid-solid), thin film devices
- Processing of soft solids: relationship between microscopic structure and bulk properties (rheology) in industrially relevant fluid fields
- Self-assembly: structure of lyotropic mesophases, micro-emulsions and vesicles, with emphasis on dynamics of structural phase changes, association and disassociation, and self-assembly in super-critical fluids
- In-situ electrochemistry

New opportunities for bio-science

- Pharmaceuticals, drug delivery formulations, membrane-protein interactions, bio-compatibility and functionality, food technology
- Interfaces and membranes: structural organisation of membranes and membrane-protein systems
- Macromolecular assemblies: low resolution studies on macromolecular assemblies, in systems not tractable by high-resolution crystallography, viruses, glyco-proteins, protein folding, protein-nucleic acid interactions. Solvent structure. Meso-scale structure
- Pharmaceuticals: determination of new drug structures, where the role of hydrogen atoms is essential in understanding drug-receptor interactions. Molecular engineering
- Food technology: study of solvent distribution and structural changes in complex assemblies (for example starches) during processing. Protein fouling. Protein adsorption and colloidal stability. Mechanism of foam and gel formation

New opportunities for advanced materials science

- Crystalline, magnetic, disordered and engineering materials, including complex inorganic and organic assemblies, clathrates, intercalates, zeolites, nano-structured materials, high temperature superconductors, giant magneto-resistance materials, magnetic films and multi-layers, spin valves, glasses, complex fluids, porous media
- Structural details of giant/colossal magneto-resistive materials, non-stoichiometric oxides, piezoelectric, ferroelectric and negative thermal expansion materials
- Composite multi-crystalline materials, such as mixed geological phases, magneto-

resistive manganates, toughened engineering materials and high-temperature superconductor materials

- Studies under extreme conditions, catalysis, in-situ chemical reactions (including electrochemistry and battery function), ultra-high pressures, novel processing routes
- Structure of nano-scale materials, sol-gel processing, ceramics
- Structure of complex materials: role of zeolites in ion exchange materials and catalysis, novel electrodes and electrolytes, clathrate formation, nano-structured materials
- Determination of new magnetic structures: materials with novel ground states
- Magnetic thin films, multi-layers, spin electronics
- Nucleation and growth processes, molecular clustering, glasses
- Complex fluids in porous media; oil recovery; waste disposal; supercritical fluids
- Stress/strain mapping in engineering materials

New opportunities for geoscience

At present the combination of flux and resolution limit the time-step of minerals reactions under *in situ* ore processing conditions to around ten minutes. The higher flux of the new Diamond source should enable kinetic processes to be studied on a time scale of less than 1 minute. This will open new horizons for *in situ* ore processing research and could be a great boon to the Australian Mining industry.

The enhancing ISIS facilities will continue to open up international networking and collaboration in science and instrument design. OPAL / ISIS complementarity will be important aspects.

Furthermore, the new state of the art synchrotron for the UK (DIAMOND) is now under construction (see background in frontis piece front cover of this review document), situated next to the ISIS facility on the Rutherford-Appleton Laboratory site. One of the thrusts of this submission is the value of joint neutron – X-ray work. It is likely that the combination of DIAMOND and ISIS (with the second target station), the “golden triangle” of Oxford, Cambridge and London Universities nearby and the close collaborations of Australian scientists established with other British and continental universities through ISIS, will be to Australia’s advantage. Already we are seeing a complementarity in the fast beam line proposed for DIAMOND and these envisaged for the Australian Synchrotron.

Chapter 3

The excellence of the researchers and research activity to be supported

69. **General performance of the participating groups**

As a measure of the general performance of the participating groups we supplement the comments above on success in international competition at the ISIS facility with standard performance indicators related to the Australian based work from the user groups. The chosen indicators are: success in ARC Grants, Prizes, Awards and Distinctions, PhD Student Theses, Honours Students Theses, Conference Invitations and Presentations, Fellowships of learned academies, and Promotions. These are listed in Appendix 3.

70. Over the past five years there have been thirteen postdoctoral fellows trained through access with the ISIS program. In that same period the number of participating graduate students (PhD and Honour students) has been 77. The postdoctoral fellows have all finished in the expected time of their contracts. The presence of postdoctoral fellows in this program and their being able to accept partial responsibility for student guidance in the overseas campaigns has been a useful training experience. The PhD students listed have achieved or are achieving theses of high standard (as judged by examiners comments) and some have finished in the minimum time. High Honours have been obtained for Honours students participating and one was awarded the Rhodes scholarship to Oxford University as well as the University Medal and First Class Honours.

71. **Current Research Programs**

To illustrate current research programs of the proposer groups and their research activity, we also show in Appendix 3 the publications lists, PhD Theses completed, Honours Theses completed, Current Theses projects and Industrial Collaborations.

The Excellence of Researchers and Research Activity to be Supported

Name: **A/Professor Craig BUCKLEY**

Qualifications: B.Sc. (Hons, First Class) (Griffith, 1990). PhD (Griffith, 1994).

Current Appointment: Associate Professor in Physics, Curtin University.

Employment History: 1993 – 1994. Leverhulme Post Doctoral Fellow, *Salford*
 1995 – 1998. Research Associate, *University of Illinois, Urbana*
 1998 – 2002. Curtin Research Fellow, *Curtin*
 2002 – 2003. Senior Lecturer, *Curtin*
 2004 – Associate Professor, *Curtin*

Research Grants

2000	ARC - Small	C E Buckley, A Rohl et al	The Determination of the Structure of γ -Alumina from First Principle Calculations.	\$12,200
2000-2002	ARC - Large grant	J Low, B Lawn, C E Buckley	Microstructural design of layered and graded alumina-based composites	\$144,629

2001	ARC - RIEF	C E Buckley, B O'Connor et al	A Small Angle X-Ray Scattering Facility for Western Australia	\$300,000
2001	ARC - RIEF	M Middleton, C E Buckley et al	Portable Neutron Generator for Resource Applications	\$130,000
2003	ARC Discovery	R De Marco, C E Buckley, A Rohl	Probing the Interfaces of Electrochemical Sensors	\$160,000
2004	ARC Discovery	G Parkinson, C E Buckley et al	Ferrhydrite: Fundamentals of a Natural Nanomaterial	\$435,000
2004-2006	ARC - LIEF	D Mather, C E Buckley et al	Access for Australian Researchers to Advanced Neutron Beam Techniques	\$715,000
2005	ARC Linkage	M I Ogden, C E Buckley, G A Carter	Controlling precipitation processes in the production of value-added zirconia	\$72,444
2005-2009	ARC Research Networks	C Kepert, C E Buckley et al	Molecular and Materials Structure Network	\$1,500,000
2006-2008	CSIRO flagship NHMA	Gray et al	Hydrogen Storage Stream	\$2,152,000

Significant Publications 2000-2005 (total in last five years: 32)

1. Characterisation of H-Defects in the Aluminium-Hydrogen System using Small Angle Scattering Techniques by C.E. Buckley, H.K. Birnbaum, J.S. Lin, S. Spooner, D. Bellmann, P. Staron, T.J. Udovic and E. Hollar. *J. Appl. Cryst.* **34**, (2001) 119 - 129.
2. A Computational Investigation of the Structure of κ -Alumina using Interatomic Potentials by G. Paglia, A.Rohl, C.E. Buckley and J.D. Gale. *J. of Mater. Chem.* **11**, (2001) 3310 - 3316.
3. Characterisation of the Charging Techniques used to introduce Hydrogen in Aluminium, C.E. Buckley and H.K. Birnbaum. *J. Alloys and Compds.* **330-332**, (2002) 649 - 653.
4. Diagnostic X-ray Dosimetry using Monte Carlo Simulation. J.L. Ioppolo, R.I. Price, T. Tuchyna and C.E. Buckley. *Physics in Medicine and Biology*, **47**, (2002) 1707 – 1720.
5. A New Structural Model for Boehmite-derived γ -Alumina. G. Paglia, C.E. Buckley, A.L. Rohl, B.A. Hunter, R.D. Hart, J.V. Hanna and L.T. Byrne. *Phys. Rev.B.*, **68**, (2003) 144110-1 – 144110-11.
6. Delamination and Re-assembly of Surfactant-Containing Li/Al Layered Double Hydroxides." M. Singh, M.I. Ogden, G.M. Parkinson, C.E. Buckley and J. Connolly. *J. Mater. Chem.*, **14**, (2004) 1 - 4.
7. The boehmite-derived γ -alumina system I: structural evolution with temperature, with the identification and structural determination of a new transition phase, γ' -alumina." G. Paglia, C.E. Buckley, A.L. Rohl, R.D. Hart, K. Winter, A.J. Studer, B.A. Hunter, and J.V. Hanna. *Chemistry of Materials*, **16**, (2004) 220 - 236.
8. Evidence of the Iron Nanostructure in the $\text{Fe}_x(\text{Ge}_{28}\text{Sb}_{12}\text{Se}_{60/100-x})$ Glass Ion-Selective Electrode using Small Angle Neutron Scattering and Electrochemical Impedance Spectroscopy." B. Pejicic, R. De Marco, C.E. Buckley, C.F. Maitland and R. Knott. *Talanta*, **63**, (2004) 149 – 157.
9. The boehmite-derived γ -alumina system, 2: consideration of hydrogen and surface." G. Paglia, C.E. Buckley, T.J. Udovic, A.L. Rohl, F. Jones, C.F. Maitland, and J. Connolly. *Chemistry of Materials.*, **16**, (2004) 1914 - 1923.
10. Determination of the Structure of γ -Alumina from Interatomic Potential and First Principle Calculations – The Requirement of Significant Numbers of Non-Spinel Positions to Achieve an Accurate Structural Model" G. Paglia, A.L. Rohl, C.E. Buckley and J.D. Gale. *Phys. Rev. B.*, **71**, (2005) 224115-1 – 224115-16.

Name: **Professor Stewart CAMPBELL**

Qualifications: BSc (Hons; 1966 Aberdeen Univ); MSc (1969 Salford Univ); PhD (1974 Monash Univ), FInstP (UK 1985) FAIP (1982) CPhys

Current Appointment: Professor (Physics Discipline), School of Physical, Environmental and Mathematical Sciences, University College, UNSW@ADFA (Emeritus Professor from July 2005)

Previous appointments:

2003 (6 months SSP) Alexander von Humboldt Fellow, Technical University Munich, Germany

2000 (6 months SSP) Alexander von Humboldt Fellow, University of Mainz, Germany

1983–1998 Lecturer/Senior Lecturer/Associate Professor, Department of Physics, Faculty of Military Studies, UNSW and University College, UNSW@ADFA

1989 (9 months SSP) Alexander von Humboldt Fellow, University of Saarland, Germany

1983 (6 months) Alexander von Humboldt Fellow, University of Saarland, Germany

1979–1983 Research Fellow, Australian National University

1976–1979 ARGC Research Fellow, Faculty of Military Studies, UNSW

1974–1976 Design/Project Engineer, The Oxford Instrument Co. Ltd, England

Research Grants 2000-2005

Granting Body	Investigators	Title	Years	Amount
ARC Discovery (C)	Y Chen (ANU), S J Campbell <i>et al.</i>	Formation Mechanism of Boron Nitride Nanotubes Produced by Reactive ball Milling	2000-2002	\$211 000
ARC Small URSP (P)	S J Campbell	Rare-Earth Magnetism – Novel Quaternary Compounds	2002	\$17 071
AINSE (P) (C)	S J Campbell <i>et al.</i>	Neutron Scattering (9 Projects)	2000-2005	\$160 000
ANSTO (P) (C)	S J Campbell	Visits to Major Facilities (6 projects)	2000-2005	\$24 000
ARC (LIEF) (P) (C)	AINSE, D Mather <i>et al.</i>	Access for Australian researchers to advanced neutron-beam techniques	2002-2005	\$960 000
ARC (LIEF) (P)	H O'Neill (ANU), S J Campbell <i>et al.</i>	An Electron Microprobe	2000	\$500 000
ARC Discovery (C)	J M Cadogan and S J Campbell	Insight and Understanding in Rare-Earth Magnetism	2003-2005	\$310 000

Significant Publications 2000-2005

(Over 42 refereed publications in past 5 years; co-editor of ICAME87, ICM 97, ICNS2005 Conf Proc; 3 Invited Book Chapters; over 242 career publications)

1. M Hofmann **S J Campbell**, and S J Kennedy, Competing Magnetic Interaction in $\text{La}_{0.8}\text{Y}_{0.2}\text{Mn}_2\text{Si}_2$, J. Phys.: Condensed Matter, **12** 3241-3254 (2000)
2. Heng Zhang, **S J Campbell** and A V J Edge, Formation and Structure of Rare-Earth Intermetallic Compounds $\text{R}_3\text{Co}_{29}\text{M}_4\text{B}_{10}$, Journal of Physics: Condensed Matter, **12** L159-

- L166 (2000)
3. M. Hofmann, **S J Campbell**, A V J Edge and A Studer, The Magnetic Structures of YbMn_2Si_2 , *J Phys: Condensed Matter* **13** 9773-9780 (2001)
 4. M Schmidt and **S J Campbell**, *In Situ* Neutron Diffraction Study (300-1273 K) of Non-Stoichiometric Strontium Ferrite SrFeO_x , *Journal of Solid State Chemistry* **63** 2085-2092 (2002)
 5. Heng Zhang and **S J Campbell**, Molecular Mean Field Study of Rare-Earth Intermetallic Compounds $\text{R}_3\text{Co}_{29}\text{Si}_4\text{B}_{10}$, *J Applied Physics*, **93** 9177-9180 (2003)
 6. **S J Campbell**, V. Ksenofontov, Y. Garcia, J. S. Lord, Y. Boland and P. Gütlich, Muon Spin Rotation and Mössbauer Investigations of the Spin Transition in $[\text{Fe}(\text{ptz})_6](\text{ClO}_4)_2$, *Journal of Physical Chemistry B* **107** 14289-14295 (2003)
 7. M Hofmann, **S J Campbell**, H Ehrhardt and R Feyerherm, The Magnetic Behaviour of Nanostructured Zinc Ferrite (**Invited**), *Journal of Materials Science* **39** 5057-5065 (2004)
 8. M Hofmann, **S J Campbell** and A V J Edge, EuMn_2Ge_2 and EuMn_2Si_2 - Magnetic Structures and Valence Transitions, *Phys Rev B* **69** 174432-1 to 174432-9 (2004)
 9. J L Wang, **S.J. Campbell**, J M Cadogan, O Tegus and A.J.V. Edge ^{57}Fe Mössbauer and Magnetic Studies of $\text{ErFe}_{12-x}\text{Nb}_x$, *Journal of Physics: Condensed Matter* **17** 3689-3700 (2005)
 10. J L Wang, S.J. Campbell, J M Cadogan, O Tegus, A J Studer and M. Hofmann Magnetic Properties of $\text{PrMn}_{2-x}\text{Fe}_x\text{Ge}_2$ - ^{57}Fe Mössbauer Spectroscopy, *Journal of Physics: Condensed Matter* **18** 189-204 (2005)

Name: **Ian Ross GENTLE**

Qualifications: BSc (Hons, University Medallist) (U. of Sydney, 1983). PhD (U. of Sydney, 1988)

Current Appointment: Reader in Chemistry; Program Leader - ARC Centre for Functional Nanomaterials; Director, Brisbane Surface Analysis Facility, The University of Queensland

Previous appointments: 2003-present, Reader, Department of Chemistry, UQ; 1998-2002, Senior Lecturer, Department of Chemistry, UQ; 1993-1998, Lecturer, Department of Chemistry, UQ; 1990-1993, Postdoctoral Fellow, Research School of Chemistry, ANU

Research Grants 2000-2005 (smaller grants, total additional \$200K not listed due to lack of space)

Grant Body	Investigators	Title	Years	Amt
ARC	Lu, et al. (19 CI's including Gentle)	ARC Centre for Functional Nanomaterials	2003-2007	\$1.53M
ARC Discovery Project	Gentle, Ashwell, Foran	Greatly improved rectification by molecular diodes	2006-2008	\$273k
ARC LIEF	Gentle, Lu, Trau, Drennan, Whittaker, Martin, Frost, Kloprogge, Brown	Small Angle Scattering Facility for the Materials and Biological Sciences	2006	\$300k
ARC LIEF	Martin, Gentle, Kepert, Turner, Guss	e-Research Infrastructure for the Molecular and Materials Structure Sciences	2006	\$1M
ARC LIEF	Gentle, Lu, George, Drennan, Frost	An advanced scanning probe microscopy facility	2005	\$168k
AusIndustry	Williams, Lamb, Gentle, Muddle, Wilkes	Australian Materials Technology Network	2004-2006	\$2.6M

ARC LIEF, AINSE and universities	Gray et al.	Access for Australian researchers to advanced neutron beam techniques	1998-2000	\$ 1100k
ARC Discovery	Gentle and Foran	Patterned assemblies of molecules on surfaces	2002-2004	\$180k
ARC LIEF	Gentle, George, Lu and Bell	An advanced facility for materials characterisation	2002	\$580k
UQ Research Develop. Grant	Gentle and Gahan	Multilayer porphyrin arrays constructed by layer self assembly	2004	\$45k
UQ Research Develop. Grant	Drennan, Riley and Gentle	A new initiative in materials chemistry	2002	\$54k
UQ Research Develop. Grant	Bhatia and Gentle	Studies of adsorption equilibria over surface engineered microporous solids	2001	\$56k
ARC Small	Gentle	Controlled Formation of Q-State Semiconductor Particles in Thin Films	2000	\$24k

Significant publications (total 21 refereed articles, 1 book and 20 conference papers (2000-2005))

1. Barnes, G.T. and **Gentle, I.R.**, *Interfacial Science: An Introduction*, Oxford University Press, Oxford (2005).
2. O'Driscoll, B.M.D., Ruggles, J.L., and Gentle, I.R., Mixed Thin Films of a Cationic Amphiphilic Porphyrin and n-Alkanes. *Langmuir* 20 6246-6251 (2004).
3. Tran, M.L., Gahan, L.R., and **Gentle, I.R.**, Structural Studies of Copper(II)-Amine Terminated Dendrimer Complexes by EXAFS. *J. Phys. Chem. B* 108 2130-2136 (2004).
4. Fullagar, W.K., Aberdeen, K.A., Bucknall, D.G., Kroon, P.A., and **Gentle, I.R.**, *Conformational Changes in SP-B as a Function of Surface Pressure*. *Biophys. J.*, 85, 2624-2632 (2003).
5. Peng, J.B., Foran, G.J., Barnes, G.T., and **Gentle, I.R.**, *Multiple Ordered Phases in Langmuir-Blodgett Films of Cadmium Arachidate at Elevated Temperatures*. *Langmuir*, 19, 4701-4706 (2003).
6. B. M. D. O'Driscoll, **I. R. Gentle**, *Structural changes in mixed Langmuir-Blodgett films upon nanoparticle formation*, *Langmuir* 18, 6391-6397 (2002).
7. Peng, J. B., Barnes, G. T. and **Gentle, I. R.** *The structures of Langmuir-Blodgett films of fatty acids and their salts* *Adv. Colloid Inter. Sci.*, 91, 163-219 (2001). (Review article)
8. G. J. Ashwell, R. Hamilton, B. J. Wood, **I. R. Gentle**, D. Zhou, *Molecular Lego: non-centrosymmetric alignment within interdigitating layers*, *J. Mater. Chem.* 11, 2966-2970 (2001).
9. Peng, J. B., Barnes, G. T., Foran, G. J., Crossley, M. J. and **Gentle, I. R.** *Structures of mixed Langmuir-Blodgett films of tetrakis(3,5-di-tert-butylphenyl)porphyrinocopper(II) with cadmium arachidate: a grazing incidence X-ray diffraction study*, *Langmuir* 16 607-611 (2000).
10. J. B. Peng, G. T. Barnes, **I. R. Gentle**, G. J. Foran, *Superstructures and correlated metal ion layers in Langmuir-Blodgett films of cadmium soaps observed with grazing incidence X-ray diffraction*, *J. Phys. Chem. B* 104, 5553 (2000).

Name: **Evan M^{ac}Alpin GRAY**

Qualifications: BSc(Hons), First Class, Monash, 1974. PhD, Monash, 1979.

Current Appointment: Associate Professor of Physics, Griffith University

Previous Appointments: Griffith University Lecturer, (1988-1993), Senior Lecturer, (1994-

1997)

Research Grants 2000-2005

Granting Body	Investigators	Title	Years	Amount
ARC (RIEF), DISR	Gray, White et al.	Access for Australian researchers to advanced neutron beam techniques	1998-2003	
ARC (Small)	Gray	Carbon-based hydrogen storage	2001	\$27,000
AMRFP, ASRP	Gray	Travel grants for overseas neutron, x-ray and muon beam experiments	2001-2006	\$95,000
ARC (Discovery)	Gray, Dobson	Hydrogen absorption by nanostructured carbons	2003-2005	\$265,000
ARC (LIEF)	Mather, Gray, White et al.	Access for Australian researchers to advanced neutron beam techniques	2003-2004	\$475,000
ARC (Linkage)	Bell, Gray, Kavanagh	Electronic properties of diamond-like carbon for applications in planar optical waveguides	2002-2004	\$69,000
ARC (LIEF)	Buckman et al.	National Positron Beamline	2004	\$512,000
ARC (LIEF)	Mather, White, Gray et al.	Access for Australian researchers to advanced neutron beam techniques	2005-2006	\$480,000
ARC (LIEF)	Kisi et al.	The rapid kinetics facility	2006	\$195,000

Significant Publications

(8 refereed papers, 10 conference papers (incl. 4 Invited and 1 Keynote) 2001-present)

1. **E.MacA. Gray**, T.P. Blach, D.J. Cookson and M.P. Pitt, "*Mechanism of the phase transformation in the $\text{LaNi}_5\text{-H}_2$ system.*", Phys. Rev. Lett. submitted.
2. T.P. Blach and **E.MacA. Gray**, "*MuSR study of graphite intercalation compounds as potential hydrogen absorbers.*", Europhys. Lett., **65** 130 (2004)
3. K.G. McLennan and **E. MacA. Gray**, "*Equation of state for deuterium gas to 1000 bar.*", Meas. Sci. Technol. **15** 1(2004).
4. I.F. Bailey, R.B. Done, J.W. Dreyer and **E.MacA. Gray**, "*A high-temperature high-pressure gas-handling cell for neutron scattering experiments.*", Int. J. High Press. Res. **24** 309 (2004).
5. M.P. Pitt and **E.MacA. Gray**, "*Tetrahedral occupancy in the Pd-D system observed by in situ neutron powder diffraction*", Europhys. Lett. **64** 344-350 (2003)
6. L.D. Cussen, **E.MacA. Gray**, A.P. Murani, S.J. Kennedy and B.A. Hunter, "*Long range atomic order in irradiated $\text{Cu}_{80}\text{Mn}_{20}$* ", Europhys. Lett., **58** 243 (2002)
7. **E.MacA. Gray**, L.D. Cussen, A.P. Murani and S.J. Kennedy, "*Magnetic scattering in irradiated MnCu_4* ", Applied Phys. A **74** S935 (2002).
8. E. Wu, **E.MacA. Gray** and D.J. Cookson, "*Synchrotron powder diffraction line broadening analysis of dislocations in $\text{LaNi}_5\text{-H}$* ", J. Alloys and Compounds, **330-332** 229 (2002)
9. M.P. Pitt and **E.MacA. Gray**, "*Evolution of microstructure in the $\text{LaNi}_5\text{-D}$ system during the early absorption-desorption cycles*", J. Alloys and Compounds, **330-332** 241 (2002)

Name: **Brendan J KENNEDY**

Qualifications: 1980 BEd (Sci) Melbourne State College; 1984 PhD in Chemistry, Monash University; 1984-1987

Current Appointment:

Previous Appointments: Post Doctoral Fellow, Inorganic Chemistry Laboratory, The University of Oxford; 1985-1987 Lecturer, Corpus Christi College, Oxford; 1987 Appointed as Lecturer in the School of Chemistry, University of Sydney; 1995-1998 Junior Research Fellow, Corpus Christi College Oxford; Promoted to Senior Lecturer and Associate Professor (2000).

Research Grants 2000-2005

Granting Body	Investigators	Title	Years	Amount
ARC (RIEF), DISR and universities	Gray et al.	Access for Australian researchers to advanced neutron beam techniques	2000-2005	\$M 1.5
ARC LGS	B.J. Kennedy, C.J. Howard, T. Vogt and B.A. Hunter	Structural and Bonding Trends in Bismuth Oxides	2000-2002	\$148K
ARC Spirt	Davies, Weder, Hambley, Kennedy, Regtop, et al	New Metal Complexes of NSAIDs as Veterinary Eye Ointments, Anti-Cancer Drugs and General Anti-inflammatory Agents	2001-2003	\$437K
ARC LGS	B.J. Kennedy and C.J. Howard	Structural Variants and Phase Transitions in Perovskites	2001-2003	\$146K
ARC Discovery	B.J. Kennedy	Structural and Electronic Properties of Layered Bismuth Oxides	2003-2004	\$170K
ARC Discovery	Kennedy, Withers and Schmid	Structural Variants and Phase Transitions in Perovskites	2005-2007	\$390K
AMREP	Kennedy	Access to Major Facilities	2000-2005	\$72K
AINSE	Kennedy	Neutron Scattering	2000-2005	\$380K
ASRP	Kennedy & Howard	Synchrotron Studies	2000-2005	\$96K

Significant Publications (Dr Kennedy has published almost 200 referred papers, 2 book chapters, 3 patents and is cited in more than 2,500 publications)

1. Bismuth Ruthenium Oxides - Neutron-Diffraction and Photoelectron Spectroscopic Study of $\text{Bi}_2\text{Ru}_2\text{O}_7$ and $\text{Bi}_3\text{Ru}_3\text{O}_{11}$. G.R. Facer, M.M. Elcombe and B.J. Kennedy, *Aust. J. Chem.*, 1993 (46) 1897-1907.
2. Structural Studies of Rutile Type Metal Dioxides. A.A. Bolzan, C. Fong, B.J. Kennedy and C.J. Howard, *Acta Cryst. Section B-Structural Science* 1997 (53) 373-380.
3. High-Temperature Phases of SrRuO_3 . B.J. Kennedy and B.A. Hunter, *Physical Review B* 1998 (58) 653-658
4. Crystal Structures of AuCN and AgCN and Vibrational Spectroscopic Studies of AuCN, AgCN, and CuCN*. G.A. Bowmaker, B.J. Kennedy and J.C. Reid, *Inorganic Chemistry* 1998 (37) 3968-3974.
5. Phase Transitions in Perovskite at Elevated Temperatures – A Powder Neutron Diffraction Study. B.J. Kennedy, C.J. Howard and B.C. Chakoumakos, *J. Phys.C Condensed Matter* 1999 (11) 1479-1488
6. The Structural Phase Transitions in Strontium Zirconate Revisited. C.J. Howard, K.S. Knight, B.J. Kennedy and E.H. Kisi, *J. Phys.C Condensed Matter* 2000 (12) L677-L683.
7. Cation Disorder in the Ferroelectric Oxides $\text{ABi}_2\text{Ta}_2\text{O}_9$, A = Ca, Sr, Ba. R. Macquart, B.J. Kennedy and Y. Shimakawa, *J. Solid State Chem.*, 2001 (160) 174-177.
8. Antiferrodistortive Phase Transition in $\text{Pb}(\text{Ti}_{0.48}\text{Zr}_{0.52})\text{O}_3$: A Powder Neutron Diffraction Study. R. Ranjan, R.S.K. Mishra, D. Pandey, and B.J. Kennedy, *Physical Review B* (2002) 65 060102

9. Ordered Double Perovskites - a Group-Theoretical Analysis. C.J. Howard, B.J. Kennedy and P.M. Woodward, *Acta Cryst., Section B-Structural Science* 2003 (59) 463-471.
10. Strain Mechanism For Order-Parameter Coupling Through Successive Phase Transitions in PrAlO₃. M.A. Carpenter, C.J. Howard, B.J. Kennedy and K.S. Knight, *Physical Review B* 2005 (72) 024118.

Name: **Professor Cameron KEPERT**

Qualifications: B.Sc. (Hons I), UWA, 1991; PhD (Lond), 1996.

Current Appointments: Professor and ARC Federation Fellow 2006-present.

Previous Appointments: Junior Research Fellow (Christ Church, Oxford), 1995-1998, Lecturer (Sydney University) 1999-2001, Senior Lecturer 2002-2004, Assoc. Prof. 2005

Research Grants 2000-2005

Granting Body	Investigators	Title	Years	Amount
ARC Discovery	Kepert	Molecular Framework Materials: Nanoporosity and Anomalous Thermal Expansion	2006-2008	\$401,000
ARC Federation Fellowship	Kepert	<i>Advanced Molecular Nanomaterials</i>	2005	\$1,515,000
ARC Research Network	Kepert (Director) + 49 other CIs	<i>Molecular and Materials Structure Network</i>	2005	\$1,500,000
ARC Special e-Research Initiative	Kepert, Abramson, Chiu, Hauser, Hursthouse, McMullen, Pailthorpe, Turner, Zomaya	<i>Scientific Instruments as ICT Components in Building a GrEMLIN for e-Research</i>	2005	\$120,000
ARC Discovery Grant	Kepert, Murray, Toftlund, Steel	<i>Polynuclear Spin-Crossover Molecular Switches: Host-Guest Chemistry, Magnetism and Memory</i>	2005-2009	\$ 925,000
Sesqui R&D Scheme, USyd	Kepert, Murray	<i>Anomalous Thermal Expansion Materials</i>	2004	\$24,000
Sesqui R&D Scheme, USyd	Kepert, Murray	<i>Anomalous Thermal Expansion Materials</i>	2005	\$15,000
ARC Research Network Seed	Kepert (Director) + 19 other CIs	<i>Molecular and Materials Structure Network</i>	2003	\$30,000
ARC Discovery Grant	Kepert	<i>Nanoporous Molecular Frameworks: Chirality, Host-Guest Chemistry and Nanoscale Templation</i>	2003-2005	\$290,000
Sesqui R&D Scheme	Kepert	<i>Anomalous Expansion Materials</i>	2003	\$36,000

ARC Linkage Grant	Keper, Thomson, Anderson, Matthews	<i>Porous Mineral Formulations for Controlled Release Applications</i>	2002	\$282,186
ARC Discovery Grant	Keper, Murray, Toftlund	<i>Cooperativity in Spin-Crossover Systems: Memory, Magnetism and Microporosity</i>	2002	\$335,000
ARC Discovery	Murray, Keper, Toftlund	<i>Microporous Spin-switching materials</i>	2001	\$30,000
Sesqui R&D Scheme, USyd	Keper	<i>Advanced materials: new phases for chiral separation</i>	2001	\$30,000
ARC Linkage International	Joint with K.S. Murray	<i>Polynuclear Spin-Crossover Molecular Switches: Host-Guest Chemistry, Magnetism and Memory</i>	2006-8	\$21,000
ARC Linkage International	Joint with K.S. Murray	<i>Cooperativity in Spin-Crossover Systems: Memory, Magnetism and Microporosity</i>	2002-2004	\$31,650
ARC Linkage International	Keper, Murray, Toftlund, Steel	<i>Polynuclear Spin-Crossover Molecular Switches: Host-Guest Chemistry, Magnetism and Memory</i>	2006	\$21,000
FAST, DEST/ French Embassy	Keper, Murray, Guionneau, Letard	<i>Light induced electronic switching in nanoporous materials and supramolecular clusters</i>	2005	\$49,500
ARC Linkage International	Murray, Keper, Toftlund	<i>Cooperativity in Spin-Crossover Systems: Memory, Magnetism and Microporosity</i>	2002	\$31,650
AMRFP, AINSE, ASRP, etc	Keper	<i>Overseas synchrotron and neutron experiments</i>	2003-	\$80,000
Venture capital investment	Keper	<i>"UCOM ten: university of Sydney based start-up company"</i>	2005	\$660,000
Orica Technology Fund	Keper, Anderson, Matthews	<i>Porous mineral formulations for controlled release applications</i>	2000-2002	\$300,000
ARC Large Grant	Keper, Rosseinsky, Thomas	<i>Microporous Molecular Frameworks: Chirality and Guest-Exchange</i>	2000-2002	\$232,000
ARC Linkage Infrastructure	Martin, Gentle, Keper, Turner, Guss	<i>e-Research Infrastructure for the Molecular and Materials Structure Sciences</i>	2006	\$ 1,000,000
ARC Linkage Infrastructure	Hambley, Keper, Turner, Hibbs, Spackman, Williams, Pyne, Try	<i>Ultra-sensitive CCD Diffractometer with High Intensity X-ray Photon Generator</i>	2003	\$399,466

Significant Publications 2000-2006

1. C.J. Kepert, "Advanced Functional Properties in Nanoporous Coordination Framework Materials", *Chem. Commun.*, 40th Anniversary Focus Article (Invited), 695-700 (2006).
2. A.L. Goodwin, K.W. Chapman, C.J. Kepert, "Guest-Dependent Negative Thermal Expansion in Nanoporous Prussian Blue Analogues $M^{\text{II}}\text{Pt}^{\text{IV}}(\text{CN})_6 \cdot x\{\text{H}_2\text{O}\}$ ($0 \leq x \leq 2$; $M = \text{Zn}, \text{Cd}$)", *J. Am. Chem. Soc.*, **127**, 17980-17981 (2005).
3. K.W. Chapman, P.J. Chupas, C.J. Kepert, "Direct Observation of a Transverse Vibrational Mechanism for Negative Thermal Expansion in $\text{Zn}(\text{CN})_2$: an Atomic Pair Distribution Function Analysis", *J. Am. Chem. Soc.*, **127**, 15630-15636 (2005).
4. K.W. Chapman, P.J. Chupas, C.J. Kepert, "Selective Recovery of Dynamic Guest Structure in a Nanoporous Prussian Blue Through In-Situ X-ray Diffraction: a Differential Pair Distribution Function Analysis", *J. Am. Chem. Soc.*, **127**, 11232 - 11233 (2005).
5. G.J. Halder, C.J. Kepert, "*In-situ* Single Crystal X-ray Diffraction Studies of Desorption and Sorption in a Flexible Nanoporous Molecular Framework Material", *J. Am. Chem. Soc.*, **127**, 7891-7900 (2005).
6. A.L. Goodwin, C.J. Kepert, "Negative Thermal Expansion and Low-Frequency Modes in Cyanide-Bridged Framework Materials", *Phys. Rev. B*, **71**, 140301 (2005).
7. K.S. Murray, C.J. Kepert, "*Cooperativity in Spin-Crossover Systems: Memory, Magnetism and Microporosity*", in "Spin-Crossover in Transition Metal Compounds", *Topics Curr. Chem.*, P. Gütllich, H.A. Goodwin (Ed.), Springer-Verlag, Heidelberg, **233**, 195 (2005).
8. G.J. Halder, C.J. Kepert, B. Moubaraki, K.S. Murray, J.D. Cashion, "Guest-Dependent Spin-Crossover in a Nanoporous Molecular Framework Material", *Science*, **298**, 1762 (2002).
9. E.J. Cussen, J.B. Claridge, M.J. Rosseinsky, C.J. Kepert, "Flexible Sorption and Transformation Behavior in a Microporous Metal-Organic Framework", *J. Am. Chem. Soc.*, **124**, 9574 (2002).
10. A.J. Fletcher, E.J. Cussen, T.J. Prior, M.J. Rosseinsky, C.J. Kepert, K.M. Thomas, "Adsorption Dynamics of Gases and Vapours on $\text{Ni}_2(4,4'\text{-bipyridine})_3(\text{NO}_3)_4$: a Nanoporous Metal Organic Framework Material", *J. Am. Chem. Soc.*, **123**, 10001 (2001).

Name: **Associate Professor Erich Herold KISI**

Qualifications: B.Met (Hons 1), PhD (Newcastle, 1988)

Current Appointment: Associate Professor in Materials Science, The University of Newcastle

Previous Appointments: National Research Fellow (ANSTO 1988-90), Senior Research Associate (Griffith 1990-93), Lecturer/Senior Lecturer/Associate Professor (Newcastle 1993-)

Research Grants 2000-2005

Granting Body	Investigators	Title	Years	Amount
ARC-LGS	Kisi	Understanding the Stress-strain State in Polycrystalline Materials	00-02	\$202k
ARC-DP	Kisi and Kennedy	Combustion Synthesis of Ternary Carbides	02-04	\$210k
ARC-DP	Kisi and Forrester	Nanocrystalline processing of polycrystalline ceramics exhibiting the giant piezoelectric effect	03-05	\$135k

ARC-SGS	Kisi	Ferroelasticity in Ferroelectric Ceramics	98-00	\$48k
Univ of Ncle RMC	Murch & Kisi	Self-propagating High-temperature Synthesis of Ti_3SiC_2	00-02	\$50k
Univ of Ncle RMC	Kisi	Giant Piezoelectric Effect in PZN-PT	00	\$13k
Univ of Ncle RMC	Kisi	Diffraction Peak Shapes From Materials Containing Chemical Gradients	01	\$14k
Univ of Ncle	Kisi	Kinetic Paths in Solid State Synthesis	02	\$14k
Univ of Ncle	Kisi	Phase transitions in ferroelectrics	04	\$15k
AINSE	Kisi	In support of all of the above grants	00-05	\$145k
Neutron beam time, ILL, ISIS	Kisi, Riley & Forrester	In support of ARC funded grants above	00-05	\$700k
Access to Major Res. Fac. Prgm	Kisi	In support of the ARC-LGS grants above	00-05	\$46k
ARC (LIEF)	Offler et al.	Upgrade of X-ray Equipment at the University of Newcastle	2002	\$337k
ARC RIEF)/ (LIEF)	Gray et al., later Mather et al.	Access for Australian researchers to advanced neutron beam techniques	2000- 2005	\$1200k
ARC DP	Kisi, Forrester and Howard	Structural basis of the giant piezoelectric effect	2006- 2008	\$230k

Significant Publications 2000-2005 (Total; 28 refereed journal papers, 1 refereed conference paper)

1. E.Wu, **E.H. Kisi**, D.P. Riley and R.I. Smith *Intermediate phases in Ti_3SiC_2 synthesis from Ti/SiC/C mixtures studied by time-resolved neutron diffraction* J. Am. Ceram. Soc. (2002) **85** 3084-3086.
2. J.S. Forrester, R.O. Piltz, **E.H. Kisi** and G.J. McIntyre, *Temperature induced phase transitions in the giant piezoelectric material PZN-4.5%PT*, J. Phys.: Condens. Matter (2001) **13** 825-833.
3. **E.H. Kisi** and D.P. Riley *Diffraction thermometry and differential thermal analysis*, J. Appl. Crystallogr. (2002) **35**, 664-8.
4. E.Wu, **E.H. Kisi**, D.P. Riley and R.I. Smith, *Intermediate phases in Ti_3SiC_2 synthesis from Ti/SiC/C mixtures studies by time-resolved neutron diffraction* J. Am. Ceram. Soc. (2002) **85** 3084-3086.
5. D.P. Riley, **E.H. Kisi**, T.C. Hansen and A.W.Hewat, *Self-Propagating High-Temperature Synthesis of Ti_3SiC_2 ; I. Ultra-High Speed Neutron Diffraction Study of the Reaction Mechanism*, J. Am. Ceram. Soc. (2002) **85**, 2417-24.
6. H.T. Stokes, **E.H. Kisi**, D.M. Hatch and C.J. Howard, *Group Theoretical Analysis of Octahedral Tilting in Ferroelectric Perovskites*, Acta Cryst (2002) **B58**, 934-38.
7. **E.H. Kisi**, R.O. Piltz, J.S. Forrester and C.J. Howard, *The giant piezoelectric effect: electric field induced monoclinic phase or piezoelectric distortion of the rhombohedral parent?* J. Phys.: Condens. Matter (2003) **15** 3631-3640.
8. Y. Ma, **E.H. Kisi**, S. J. Kennedy and A.J. Studer *Tetragonal to monoclinic transformation in Mg-PSZ studied by in-situ neutron diffraction* J. Am. Ceram. Soc (2004) **87**, 465-72.
9. J.S. Forrester, **E.H. Kisi** and A.J. Studer *Direct observation of ferroelastic domain switching in polycrystalline $BaTiO_3$ using in-situ neutron diffraction* J. Europ. Ceram. Soc. (2005) **25**, 447-454.
10. E. Wu, **E.H. Kisi**, D.P. Riley and R.I. Smith *Reaction kinetics of Ti_3SiC_2 synthesis from 3Ti/SiC/C mixtures studied by in-situ neutron diffraction* J. Europ. Ceram. Soc., (2005), **25**, 2503-8.

Name: **Professor Allan PRING**

Qualifications: 1983, PhD The University of Cambridge; **1979, BSc(Hons)** Thesis, Monash University.

Current Appointment: Principal Research Scientist, Mineralogy, South Australian Museum, North Terrace, Adelaide, 5000 and also affiliated positions at University of Adelaide, University of South Australia and Flinders University.

Previous Appointments: 1984- (tenured): Research Scientist (senior and then principal, South Australian Museum. 1999-2000: Visiting fellow commoner, Trinity College, Cambridge.

Research Grants

2000-2002	ARC - large	Pring, Putnis and McCammon	The interaction between exsolution, cation ordering and magnetic properties of iron nickel sulphides	\$140,000
2003-2005	ARC - Discovery	Pring and Putnis	Nickel iron sulphide mineralogy: the link between mineral transformations and microstructure and magnetic properties	\$240,000
2003-2005	ARC Discovery	Withers, Pring, Welbery and Ishizawa	The effects of local strain on the crystal chemistry of solid solutions	\$250,00
2004-2007	ARC - linkage	Brugger, Pring, Schmidt Mumm and McPhail	Mobility of metals in hydrothermal solutions: critical experiments and numerical modelling tools to improve exploration success and ore processing	\$450,000

Significant Publications 2000-2005 (total number of peer-reviewed publications 2001 to present: 25)

1. **Pring, A., T.** The crystal chemistry of the sartorite group minerals from Lengnabach, Binntal, Switzerland: A HRTEM study. *Schweizerische Mineralogische und Petrographische Mitteilungen*. 81, 69-87, 2001.
2. Kolitsch, U and **Pring, A.** Crystal chemistry of the crandallite, beudantite and alunite groups; a review and evaluation of the suitability as storage materials for toxic metals. *Journal of Mineralogy and Petrological Sciences*. 96, 67-78, 2001.
3. **Pring, A.** and Etschmann, B. Crystal chemistry of cosalite, and its relationship to the lillianite group. *Mineralogical Magazine*, 66, 451-458, 2002.
4. Wallwork, K.S., **Pring A.**, Taylor, M.R. and Hunter, B.A. Structure solution of priceite, a basic hydrated calcium borate, by *ab initio* powder-diffraction methods. *Canadian Mineralogist*. 40, 1199-1206, 2002.
5. Etschmann B., **Pring, A.**, Putnis A., Grguric, B.A., and Studer, A. (2004) A kinetic study of the exsolution of pentlandite (Ni,Fe)₉S₈ from the monosulfide solid solution (Fe,Ni)S. *American Mineralogist*, 89, p39-50. 2004
6. Ciobanu, C.L., **Pring, A.** and Cook, N.J. Micron- to nano-scale intergrowths among members of the cuprobismutite series and pad raite: HRTEM and microanalytical evidence. *Mineralogical Magazine*, 68, 279-300, 2004
7. Snow, M.R. **Pring, A.** Self, P. Losic, D. and Shapter, J. The origin of the color of pearls in iridescence from nano-composite structures of the nacre. *American Mineralogist*, 89, 1353-58 (2004)
8. Wang, H., **Pring, A.**, Ngothai, Y., O'Neill, B. A low-temperature kinetic study of the exsolution of pentlandite from the monosulfide solid solution using a refined Avrami method. *Geochimica et Cosmochimica Acta*, 69, 415-125, 2005.
9. Tenailleau, C. **Pring, A.**, Moussa, S., Liu, Y., Withers, R.L. Tarantino, S., Carpenter,

- M. and Zhang, M. An infrared spectroscopy study of composition induced structural phase transitions in the $(\text{Ba}_{1-x}\text{La}_x)_2\text{In}_2\text{O}_{5+x}$ ($0 \leq x \leq 0.6$) system. *Journal of Solid State Chemistry* 178 882-891, 2005.
10. Wang, H., **Pring, A.**, Ngothai, Y., O'Neill, B. The kinetics of the $\alpha \rightarrow \beta$ transition in nickel monosulfide and the synthesis of α nickel monosulfide. *American Mineralogist*, 91, 171-181, 2006.

Name: **Professor Thomas Richard WELBERRY**

Current Appointment: 2001- Professor, Research School of Chemistry
Australian National University

Previous Appointments: 1975-2001 Fellow/Senior Fellow Australian National University

Qualifications: 1970 Ph.D. Chemistry University College, London, UK;
1967 B.A. Cambridge University, UK

Significant Publications

Over the last five years, Professor Welberry has published 1 book, 2 book chapters, 17 journal articles and 4 refereed full conference papers. Ten most significant publications relevant to this application:

- (1) **Welberry, T.R.** Diffuse X-ray Scattering and Models of Disorder. IUCr Monographs on Crystallography, Oxford University Press. Oxford (2004). 279pp.
- (2) **Welberry, T.R.**, *Analysis of Single-Crystal Diffuse X-ray Scattering via Automatic Refinement of a Monte Carlo Model*. Fundamental Materials Research: Beyond the Average Structure, (Eds S.J.L. Billinge, and M.F. Thorpe Plenum Press, New York and London, pp 1-22. (2002).
- (3) **Welberry, T.R.**, Diffuse X-ray scattering and disorder in p-methyl-N-(p-chlorobenzylidene)aniline, $\text{C}_{14}\text{H}_{12}\text{ClN}$ (ClMe): analysis via automatic refinement of a Monte Carlo model. *Acta Crystallogr.* **A56**, 348-358, (2000).
- (4) Butler, B.D., Haeffner, D.R., Lee, P.L. and **Welberry, T.R.** High-energy X-ray diffuse scattering using Weissenberg flat-cone geometry *J. Appl. Crystallogr.* **33**, 1046-1048, (2000).
- (5) **Welberry, T.R.**, Goossens, D.J., Edwards, A.J., David, W.I.F., Diffuse X-ray scattering from benzil, $\text{C}_{14}\text{H}_{10}\text{O}_2$: analysis via automatic refinement of a Monte Carlo model. *Acta Crystallogr.* **A57**, 101-109, (2001).
- (6) **Welberry, T.R.**, Diffuse X-ray scattering and strain effects in disordered crystals. *Acta Crystallogr.* **A57**, 244-255, (2001).
- (7) **Welberry, T.R.**, Goossens, D.J., Haeffner, D.R., Lee, P.L., Almer, J. High-energy diffuse scattering on the 1-ID beamline at the Advanced Photon Source. *J. Synchrotron Radiation.* **10**, 284-286, (2003).
- (8) Kreisel, J., Bouvier, P., Dkhil, B., Thomas, P.A., Glazer, A.M., **Welberry, T.R.**, Chaabane, B., Mezouar, M., High-pressure x-ray scattering of oxides with a nanoscale local structure: Application to $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$. *Phys. Review.* **B68**, 014113, (2003).
- (9) **Welberry, T.R.** and Heerdegen, A.P., Diffuse X-ray scattering from 4,4 'dimethoxybenzil, $\text{C}_{16}\text{H}_{14}\text{O}_4$: analysis via automatic refinement of a Monte Carlo model. *Acta Crystallogr.* **B59**, 760-769. (2003).
- (10) Campbell, B.J., **Welberry, T.R.**, Broach, R.W., Hong and H.W., Cheetham, A.K., Elucidation of zeolite microstructure by synchrotron X-ray diffuse scattering. *J. Appl. Crystallogr.* **37**, 187-192. (2004).

Research Grants

Prior to 2002 Professor Welberry was ineligible, because of the ANU Block funding, to compete for ARC competitive grants. Professor Welberry is a Chief Investigator on the following competitive grants.

Development of Methods and Strategies for the Measurement, Interpretation and Analysis of Diffuse X-ray Scattering from Disordered Materials.	ARC Discovery Grant	2003-2005	\$240,000
The effects of local strain on the crystal chemistry of solid solutions.(with Withers, Pring, and Ishizawa)	ARC Discovery Grant	2003-2005	\$240,000
Diffuse neutron scattering from benzil; temperature dependence and energy resolved diffuse scattering	AMRF grants	2003, 2004	\$22,870
High energy diffuse scattering from disordered crystals. Diffuse scattering from flexible molecular systems	ASRP grants	2000, 2003	\$14,070

Name: **Professor John WHITE**

Qualifications: 1957: B.Sc. (University of Sydney); 1959 MSc. (University of Sydney); 1963 D.Phil (Oxford University).

Current Appointments: Professor (Level E3) and Head of the Solid State Molecular Science Group, RSC, ANU: 1985–

Previous Appointments: ICI Research Fellow , Lincoln College , Oxford 1961-1963. Fellow of St Johns College , Oxford and University Demonstrator in Physical Chemistry 1963-1985, Director of Institut Laue Langevin , Grenoble, France 1975-1980, Pro-Vice Chancellor and Chairman of the Board of the Institute of Advanced Studies, ANU 1991-1994, Dean Research School of Chemistry, ANU, 1994-1997

Research Grants

2002-2004	ARC - Linkage	Yates, Henderson Goodridge, Reynolds	High Internal Phase Emulsions - Structure and Rheology Control	\$340,000 + \$280,000
2004-2007	ARC - Linkage	Reynolds, Zank, Goodridge, Such, Henderson	Designer Surfactants for Creation of Emulsion Properties	\$390,000
2004-2006	DEST	Henderson	Making Film Stars - photoactive TiO2	\$290,000

In addition for the UNIChe project linking the best school and university students to industrial projects 2000 to 2006, a grant of \$M1.3, part financed by DEST, industry and universities in 2000 supplemented by \$ 200,000 + \$400,000 (from industry and Universities)

Publications 2000-2005

1. **Polymeric Surfactant Structure.** Saville, P M, White, J W. *Chinese Journal of Polymer Science*, **2**, 135- (2001).

2. **High internal phase water-in-oil emulsions and related microemulsions studied by small angle neutron scattering: II the distribution of surfactant.** Reynolds, P A, Gilbert, E P, White, J W. *J. Phys. Chem B*, **105**, 6925-6932 (2001)
3. **An energy dispersive time resolved liquid surface reflectometer.** Garrett, R F, White, J W, King, K J, Dowling, T L, Fullagar, W. *Nucl. Instr. Meth. A*, **467-468**, 998-1000, (2001)
4. **Structure development in octadecyl trimethylammonium templated silicate films grown at the air/water interface.** Holt, S A, Ruggles, J L, White, J W, Garrett, R F. *J. Phys. Chem B*, **106** (9), 2330-2336, (2002)
5. **Thermal Denaturation of Interfacial Protein Layers.** Holt, S A, Henderson, M J, White, J W. *Aust. J. Chem.*, Special Edition of Plenary Lectures, 25 Australian Polymer Symposium, **55**, 449–459 (2002)
6. **The Interfacial Structure of a High Internal Phase Emulsion Near a Solid Surface.** Reynolds, P A, Henderson, M J, Holt, S A, White, J W. *Langmuir* **18**, 9153–9157(2002).
7. **Neutron and X-ray Reflectivity from Polyisobutylene-Based Amphiphiles at the Air-Water Interface.** Reynolds, P A, McGillivray, D J, Gilbert, E P, Holt, S A, Henderson, M J, White, J W. *Langmuir* (2003), **19**, 752-761.
8. **Expanded Mesoporous Silicate Films Grown at the Air-Water Interface by Addition of Hydrocarbons.** Ruggles, J L, Gilbert, E P, Holt, S A, Reynolds, P A, White, J W. *Langmuir* **19**, 793-800 (2003)
9. **The growth of self-assembled titania-based films at the air-water interface.** Henderson, M J, King, D, White, J W. *Aust. J. Chem.* **56**, 933-939 (2003).
10. **Structural Development of Silicated Films Self-Assembled at the Air-Water Interface.** Holt, S A, Ruggles, J L, Reynolds, P A, White, J W. *Physica B* **336**, 193-203 (2003)
11. **Characterisation of Electrosterically Stabilized Polystyrene Latex; Implications for Radical Entry Kinetics.** De Bruyn, H, Gilbert, R G, White, J W, Schulz, J C. *Polymer* **44**, 4411-4420 (2003)
12. **Time Dependent Changes in the Formation of Titania Based Films at the Air-water Interface.** Henderson, M J, King, D, White, J W. *Langmuir* **20**, 2305-2308 (2004)
13. **A Small Angle Neutron Scattering Study of the Interface Between Solids and Oil-continuous Emulsions and Oil based Microemulsions.** Reynolds, P A, Henderson, M J, White, J W. *Colloids Surf A* **232**, 55-65 (2004)
14. **Determination of domain sizes in blends of poly(ethylene) and poly(styrene) formed in the presence of supercritical carbon dioxide.** Thurecht, K J, Hill, D J T, Preston, C M L, Rintoul, L, White, J W, Whittaker, A K. *Macromolecules* **37**(16), 6019-6026 (2004)
15. **Time Dependent Changes in the Formation of Titania Based Films at the Air-**

Water Interface. Henderson, M J, King, D, White, J W. *Langmuir*, **20**(6), 2305-2308 (2004)

16. A Zirconium Oxide Film Self-Assembled at the Air-Water Interface. Henderson, M J, Gibaud, A, Bardeau, J-F, Rennie, A R, White, J W. *Physica B*, **357**, 27-33, (2005)

17. The Phase Transitions of n-alkanes in mesoscopic pores of graphite. Espeau, P, White, J W. *Carbon*, **43**, 1885-1890 (2005)

18. The Structure of n-alkane binary mixtures Adsorbed on Graphite. Espeau, P, White, J W, Papoular, R J. *Applied Surface Science*, **252**, 1350-1359 (2005)

19. Characterisation of a protein-based adhesive elastomer secreted by the frog *Notaden bennetti*. Graham, L D, Glattauer, V, Mickey G. Huson, Jane M. Maxwell, Russell Varley, Robert B. Knott, John W. White, Paul R. Vaughan, Yong Peng, Michael J. Tyler, Jerome A. Werkmeister, and John A. Ramshaw, *Biomacromolecules*, **6**(6) 3300-3312, (2005)

20. Protein-Poly(silicic) Acid Interactions at The Air/Solution Interface. Mark J. Henderson, Adam W. Perriman, Hana Robson-Marsden, and John W. White, *J Phys Chem*, **109**(44), 20878-20886, (2005)

There are five papers on high internal phase emulsions awaiting clearance by ORICA Ltd after patent proceedings have finished.

Other Evidence of Impact 2000-2005

Invited Lecturer American Chemical Society Meeting, San Francisco, March (2000)

Invited Lecturer American Chemical Society Meeting Washington, August (2000)

Invited Lecturer, IUPAC World Chemistry Congress, Brisbane, July (2001)

One of three plenary speakers at 50th Anniversary of the IUCr

25th Australian Polymer Symposium opening lecture (2002)

Plenary Lecture (International Conference on radiation) 2004

Plenary Lecture for Bionano Oliphant Conference (2005)

Leighton Medal (Royal Australian Chemical Institute) (2005)

Craig Medal for Chemistry (Australian Academy of Science)(2005)

Name: **Professor Ray WITHERS**

Qualifications: 1973-75: B.Sc. (University of Melbourne); 1976: B.Sc.Hons. (University of Melbourne); 1981: Ph.D. (University of Melbourne); Ph.D. thesis title: "*The incommensurate phase of 2H-TaSe₂*".

Current Appointments: Professor (Level E1) and Head of the Solid State Chemistry group, RSC, ANU: Jan. 2004–

Associate Dean (Students) and Prescribed Authority, RSC, ANU: October 2000- . The Associate Dean (Students) is the delegated authority for all matters relating to students within RSC.

Previous Appointments: August 1981-January 1983: Post-doctoral Fellow, Theoretical Solid State Physics, University of Toronto, Canada.

1983-1986: Post-doctoral Fellow and Research Associate, Electron Microscopy and

Microstructural characterization Group, H.H. Wills Physics Laboratory, University of Bristol, U.K.

Research Fellow, RSC, ANU: January 1986-July 1989.

Senior Research Fellow, RSC, ANU: July 1989 - December 1991.

Fellow and Head of the Solid State Chemistry group, RSC, ANU: December 1991 - September 1997.

Senior Fellow (Level D) and Head of the Solid State Chemistry group, RSC, ANU: Sept. 1997– Oct. 2003.

Convenor, Graduate Program in Chemistry, ANU: Jan. 1997 – Oct. 2000.

Research Grants

2003-2005	ARC - Discovery	Pring, Welberry, Ishizawa, Withers	The effects of local strain on the crystal chemistry of solid solutions	\$245,000
2005-2007	ARC - Discovery	Kennedy, Schmid, Howard, Withers	Understanding phase transformations through precise structural studies	\$390,000
2006-2010	ARC - Discovery	Liu, Withers	An integrated approach towards the development of new generation RF/microwave dielectric materials	\$830,000

Significant Publications 2000-2005

1. R.L.Withers, Y.Tabira, A.Valgomar, M.Aroyo and M.Dove. The inherent displacive flexibility of the hexacelsian tetrahedral framework and its relationship to polymorphism in Ba-hexacelsian. *Phys. Chem. Minerals* **27**, 747-756, 2000.

2. R.L.Withers, Y.Tabira, J.S.O.Evans, I.J.King and A.W.Sleight. A new three-dimensional incommensurately modulated cubic phase (in ZrP_2O_7) and its symmetry characterization via temperature-dependent electron diffraction. *J.Solid State Chem.* **157**, 186-192, 2001.

3. R.L.Withers, Y.Tabira, Y.Liu and T.Höche. A TEM and RUM study of the inherent displacive flexibility of the fresnoite framework structure type. *Phys. Chem. Minerals* **29**, 624-632, 2002.

4. R.L.Withers. An analytical solution for the zero frequency hyperbolic RUM modes of distortion of SiO_2 -tridymite. *Solid State Sciences* **5**, 115-123, 2003.

5. R.L.Withers, T.R.Welberry, F.J.Brink and L.Norén. Oxygen/fluorine ordering, structured diffuse scattering and the local crystal chemistry of $K_3MoO_3F_3$. *J.Solid State Chem.* **170**, 211-220, 2003.

6. R.L.Withers, M.James and D.J.Goossens. Atomic Ordering in the Doped Rare Earth Cobaltates $Ln_{0.33}Sr_{0.67}CoO_{3-\delta}$ ($Ln = Y^{3+}, Ho^{3+}$ and Dy^{3+}). *J.Solid State Chem.* **174**, 198-208, 2003.

7. R.L.Withers, T.R.Welberry, A-K.Larsson, Y.Liu, L.Norén, H.Rundlöf and F.J.Brink. Local crystal chemistry, induced strain and short range order in the cubic pyrochlore $(Bi_{1.5-\alpha}Zn_{0.5-\beta})(Zn_{0.5-\gamma}Nb_{1.5-\delta})O_{(7-1.5\alpha-\beta-\gamma-2.5\delta)}$ (BZN). *J. Solid State Chem.* **177**, 231-244, 2004.

8. R.L.Withers, L.Norén and Y.Liu. Flexible phases, Modulated Structures and The Transmission Electron Microscope. *Z.Krist.* **219**, 701-710, 2004.

9. R.L.Withers and Yun Liu. Local crystal chemistry, structured diffuse scattering and inherently flexible framework structures. Chapter in *Inorganic Chemistry in Focus* (Eds.

G.Meyer, D.Naumann and L.Wesemann) Wiley-VCH, Weinheim, 2005.

10. Ray L. Withers. Disorder, structured diffuse scattering and the Transmission Electron Microscope. *Z.Krist.* **220**, 1027-1034, 2005.

Proposal by the participating groups for the general good.

The groups and universities associated with this proposal do so on behalf of all Australian present and future users of access through AINSE to this facility. An indication of their general performance against the very fierce competition for access to ISIS is illustrated by the data above and also by the success of these groups in Australian research council discovery grants, linkage grants, and other grants from industry and industry related bodies. The groups also undertake a “mentoring role” for new users. Their participation in the ISIS access program has led to recruitment of Australians onto the ISIS staff and to new collaborations with UK and European colleagues.

They are also active on many Australian committees including those associated with AINSE, OPAL, and the Australian Synchrotron.

Chapter 4

Effectiveness of the cooperative arrangements between institutions including access and resource sharing and the extent of current usage

Evidence of collaborative arrangements including research grants and publications

The sections in Chapter 2 on complementarity to Lucas Heights illustrates the growth of close collaborations as do the illustrations of current programmes in Appendix 4(below) . We note a few of these:

A/Professor Gentle has a long-term collaboration with Professor Geoffrey Ashwell of Cranfield University, UK, on aspects of molecular electronics. Access to ISIS is central to the success (and continuation) of this collaboration. It has resulted in a number of publications and, most recently, a successful ARC Discovery Project Grant.

International work from ISIS published with Professor Pat Woodward (Ohio State University) and an ongoing collaboration with Professor Tom Vogt (ex Brookhaven National Laboratory and now South Carolina University). Also critical for ARC discovery project between Kennedy and Schmid (Sydney) Withers (ANU) and Howard (ANSTO).

Professor Welberry has a new collaboration with professor Bill David (University College London) and Professor White a long standing collaboration with Professor Jeffrey Penfold (ISIS), Dr Stephen Holt (ISIS) and Dr R.K.Thomas FRS (Oxford University).

The current cooperative arrangements between the Australian Institute of Nuclear Science and Engineering and the Rutherford-Appleton Laboratory (ISIS facility) work very well. The Australian scientific proposals are sent direct to the ISIS reviewing panels from Australia. It has not been found necessary to add a second reviewing process in Australia because of the complementarity of the ISIS and HIFAR instruments.

The AINSE access to HIFAR process has adopted strict refereeing guidelines to maximise the quality of the science done with the available facility. Experiments only suitable for ISIS are directed for resubmission in there. In addition, the AINSE Council has now earmarked funding some scholarships for students needing access to the ISIS facilities so as to encourage the international networking spoken of above.

In the last five years four different senior investigators from Australia have been invited as members of the ISIS specialist review panels. They have participated in those meetings twice a year with their travel and local accommodation costs met by ISIS. This has had a value to Australia because of the personal and scientific contacts developed in those meetings.

AINSE does not have the funding to support travel and accommodation for Australian users of the ISIS facility. This funding is obtained for most of the successful proposals through the Department of Education, Science and Training (DEST) "Access to Major Research Facilities fund (AMRF)". Often the demands on funds available result in no more than two campaigns of a few days a year for principal proposers with one or two postdoctoral or student members being supported. Often researchers have added university funds to allow an adequate team to support a long or exhausting experiment (often teams have to work shifts for instruments that are highly productive such as LOQ, GEM, SURF & CRISP). The funding availability has limited the access in the last two years; only partial funding being available.

A Memorandum of Understanding between AINSE and the ISIS facility covers the access process of Australian users as well as all of the radiation safety and other user matters performed by ISIS for Australian users. In all respects Australian users appear to be treated on an identical footing as those from the UK.

As mentioned above, Australian users are accessing much more of the facility than they pay for. There have been occasional reminders that we should attempt to pay “more of our way” but there has never been any discrimination on the basis that we have been unable to do that.

The year 2005 was a more difficult year for Australian and other ISIS users than any previously because the source was shutdown for upgrading for approximately seven months of the year. Despite this, Australian proposals have remained very successful and it is expected that some proposals that did not get through because of reduced facility time will be funded as a priority after resubmission in 2006.

As a further illustration of the effectiveness of cooperation, a number of Australians have participated in joint planning meetings and workshops for instrument development at ISIS. Examples include:

- Planning and partial funding of the SURF facility;
- Support for the GEM proposal;
- Invited participants (speaking) at the scientific foresight meeting for the Second Target Station proposal and in the working groups on Second Target Station instruments.

In addition to this collaboration there have been collaborative publications between Australian groups themselves and between Australian and UK groups. Examples of this are indicated in the list of publications by the symbol.

Chapter 5

The Commitment of the Lead and Collaborating Institutions, including clear evidence of the extent of financial and other support, consistent with relevant research management plans.

AINSE has a forty-eight year track record of innovation in collaborative arrangements between the Australian Nuclear Science and Technology Organisation (ANSTO), and Australian universities. The success of the collaboration with the ISIS facility has added a new dimension to that track record and the Council is committed to maintaining and developing this role. The process of a substantial AINSE financial commitment to the access to ISIS combined with separate contributions from the universities of the major users is one that AINSE expects to continue as the chief current international outreach.

The contributions from universities towards the ISIS access program have all been agreed in the past by the Deputy Vice-Chancellors (Research) of the participating universities as an additional sum as to that provided by the universities for access to ANSTO facilities. This process is intended to continue in the proposal for the next five-year period of the Large Infrastructure Equipment Fund (LIEF) grant, which will be sought in association with this submission. These commitments are key components of the research management plans of the Departments, schools and universities concerned and of AINSE.

The financial relationship between AINSE and the individual collaborating institutions is a stable one. The contributions to AINSE, both from universities and ANSTO, have been planned into budgets and a new Memorandum of Agreement between AINSE and ANSTO, valid until the operation of instruments for the Replacement Research Reactor, has just been signed between AINSE and ANSTO, valid until the operation of instruments for the Replacement Research Reactor.

96. AINSE's objectives are:

1. To provide a mechanism for users in member organisations of AINSE to have access to major nuclear science and engineering and associated facilities at ANSTO and other agreed sites for research purposes;
2. To facilitate graduate and undergraduate education and training experience utilising major nuclear science and technology facilities at ANSTO and other agreed sites;
3. To encourage collaboration and cooperation between member organisations of AINSE in areas primarily related to nuclear science and engineering and their applications; and
4. To sustain and support the development of major nuclear science and technology facilities at ANSTO and other agreed sites for shared use by member organisations of AINSE.

The access to ISIS thus falls squarely within the mission and all of the objectives of AINSE.

Chapter 6

The financial relationship between AINSE and the individual collaborating institutions

AINSE took over the leadership of access to ISIS in 1997. Since then there has been consistent support for the program from the collaborating institutions. Levels of support range from \$5,000 to \$30,000. Over the period the number of collaborating universities has increased from seven and in 2007 there will be nine. Over the period ANSTO has contributed \$25,000 pa up to and including 2006.

Over the contract with ISIS has maintained a subscription at AUD\$400,000 pa. Over the period the contribution from collaborating institutions has represented about 40% of the subscription, the remainder coming from the ARC LEIF Grants.

Since then the ARC, with the exception of 1999, has supported the program. In that year AINSE gained other support and thereby managed to maintain the continuity of the collaboration with ISIS.

Organisation	2003	2004	2005	2006	Anticipated 2007
AINSE	20,000	8750	8750	7750	12,750
Griffith University	20,000	20,000	15,000	15,000	15,000
The Australian National University	30,000	30,000	30,000	30,000	30,000
The University of Queensland	20,000	20,000	20,000	20,000	20,000
Curtin University of Technology	10,000	10,000	10,000	10,000	10,000
The University of Newcastle	10,000	10,000	10,000	10,000	10,000
The University of Sydney	10,000	20,000	20,000	20,000	20,000
The University of New South Wales	5,000	16,250	16,250	16,250	16,250
ANSTO	25,000	25,000	25,000	25,000	20000
Monash University	5,000	5000	5000	6000	6000
The University of Adelaide					5000
	155,000	165,000	160,000	160,000	132,250
Awarded	245,000	235,000	240,000	240,000	240,000
Total	400,000	400,000	400,000	400,000	400,000

Table 3. Summary of university cash contributions to LIEF “access to ISIS” proposals.

Chapter 7

Summary and Conclusion

This document responds to the request of the Australian Research Council for its review of Australian Access to the worlds most powerful spallation neutron source, ISIS, at the Rutherford Appleton Laboratory, Oxfordshire UK. Information gathered from the principle groups using ISIS illustrates the breadth of science possible there and the complementarity of this science to that accessible in Australia. This science is representative of the whole spectrum of Australian use of the facility. It is also iredcently of future trends in Australian condensed matter science if the experience of Europe, the United States and Japan can serve as a guide.

The much broader community served by the ISIS source spans Japan, India, countries of Europe, Canada and the United States in addition to Australia. Judging by the experience in those countries Australia will require access to a broader range of instruments at ISIS than we currently have. Some of this demand will be met by the Replacement Research Reactor, but weaknesses in the current condensed matter science community in Australia, such as in the structure and dynamics of fluids, the dynamics of crystalline and amorphus solids may eventually be met or be initiated in Australia through ISIS access.

The terms of reference set out by the Australian Research Council have been addressed sequentially in this report, and ancillary material requested has been incorporated as appendixes to the report. This relates to the track record of the principle investigators for grants and publications, prizes and promotions, and also to the comprehensive publication record of those proposers as well as all Australian ISIS users.

We draw the attention of the review committee to the increasing Australian-overseas collaborations initiated through ISIS access. This is the more mature aspect of an initial mentoring process provided both by ISIS scientists as part of their role for visitors, as well as by groups in Australia who have helped new groups to start up on suitable problems.

From the point of view of the authors of this report, ISIS access has provided a scientifically exciting avenue to new areas of science and international collaborations. The success rate of Australian proposals in the contestable situation at ISIS indicates that Australia not only gets good value for money, but also a benchmark for its own scientific originality.

Appendix 1

Issues to be addressed in submission to the ARC

- Evidence of significant benefits to Australia resulting from access to a major facility not otherwise available to Australians.
 - Including benefits realised to date by research and research training, the public sector and industry.
- The relevance of the facility to national needs and the availability of comparable infrastructure in Australia.
 - In particular, the benefits to Australia of continued participation.
- The excellence of the researchers and research activity to be supported.
 - The general performance of the participating groups
 - The success of current research programs
- The effectiveness of the cooperative arrangements between institutions, including access and resource sharing and the extent of current usage.
 - Evidence of collaborative arrangements including research grants, publications
- The commitment of the collaborating institutions and AINSE as the peak body, including clear evidence of the extent of financial and other support, consistent with relevant research management plans.
- The financial relationship between AINSE and individual collaborating institutions.
- The relationship between the strategic plans of AINSE and individual collaborating institutions.

Appendix 2

List of Australian Users 1998 – 2005 (Alphabetical, from Proposals)

Dr G Allan	Minerals, CSIRO
Dr David Antelmi	Research School of Chemistry, ANU
Mr Esteban Astudillo	University of Western Sydney
Ms Katie Baldwin	Dept of Chemistry, university of Queensland
Dr Krisztian Baranyai	Research School of Chemistry, ANU
Mr Andrew Beasley	Research School of Chemistry, ANU
A/Prof James Beattie	School of Chemistry, University of Sydney
Dr T P Blach	School of Science, Griffith University
Dr Annabelle Blom	School of Chemistry University of Sydney
Dr Till Boecking	School of Physics, University of New South Wales
A/Prof Craig Buckley	Dept of Applied Physics, Curtin University of Technology
Prof Stewart Campbell	School of Physics, ADFA, University of NSW
Ms Karena Chapman	School of Chemistry, University of Sydney
Dr Caroline Curfs	University of Newcastle
Dr Gary Dennis	Dept of Chemistry, University of Western Sydney
Dr B Etschmann	South Australian Museum
Dr Yang Fei	Neutron Scattering Group, ANSTO
Mr Bradley Finnigan	Department of Chemistry University of Queensland
Dr Jenny Forrester	School of Engineering, University of Newcastle
Dr Christopher Garvey	Neutron Scattering Group, ANSTO
Dr Ian Gentle	Dept of Chemistry, University of Queensland
Dr Elliot Gilbert	Research School of Chemistry, ANU
Dr Darren Goossens	Research School of Chemistry, ANU
A/Prof Evan Gray	School of Science, Griffith University
Dr Mark Hagen	Bragg Institute, ANSTO
Dr Mark Henderson	Research School of Chemistry, ANU
Dr Trevor Hicks	Dept of Physics, University of Monash
Professor Greg Hope	School of Science, Griffith University
Dr Chris Howard	Australian Science and Technology Organisation (ANSTO)
Dr Michael James	Neutron Scattering Group, ANSTO
Dr Brendan Kennedy	School of Chemistry, University of Sydney
Dr Cameron Kepert	School of Chemistry, University of Sydney
A/Prof Erich Kisi	School of Engineering, University of Newcastle
Dr Wim Klooster	ANSTO
Dr Robert Knott	ANSTO
Dr Chris Ling	Research School of Chemistry, ANU
Dr I-M Low	Dept Applied Physics, Curtin University of Technology
Dr Y Ma	Dept of Mechanical Engineering, University of Newcastle
Dr Rene Macquart	School of Chemistry, University of Sydney
Dr David Martin	University of Queensland
Mr Keith McLennan	Griffith University
Dr Paul Meredith	University of Queensland
Assoc Prof Tom Millar	University of Western Sydney
Dr Sandra Moussa	School of Chemistry, University of Sydney
Dr Andrew Nelson	Bragg Institute, ANSTO
Prof Brian O'Connor	Dept of Applied Physics, Curtin University of Technology
Dr Ben O'Driscoll	Dept of Chemistry, University of Queensland
Mr Adam Perriman	Research School of Chemistry, ANU
Mr Allan Pring	Principal Curator of Minerals, South Australian Museum

Dr Philip Reynolds	Research School of Chemistry, ANU
Mr Daniel Riley	Dept of Engineering, University of Newcastle
Dr Jeremy Ruggles	Dept of Chemistry, University of Queensland
A/Prof Tim St. Pierre	Dept of Physics, University of Western Australia
Mr Paul Saines	School of Chemistry, University of Sydney
Dr Brian Saunders	Dept of Chemistry, University of Adelaide
Dr Siegbert Schmid	Research School of Chemistry, ANU
Dr Jamie Schulz	Neutron Scattering Group, ANSTO
Dr M Singh	Dept of Applied Physics, Curtin University of Technology
Dr Christophe Tenailleau	The South Australian Museum
Ms Valseka Ting	Research School of Chemistry, ANU
Dr Arie van Riessen	Dept of Applied Physics, Curtin University of Technology
Dr Maarten Vos	Research School of Physical Sciences, ANU
A/Prof Gregory Warr	School of Chemistry, University of Sydney
Dr Richard Welberry	Research School of Chemistry, ANU
Dr Ray Withers	Research School of Chemistry, ANU
Prof John White	Research School of Chemistry, ANU
Dr Wong	University of Wollongong
Dr E Wu	Dept of Mechanical Engineering, University of Newcastle
Dr Johann Zank	Research School of Chemistry, ANU
Dr Zhaoming Zhang	Materials and Engineering Science ANSTO

Appendix 3

The excellence of the researchers and research activity to be supported

Performance of the participating group

As a metric of the general performance of the participating groups we have used the following:

Success in ARC Grants

Year	Grant	Investigators	Title	Amount
2000	ARC Discovery	Y Chen (ANU), SJ Campbell et al	Formation Mechanism of Boron Nitride Nanotubes Produced by Reactive Ball Milling	\$81,000
2000	ARC RIEF	H O'Neill (ANU), S J Campbell et al	An Electron Microprobe for High Accuracy Chemical Microanalysis	\$510,799
2000	ARC - Small	C E Buckley, A Rohl et al	The Determination of the Structure of γ -Alumina from First Principle Calculations.	\$12,200
2000-2002	ARC -Large grant	J Low, B Lawn, C E Buckley	Microstructural design of layered and graded alumina-based composites	\$144,629
2001	ARC - RIEF	C E Buckley, B O'Connor et al	A Small Angle X-Ray Scattering Facility for Western Australia	\$300,000
2001	ARC - RIEF	M Middleton, C E Buckley et al	Portable Neutron Generator for Resource Applications	\$130,000
2003	ARC Discovery	R De Marco, C E Buckley, A Rohl	Probing the Interfaces of Electrochemical Sensors	\$160,000
2004	ARC Discovery	G Parkinson, C E Buckley et al	Ferrihydrite: Fundamentals of a Natural Nanomaterial	\$435,000
2005	ARC Linkage	M I Ogden, C E Buckley, G A Carter	Controlling precipitation processes in the production of value-added zirconia	\$72,444
2005-2009	ARC Research Networks	C Kepert, C E Buckley et al	Molecular and Materials Structure Network	\$1,500,000
2006-2008	CSIRO flagship NHMA	Gray et al	Hydrogen Storage Stream	\$2,152,000
2001	UQ RDG	S Bhatia, I Gentle	Studies of adsorption equilibria over surface engineered microporous solids	\$56,000
2001	UQ Enabling Grant	I Gentle, M Crossley	Supramolecular assemblies of porphyrins in thin films	\$10,000
2002	ARC Discovery	IR Gentle and GJ Foran	DP021067, Patterned Assemblies of Molecules on Surfaces	\$183,000
2002	UQ RDG	J Drennan, M Riley, I Gentle	A new initiative in materials chemistry	\$54,000
2001	ARC Small	E Gray	Carbon-based hydrogen storage	\$26,500
2001	ARC RIEF	AINSE, E Gray et al	Access for Australian researchers to advanced neutron-beam techniques	\$245,000
2002	ARC, Linkage	J Bell, E Gray, J Kavanagh	Electronic properties of diamond-like carbon for applications in planar optical waveguides	\$23,000
2003	ARC Discovery	E Gray, J Dobson	Hydrogen absorption by nanostructured carbons	\$95,000
2000	ARC (Small)	B Kennedy	Structural Variants and Phase Transitions in Perovskites	\$15,000
2000	ARC (Large)	B Kennedy, CJ Howard, T Vogt	Structural and Bonding Trends in Bismuth Oxides	\$144,000

2001	ARC (Large)	B Kennedy, CJ Howard	Structural Variants and Phase Transitions in Perovskites	\$144,000
2001	ARC SPIRT	B Kennedy, PA Lay, N Davies, E Weder, TW Hambley	New Metal Complexes of NSAIDs as Veterinary Eye Ointments, Anti-Cancer Drugs and General Anti-inflammatory Agents.	\$437,860
2003	ARC (Large)	B Kennedy	Structural and Electronic Properties of Layered Bismuth Oxides	\$85,000
2002	ARC Linkage (LIEF)	C Offler, E Kisi et al.	Upgrade of X-ray Equipment at the University of Newcastle	\$337,000
2002	ARC Discovery	E Kisi and S Kennedy	Combustion Synthesis of Ternary Carbides	\$210,000
2003	ARC Discovery	E Kisi and J Forrester	Nanocrystalline Processing of Polycrystalline Ceramics Exhibiting the Giant Piezoelectric Effect	\$135,000
2002	ARC Linkage (LIEF)	JW White	Nanostructures of High Internal Phase emulsions	\$340,000
2002	ARC Linkage (LIEF)	AINSE, J W White, D Mather et al	Access for Australian researchers to advanced neutron-beam techniques	\$245,000

2006	ARC-LIEF	EH Kisi, CC Curfs, DP Riley, BV King, T Maschmeyer, EM Gray, RF Garrett, I Madsen and SA Schmid	The Rapid Kinetics Research Facility - an Integrated system for rapid kinetic studies of materials using synchrotron radiation	\$195,000
2006-2008	ARC-Discovery	EH Kisi, JS Forrester & CJ Howard	Structural Origins of the Giant Piezoelectric Effect in Relaxor Ferroelectrics	\$232,000
2005-2007	ASRP - Fellowship	CC Curfs & EH Kisi	Combustion Synthesis studies using synchrotron radiation	\$228,000
2003-2005	ARC-Discovery	EH Kisi & JS Forrester	Nanocrystalline Processing of Polycrystalline Ceramics Exhibiting the Giant Piezoelectric Effect, ARC Discovery Project. **	\$135,000
2002-2004	ARC-Discovery	EH Kisi (CI) & SJ Kennedy (PI)	Combustion Synthesis of Ternary Carbides	\$210,000
2005	U of Ncle RGC Project grant	G Suaning & EH Kisi	Controlled Sintering of Alumina Powder at Low Temperatures	\$9,100
2005	U of Ncle RGC Project grant	EH. Kisi & G. Suaning	Diffusion Machining of Microcavities: A First Step	\$9,500
2006	ARC-LIEF	Bilek, Valanoor, McKenzie, O'Connor, Green, Lay, Ekins-Daukes, King, James, Conibeer, Kable, Schmidt, Ostrikov, Hoffman, Riley and Ferry.	Combinatorial Deposition and Characterisation Facility for New Alloy Thin Film Materials	\$1,250,000
2004-2006	ARC-Discovery (APD)	DP Riley	Engineering of Crystalline Ternary Ceramic Precursors, ARC-DP *, **	\$225,000
2005	U of Ncle RMC Coop'Ve Research Grant	DP Riley & EH Kisi	New Laser Clad Wear Resistant Coatings,	\$10,000

2002	ARC-LIEF	C Offler, EH Kisi et al.	Upgrade of X-ray Equipment at the University of Newcastle	\$337,000
2006-2008	ARC Discovery	Low	Synthesis of Novel Nanostructured Ternary Carbide Composites	\$120,000
2002-2004	ARC Linkage-International	Low	Damage Micromechanisms in Alumina Hybrid Bilayers with Graded Interfaces	\$36,400
2002-2004	Systemic Infrastructure Initiative	Low	Nanofabrication Facilities for Processing of Novel Multilayer Materials	\$1,477,500
2005	AINSE	Low	Effect of Grain Size on the Thermal Stability of Al ₂ TiO ₅	\$12,360
2005	AINSE	Low	Depth-profiling of Composition in Vacuum-Treated and Air-Oxidised Titanium Silicon Carbide Using SIMS	\$17,500
2006	ASRP	Low	Depth-profiling of Near-Surface Compositions in Air-Oxidised Titanium Silicon Carbide (Ti ₃ SiC ₂)	\$4,300
2001	AMFP 01/115P	Pring	Exsolution and cation ordering in iron nickel sulphides.	\$9,600
2002	02/102	Pring	A new type of copper and rare earth element mineralisation at Paratoo, SA: a natural laboratory for the mobility of elements in the regolith	\$12,300
2002	02/103	Pring	The kinetics of exsolution in the pentlandite-pyrrhotite system ((Fe,Ni) ₉ S ₈ -FeS)	\$32,699
2003	03/094	Pring	The effects of S fugacity on the kinetics of exsolution in iron nickel sulfides	\$16,782
2005	05/209	Pring	Transformations in nickel sulfides under hydrothermal conditions	\$8,540
2000-2002	ARC Large	Pring, Putnis and McCammon	The interaction between exsolution, cation ordering and magnetic properties of iron nickel sulphides	\$140,000
2003-2005	ARC Discovery	Pring and Putnis	Nickel iron sulphide mineralogy: the link between mineral transformations and microstructure and magnetic properties	\$240,000
2003-2005	ARC Discovery	Withers, Pring, Welberry and Ishizawa	The effects of local strain on the crystal chemistry of solid solutions	\$250,000
2004-2007	ARC Linkage	Brugger, Pring, Schmidt Mumm and McPhail	Mobility of metals in hydrothermal solutions: critical experiments and numerical modelling tools to improve exploration success and ore processing	\$450,000
1998-2003	ARC (RIEF), DISR	Gray, White et al.	Access for Australian researchers to advanced neutron beam techniques	\$1,480,000
2000-2005	AMRFP	Kennedy	Access to major facilities	\$72K
2000-2005	ASRP	Kennedy and Howard	Synchrotron studies	\$96K
2001	ARC (Small)	Gray	Carbon-based hydrogen storage	\$27,000
2001-2006	AMRFP, ASRP	Gray	Travel grants for overseas neutron, x-ray and muon beam experiments	\$95,000
2003-2005	ARC (Discovery)	Gray, Dobson	Hydrogen absorption by nanostructured carbons	\$265,000
2003-2007	ARC	Lu et al (19 CIs including Gentle)	ARC Centre for functional Nanomaterials	\$1.53M

2006-2008	ARC Discovery Project	Gentle, Ashwell, Foran	Greatly improved rectification by molecular diodes	\$273K
2006	ARC LIEF	Gentle, Lu, Trau, Drennan, Whittaker, Martin, Frost, Klopogge, Brown	Small Angle Scattering facility for the Materials Structure Sciences	\$300K
2006	ARC LIEF	Martin, Gentle, Kepert, Turner, Guss	E-Research Infrastructure for the Molecular and Materials Structure Sciences	\$1M
2005	ARC LIEF	Gentle, Lu, George, Drennan, Frost	An advanced scanning probe microscopy facility	\$168K
2004-2006	AusIndustry	Williams, Lamb, Gentle, Muddle, Wilkes	Australian Materials Technology Network	\$2.6M
2002	ARC LIEF	Gentle, George, Lu and Bell	An advanced facility for materials characterisation	\$580K
2004	UQ Research Development	Gentle and Gahan	Multilayer porphyrin arrays constructed by layer self assembly	\$45K
2003-2004	ARC (LIEF)	Mather, Gray, White et al.	Access for Australian researchers to advanced neutron beam techniques	\$475,000
2002-2004	ARC (Linkage)	Bell, Gray, Kavanagh	Electronic properties of diamond-like carbon for applications in planar optical waveguides	\$69,000
2004	ARC (LIEF)	Buckman et al.	National Positron Beamline	\$512,000
2005-2006	ARC (LIEF)	Mather, White, Gray et al.	Access for Australian researchers to advanced neutron beam techniques	\$480,000
2006	ARC (LIEF)	Kisi et al.	The rapid kinetics facility	\$195,000
00-02	ARC-LGS	Kisi	Understanding the Stress-strain State in Polycrystalline Materials	\$202k
02-04	ARC-DP	Kisi and Kennedy	Combustion Synthesis of Ternary Carbides	\$210k
03-05	ARC-DP	Kisi and Forrester	Nanocrystalline processing of polycrystalline ceramics exhibiting the giant piezoelectric effect	\$135k
98-00	ARC-SGS	Kisi	Ferroelasticity in Ferroelectric Ceramics	\$48k
00-02	Univ of Ncle RMC	Murch & Kisi	Self-propagating High-temperature Synthesis of Ti ₃ SiC ₂	\$50k
00	Univ of Ncle	Kisi	Giant Piezoelectric Effect in PZN-PT	\$13k
01	Univ of Ncle RMC	Kisi	Diffraction Peak Shapes From Materials Containing Chemical Gradients	\$14k
02	Univ of Ncle	Kisi	Kinetic Paths in Solid State Synthesis	\$14k
04	Univ of Ncle	Kisi	Phase transitions in ferroelectrics	\$15k
00-05	AINSE	Kisi	In support of all of the above grants	\$145k
00-05	Neutron beam time, ILL, ISIS	Kisi, Riley & Forrester	In support of ARC funded grants above	\$700k
00-05	Access to Major Res. Fac. Prgm	Kisi	In support of the ARC-LGS grants above	\$46k
2002	ARC (LIEF)	Offler et al.	Upgrade of X-ray Equipment at the University of Newcastle	\$337k
2000-2005	ARC RIEF)/ (LIEF)	Gray et al., later Mather et al.	Access for Australian researchers to advanced neutron beam techniques	\$1200k
2006-2008	ARC DP	Kisi, Forrester and Howard	Structural basis of the giant piezoelectric effect	\$230k
2000-2002	ARC Discovery (C)	Y Chen (ANU), S J Campbell <i>et al.</i>	Formation Mechanism of Boron Nitride Nanotubes Produced by Reactive ball Milling	\$211 000
2000-2005	AINSE (P) (C)	S J Campbell <i>et al.</i>	Neutron Scattering (8 Projects)	\$125 000

2000-2005	ANSTO (P) (C)	S J Campbell	Visits to Major Facilities (6 projects)	\$24 000
2002-2004	ARC (LIEF) (P) (C)	AINSE, D Mather <i>et al.</i>	Access for Australian researchers to advanced neutron-beam techniques	\$720 000
2000	ARC (LIEF) (P)	H O'Neill (ANU), S J Campbell <i>et al.</i>	An Electron Microprobe	\$500 000
2003-2005	ARC Discovery (C)	J M Cadogan and S J Campbell	Insight and Understanding in Rare-Earth Magnetism	\$310 000
2005-2007	ARC Discovery	Kennedy, Schmid, Howard, Withers	Understanding phase transformations through precise structural studies	\$390,000
2006-2010	ARC Discovery	Liu, Withers	An integrated approach towards the development of new generation RF/microwave dielectric materials	\$830,000

Awards and Distinctions

Allan Pring was awarded the John Sanders Medal, by the Australian Microscopy Society for his work on the minerals in 2004 and the Sir Joseph Verco Medal, of the Royal Society of South Australia in 2005.

A/Prof. Ian Gentle was invited to give one of the two keynote lectures at the 2004 ISIS Large Scale Structures User Group Meeting, held at the Rutherford Appleton Laboratory. The lecture was entitled "Probing the behaviour of lung surfactant peptides with neutron reflectometry". About 50 users of small angle scattering and reflectometry attended the meeting.

PhD Student Theses

Student name	University	Year	Thesis Title
Dr Sandra Moussa	University of Sydney	2000	A study of classical Metal (II) aminoacidato Coordination compounds using powder Diffraction Methods
Dr Gavin F. Kirton, BSc (Hons)	Australian National University	2000	Reflectometry of Molecular Films of Linear and Dendritic Polymers
M W Schmidt	Australian National University	2001	Phase Formation and Structural Transformation of Strontium Ferrite SrFeO ₃
Dr Jean Kim	University of Sydney	2001	Structural Studies of Lead Containing Apatites
Dr Prodjostanso	University of Sydney	2001	Synthesis and Structural Studies of Common Cement Phases
Jennifer Forrester	University of Newcastle	2002	In-situ diffraction study of perturbed ferroelectric crystal structures
Dr Rene Macquart	University of Sydney	2003	Layered Ferroelectric Oxides
Dr Leqing Li	University of Sydney	2003	Structural Studies of Bi containing oxides
Dr Jeremy Ruggles	Australian National University	2002	A study of the formation of mesoporous silicate films at the air-water interface
Dr Tomasz Blach	Griffith University	2002	Effects of hydrogen absorption on the structure and properties of LaNi ₅
Dr Mark Pitt	Griffith University	2003	Neutron powder diffraction investigation of microstructure in some metal-hydrogen systems
Dr Haipeng Wang	University of Adelaide	2005	Kinetic studies of some solid-state reactions of metal sulfides

Keith McLennan	Griffith	2005	Structural Studies of the Palladium-Hydrogen System
Daniel Riley	University of Newcastle	2003	In-situ neutron diffraction analysis of Ti_3SiC_2 during self-propagating high-temperature synthesis (SHS)
Ben O'Driscoll	The University of Queensland	2004	

111. Honours Students Theses

Name	University	Year	Awards etc.
Duncan J McGillivray, BA BSc Auck.	Australian National University	1999	First Class Honours, University Medal – ANU, Rhodes Scholarship to Oxford University
Kylie Dean	University of Queensland	2001	Interactions of Pulmonary Surfactant at the Air-Water Interface
Adam Perriman	Australian National University	2002	First Class Honours

Conference Invitations and Presentations

- **AsCA '03/Crystal 23 – Combined meeting of the Asian Crystallographic Association and the Society of Crystallographers in Australia and New Zealand**, Broome WA, August 2003 where E. Kisi gave a plenary lecture
- **Ultra-high speed neutron diffraction studies: combustion synthesis of Ti_3SiC_2 and related compounds.** (E Kisi invited)
- **International Conference on Neutron Scattering**, Sydney 27 Nov – 2 Dec 2005, attended by E. Kisi, et al.
- **XIX International Union of Crystallography Congress and General Assembly**, Geneva, Switzerland, August 2002, attended by E. Kisi, C. Howard and D. Riley who gave the following presentations:
E. Kisi (invited)
Ultra-high Speed Neutron Diffraction Studies of the Combustion Synthesis of Ti_3SiC_2 and Related Compounds
C Howard, B Kennedy, E Kisi, K Knight and V Luca (oral)
On structural phase transitions in perovskites
D Riley and E Kisi (poster)
Diffraction thermometry and differential thermal analysis
- **IUCr Satellite Meeting – Crystal Chemistry of New Materials and Soft Matter**, Grenoble France, August 2002 was attended by E Kisi who gave an invited paper:
E Kisi and D Riley
In-situ Neutron Diffraction Studies of Ti_3SiC_2 Synthesis Over Four Decades of Time Resolution: From Stalemate to Combustion Synthesis
- **International Conference on the Applications of the Mössbauer Effect (ICAME2001)**, Germany, September 2001. SJ Campbell invited lecture

- **E Gray** and students presented numerous neutron scattering papers at the International Symposium on Metal-Hydrogen Systems (Hangzhou, China, October 1998; Noosa, Australia, October 2000; Annecy, France, September 2002)
- **User Consultation Meeting 'A second target station at ISIS'**, Rutherford–Appleton Laboratory, Didcot, UK, 19 May 2000. J. W. White gave the invited lecture:
The application of neutron scattering techniques to advanced materials.
- **Chemeca 2000 Conference**, Perth, 9–12 July 2000. J. W. White gave the following invited lectures:
Self-assembly of nanostructured material. Template induced crystal growth.
- **220th American Chemical Society Meeting**, Washington, DC, 21–24 August 2000. J. W. White gave an invited lecture at the Physical Chemistry Division's symposium on *Neutron Scattering: Biomimetic films and oil/water emulsions.*
- In July 2000, J. W. White gave a seminar at **Griffith University, Queensland**: *The chemical physics of intercalation compounds and hydrogen storage.*
- **219th National Meeting of the American Chemical Society**, San Francisco, USA, 26–30 March 2000. J. W. White gave an invited lecture at the symposium on *Application of X-ray Neutron Methods to Complex Systems in Energy and Fuels Science: Template-induced crystal growth.*
- **Workshop for Replacement Research Reactor Neutron Reflectometer**, ANSTO, 8–9 May 2001. J. W. White gave the invited lecture:
The study of molecular self-assembly using neutron and X-ray reflectometry.
- **Neutrons for Biology Workshop**, University of Melbourne, 10–11 July 2001. J. W. White gave the invited lecture:
The study of molecular self-assembly using neutron and X-ray reflectometry.
- **World Chemistry Congress, International Union of Pure and Applied Crystallography 38th Congress, 9th Asian Chemistry Congress**, Brisbane, Queensland, 1–6 July 2001. J. W. White gave two invited lectures:
Template induced crystal growth (at 9ACC); and *The structure of proteins at interfaces* (at IUPAC Polymer Satellite Meeting).
- **International Conference on Neutron Scattering 2001**, Munich, 9–13 September 2001. J. W. White gave two lectures:
Template induced crystal growth; and Structure and reactions of proteins at interfaces.
- **National Conference of the Australian Association of Constitutional Law 2001**, Perth, Western Australia, 21–23 September 2001. J. W. White gave the invited lecture:
National science and industry policy – balancing the centrifugal tendency.
- **Orica Emerging Science Symposium**, Melbourne, Victoria, 31 October 2001. P. A. Reynolds gave the invited lecture:
Microstructure of high internal phase emulsions.
- **Creation and Complexity Workshop**, Australian National University, Canberra, 25–30 January 2002. J. W. White gave the invited lecture:
Developments in Human Stem Cell Research: Science and Christian Ethics.

- **Polymers in Dentistry**, University of Queensland, Brisbane 7 February 2002. J. W. White gave the invited lecture:
Template-Induced Biomineralisation.
- **Analytical X-rays for Industry and Science**, University of Newcastle, 11 – 15 February 2002. J. W. White gave the invited lecture:
X-ray Small Angle Scattering and Reflectivity – Novel Applications.
- **25th Australasian Polymer Symposium**, University of New England, Armidale, 10 – 13 February 2002. J. W. White gave the invited lecture:
Biological Macromolecules – Structure and Function at Interfaces.
- **Australia-NZ Milkfat Workshop**, Food Science Australia, Melbourne, 18 – 20 March 2002. J. W. White gave the invited lecture:
Neutron Scattering from the Milk Fat Membrane – first results.
- **Australian Institute of Physics-RACI joint meeting**, Research School of Physics, Science and Engineering, Canberra, 6 June 2002. J. W. White gave the invited lecture:
Developments in Human Stem Cell Research.
- **SETnet meeting**, Australian Academy of Science, Canberra, 12 June 2002. J. W. White gave the invited lecture:
National research priorities
- **International Union of Crystallography Satellite Meeting**, Grenoble, France, 1 August 2002. J. W. White gave the invited lecture:
Measuring Time Dependent Interfacial Structures.
- **1st National Conference and Exhibition on Nanotechnology**, Sydney, 25 – 27 September 2002. J. W. White gave the invited lecture:
Biologically Directed Assembly of Soft Matter.
- **SMART-RACI Industrial Symposium**, RMIT, Melbourne, 11 October 2002. J. W. White gave the invited lecture:
Marriage between Industry and Academia – how to develop this relationship.
- **The Financial Future of Australia's Universities**, Australian Academy of Science, Canberra, 11 – 12 September 2002. J. W. White gave the invited lecture:
Research Funding and the UK Experience.
- **Nano-Composite Materials Workshop, Canberra**, 22 October 2002. J. W. White gave the invited lecture:
Self-directed Assembly
- **Australian and New Zealand Institute of Physics 28th Annual Condensed**
- **Matter Physics Meeting**, Wagga Wagga, 2003, 'The antiferromagnetic structure of BaPrO₃', R.A.Robinson, D.J.Goossens and M.F.Telling.

- **Asian Crystallography Association Meeting**, Hong Kong, June 2004, 'Diffuse neutron scattering in benzil, C₁₄D₁₀O₂, using the time-of-flight Laue technique', T.R.Welberry, D.J.Goossens, W.I.F.David, M.J.Gutmann, M.J.Bull and A.P.Heerdegen.
- **International Conference Neutron Scattering 2005**, Sydney, Nov 28 to Dec 2, 'Monte Carlo Analysis of Neutron Diffuse Scattering Data', D.J. Goossens, T.R. Welberry, A.P. Heerdegen and M.J. Gutmann.
- **Diffuse Neutron Scattering from Benzil'**, BCA Physical Crystallography Group and the IoP Structural Condensed Matter Physics Group Winter Meeting 2003 Probing Structure at the Nanoscale:- Fact, Fiction or Hype? M.J.Gutmann, T.R.Welberry and D.J.Goossens.
- The magnetic structure of BaPrO₃', **Australian and New Zealand Institute of Physics 28rd Annual Condensed Matter Physics Meeting**, Charles Sturt University, Wagga Wagga, 2004. R.A.Robinson, D.J.Goossens and M.F.Telling.

Talks:

- **Australian and New Zealand Institute of Physics 28rd Annual Condensed Matter Physics Meeting**, Charles Sturt University, Wagga Wagga, 2004 Measuring diffuse scattering' D. J. Goossens, T. R. Welberry and A. P. Heerdegen.
- **The magnetic structure of BaPrO₃'**, APS March Meeting, Montreal, Canada, 2004. R. A.Robinson, D.J.Goossens and M.F.Telling.
- **Neutron Diffuse Scattering and Monte-Carlo Study of the Relaxor Ferroelectric PbZn_{1/3}Nb_{2/3}O₃, (PZN)**', Society of Crystallographers in Australia and New Zealand Conference Crystal 24, Victoria, March 2005. T.R.Welberry, D.J.Goossens and M.J.Gutmann.
- **XX Congress of the International Union of Crystallography** Florence, 23-31 August 2005 "Diffuse Scattering and Monte Carlo Studies of Relaxor Ferroelectrics" T. R. Welberry

Prizes and Fellowships

S J Campbell – Alexander von Humboldt Research Fellowship, University of Mainz, 2000

114. **Promotions**

A/Prof Craig Buckley	Curtin University
A/Prof Brendan Kennedy	The University of Sydney
A/Prof Ian Gentle	The University of Queensland

Current Research Programs

Publications list

Australian researchers are in bold; * indicates international collaboration; # indicates ISIS collaboration.

2000

* # F J Burghart, W Potzel, G M Kalvius, E Schreier, G Grosse, D Noakes, W Schafer, W Kockelmann, **S J Campbell, W A Kaczmarek**, A Martin, M K Krause
Magnetism of crystalline and nanostructured ZnFe_2O_4
Physica B 289-290 286 (2000)

* # M Hofmann, **S J Campbell, A Calka**
The synthesis of TiN by ball-milling - a neutron diffraction study
Physica B 276-278 899 (2000)

S A Holt, **P A Reynolds, and J W White**,
Growth of silicated films at the solid/liquid interface
Phys Chem Chem Phys, **2**, 5667–5671 (2000).

C.J. Howard, K.S. Knight, B.J. Kennedy and E.H. Kisi
Structural Phase Transitions in Strontium Zirconate Revisited (2000),
J Phys:Condens Matter, **12**, L677-L683.

P A Reynolds, E P Gilbert, and **J W White**,
High internal phase water-in-oil emulsions studied by small angle neutron scattering,
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Materials Science LOQ

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Industrial Collaborations

Through access to ISIS new science – technology linkages have been created. We cite here two of the programs for which access to ISIS has been essential. For both there is a component of underlying research, which could not have been done without this access and which has potential and actual benefits to Australian health science and industry. The two programs are the work of Professor Ian Gentle, at the **University of Queensland**, on “Lung Surfactants” and the work of Professor John White and his group at the Research School of Chemistry on emulsion structure.

The processes of ore formation in nickel deposits and the mineral reactions that occur during their weathering and ore processing have been studied using the high resolutions and high flux offered by the ISIS source. This work has recently been extended to *in situ* studies under hydrothermal conditions in specially designed hydrothermal cells for *in situ* neutron powder diffraction. The research has been undertaken as part of a collaboration with scientist at the **University of Adelaide**, Western Mining Corporation (now BHP Billiton) and the Universities of Münster and Cambridge.

New PhD & new Honours Students

One current PhD student and 1 honours student to date (Newcastle)

Ben O’Driscoll, PhD student, who will visit ISIS later this year (UQ)

Post-doc - Jeremy Ruggles (UQ)

Katie Baldwin - new Honours student on lung surfactant project (UQ)

Daniel Riley PhD (Newcastle)

Ms Robin Kelly Hons (Newcastle)

Mr Rene Macquart “ Layered Ferroelectric Oxides “ to be submitted March 2003 (U Syd)

Mr Leqing Li “ Structural Studies of Bi containing oxides” To be submitted December 2003 (University of Sydney)

Mr Adam Perriman The Australian National University

Ms Karena Chapman The University of Sydney

Mr Paul Saines The University of Sydney

Appendix 4

Excellence of the researchers and research activity - lead researchers and programs for 2003- 2005

Group Research Projects

DISORDERED MATERIALS

Lead Researcher: Professor Richard Welberry, Australian National University

Overview

This group combines diffuse X-ray scattering methods with computer simulation to deduce the arrangement of atoms and molecules in disordered crystals. Conventional crystal structure determination reveals only averaged arrangements, inadequate to explain some of the basic properties of many minerals, inorganic compounds, organic compounds and alloys that exhibit crystalline disorder. Diffuse scattering gives information on how neighbouring atoms or molecules interact with each other. Quantitative studies of diffuse scattering are, however, still rare because of the intrinsically very low intensities involved.

The group's interests span a wide range of different fields, each presenting problems for which this specialised technique can give unique information. Areas in which we have applied the techniques include: disordered molecular crystals, guest/host systems such as urea inclusion compounds, non-stoichiometric inorganic materials and minerals, (for example, the cubic stabilised zirconias, mullite and wüstite), flexible framework structures such as silica polymorphs and their analogues, alloys, and quasicrystal phases.

Much of present day knowledge of the solid-state derives from crystallographic studies using Bragg diffraction. However this gives information only about the *average* structure of a material. The properties of many technologically important materials are dependent not just on the average structure but are often also crucially dependent on local deviations from the average (disorder). Such disorder gives rise to *diffuse scattering* and this scattering is a rich source of information about local structure and dynamics and the way atoms and molecules interact with each other. It thus often provides the key to understanding a material's properties.

Single crystals provide the most complete information in any type of experiment. For neutron diffuse scattering complete data can be recorded only with the aid of specialised instruments such as SXD. SXD uses time-of-flight diffraction and multi-pixel banks of detectors, to record simultaneously large sections of reciprocal space. The amount of data present in 3D reciprocal space is enormous. Even when the data have been obtained, analysis is not a simple problem and current methodology relies on comparison of the data to computer models of the disordered material. It would be most desirable if quantitative agreement between observed and calculated data could be obtained for the full 3D data using a rigorous least-squares procedure as is routinely done in a standard crystallographic (Bragg scattering) analysis. Such an analysis would, however, require computational resources well beyond any currently available and as yet it is only feasible to make comparisons for sections of data.

The present experiment is part of an extended study of benzil, $C_{14}D_{10}O_2$, (Figure 1), which is aimed at understanding the role that molecular flexibility plays in crystal packing and polymorphism. The molecules essentially consist of two phenyl rings linked by a flexible O–C–C–O bridge. The molecular flexibility may be characterised by three dihedral angles that define intramolecular rotations (see Figure 16). The compound crystallises in the trigonal space group $P3_121$.

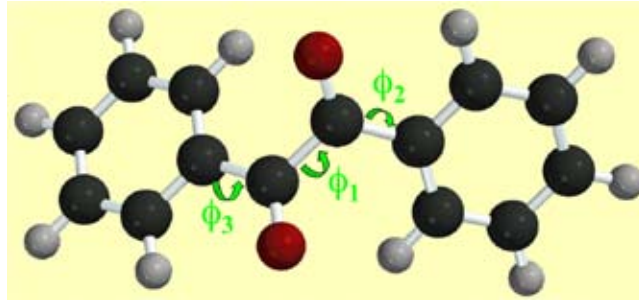


Figure 16. Intramolecular rotations in benzil

Neutron scattering offers access to information not available using X-rays. First, the scattering power of D is large for neutrons but small for X-rays and so their behaviour is reflected more strongly in neutron scattering patterns. This is particularly pertinent since these atoms occur around the periphery of the molecule and play an important role in intermolecular interactions. Secondly, neutron scattering cross-sections extend out to high values of the scattering vector Q so information is accessible well beyond the range possible with X-rays. Thirdly, the torsional energy of the dihedral angles in the free benzil molecule has been estimated to be ~ 3.1 meV from *ab initio* molecular orbital calculations. This means that correlated motion of the molecules within the crystal should lead to observable inelastic effects in a neutron diffraction experiment—information over and above anything available using X-rays.

SXD has been used to carry out a large-scale survey of reciprocal space. Three exposures are sufficient to get complete coverage of the $(hk0)$ plane when the $\bar{3}m$ crystal symmetry is used (Figure 17). Not only have hitherto unknown features been observed but also the diffuse scattering appears qualitatively different when measured in different detectors. Most striking is the splitting of the diffuse lines around the (400) reflection (Figure 17a). By observing the same feature in reciprocal space in the different detectors, one has effectively probed it with different incident neutron energies. Thus, the same feature in Figure 17b shows no splitting because for that detector the neutron energies used are much greater and the pattern is much more like the X-ray patterns.

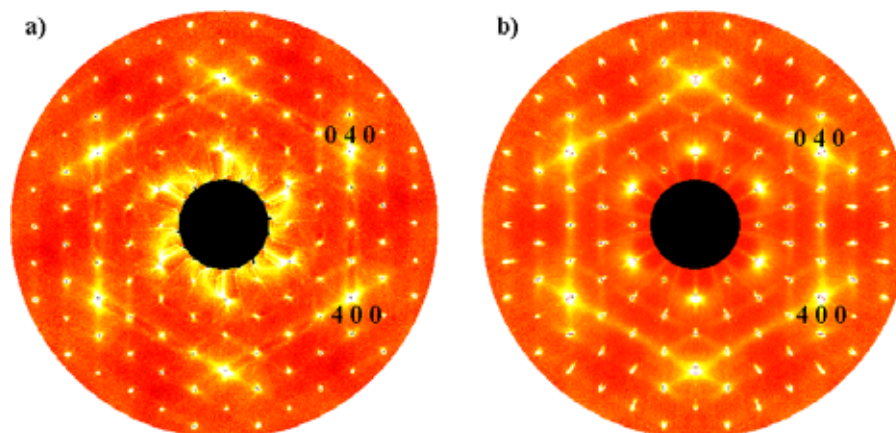


Figure 17 (a) and (b) Diffuse neutron scattering from a benzil crystal

The splitting of the diffuse line near the (400) reflection makes it possible to estimate the energy of the phonon mode involved to be 1.11 meV. This value is somewhat lower than any known phonon frequency observed for the hydrogenous compound. This mode has now been seen directly using PRISMA (Figure 18).

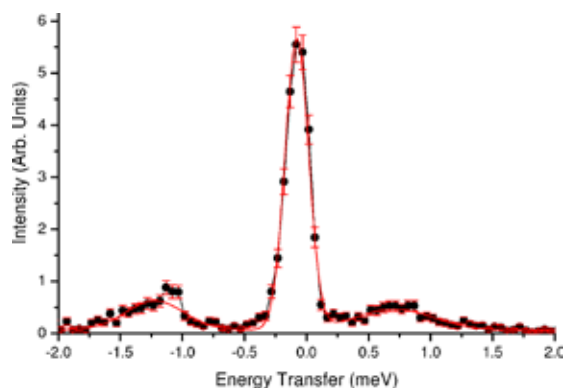


Figure 18. Inelastic neutron scattering from "soft modes" in benzil

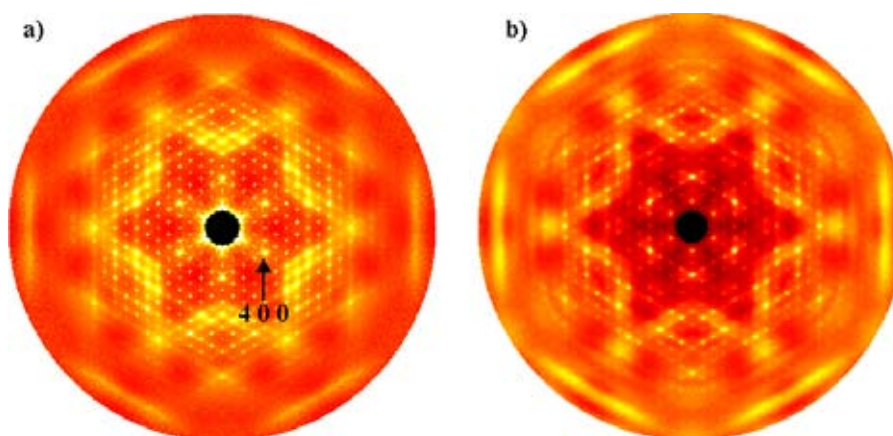


Figure 19 shows data for the $(hk0)$ plane for a much wider Q-range together with a calculated pattern obtained from a Monte-Carlo simulation model derived from an earlier X-ray analysis. The agreement is remarkable given that the X-ray data covered only about one quarter of the Q-range of the neutron data. Any remaining differences that may be seen should allow further refinement of the Monte Carlo model.

SOLID STATE MOLECULAR SCIENCE

Lead Researcher: Professor John White, Australian National University

Overview

Neutron and X-ray scattering methods, developed by this research group, are used to study the structure and dynamics on nanometre and picosecond space/time scales. Adsorption, self-assembly at interfaces, polymers, the imitation of biomineralisation phenomena using "template" molecules and, most recently, the structure and denaturation of proteins at interfaces are current areas of interest. The insights gained are used to guide chemical synthesis in making new materials with interesting physicochemical properties. One recent highlight has been the first determination of the thermodynamic parameters for protein denaturation in the 50 Å surface layer of a protein solution. By comparison with denaturation in the bulk, the contribution of the surface forces can be measured quantitatively. Another highlight is the first measurement of the interfacial structure of an emulsion surface by neutron reflectivity and the extension of this program to new surfactant design. Our collaboration with Orica Ltd and Food Science Australia on the structure and stability of emulsions has produced scientifically interesting and useful practical information. We continue to show that structural relationships at the nanoscale have importance for rheological and other properties.

Current research also includes polymer phase separation and polymer surfactant structure at interfaces where unusual and potentially controllable supramolecular aggregation can be seen. The first observations of off-specular neutron reflectivity from Langmuir films of dendrimers was recently made and the pathological behaviour of their Π -A isotherms are commencing to be understood in terms of intramolecular conformational change in response to mechanical stress.

The projects described below combine the unique facilities available at the ISIS neutron source, UK, and the X-ray facilities developed in our group at the Research School of Chemistry.

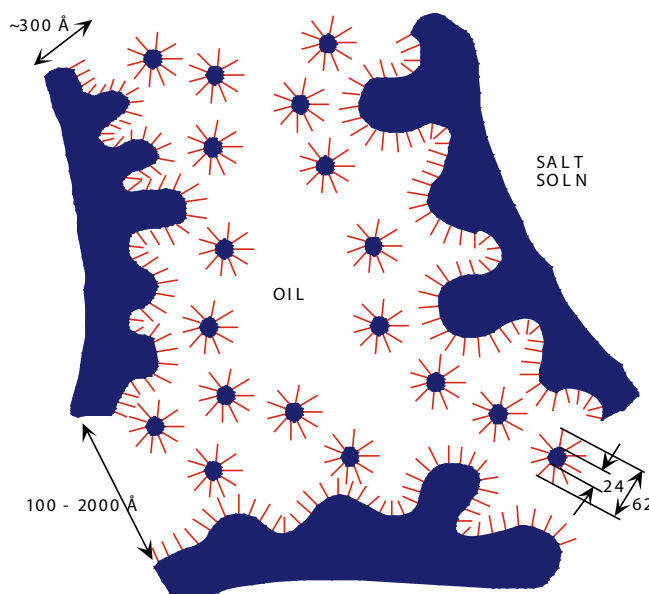


Figure 20. A cartoon of an emulsion structure. Blue is water and red is surfactant.

Growth of Highly Ordered Thin Silicate Films at the Air-Water Interface

Dr A.S. Brown, Dr S.A. Holt, Dr P.A. Reynolds, Dr J. Penfold (ISIS), Professor J.W. White (Note ISIS Collaboration)

The growth of thin silicate-organic films at the air-water interface of surfactant solutions has been discovered and studied *in situ* by X-ray and neutron reflectivity to a resolution of ca. 5 Å. The combination of X-ray and neutron reflectivity (several scattering contrasts using H₂O/D₂O mixtures) has been of key value in solving the structures produced. The combined X-ray and neutron data showing fringes at later times in the growth process are shown in Figure 2. Surfactant in the solution and the air-water interface itself are involved in directing the growth and final structure of the films. Following this induction period a rapid crystallisation occurs to give a structure with a crystallographic repeat distance of 45 Å perpendicular to the surface and composed of alternating layers of mainly surfactant, and then mainly silicate material. The very narrow diffraction peaks observed indicate that the final silicate film is highly ordered.

Titanium Oxide Films for Solar Energy Capture

J W White, M J Henderson, and A Gibaud (Laboratoire de Physique de l'Etat Condense), A R Rennie (Uppsala University)

Titanium dioxide is an inexpensive and stable semiconductor material. Its wide bandgap, however, (ca. 3.2 eV) allows for the capture of only 2-8 % of the solar photon flux. A shift in the optical response of TiO₂ from the UV to the visible spectral range will increase the effect on the photocatalytic efficiency of the material. Our work concerns the preparation of thin mesoporous

TiO₂ films (800 - 3000 Å) doped to provide a shift in the optical response. The films have been prepared by a surfactant template route using evaporative induced self-assembly (EISA). During the year the collaboration identified the conditions required to form well structured films reproducibly; characterised the film structure at each step of the process with reflectometry using X-rays and neutrons; nitrogen doped the oxide framework; and removed the surfactant template with an ethanol rinsing treatment prior to calcination at 400 °C to help prevent collapse of the oxide structure.

Solvent Effects in High Internal Phase Emulsions (SANS and USANS analysis)

J W White, K Baranyai, A J Jackson, P A Reynolds, A J Scott, J Zank and J Barker (NIST)

Previous work using small angle neutron scattering (SANS) and ultra small angle neutron scattering (USANS) focused on high internal phase emulsions (90% aqueous phase/10% oil phase) in which surfactant nature, concentration and molecular weight have been varied. This year we have completed a comprehensive study on the effects of variation in the oil phase on the emulsion structure. The oil-phase consisted of mixtures of hexadecane and toluene in different ratios. The research has been supplemented by small angle X-ray scattering data and viscometry on surfactant solutions in the corresponding hexadecane/toluene mixtures. The combination of USANS, SANS (various neutron contrasts) and optical microscopy enabled us to develop a complete structural description of the emulsion system. The polyisobutylene-based surfactant stabilises the droplets within the emulsion by monolayer formation at the aqueous/oil interface, and by formation of nanometer-scale reverse micelles within the oil phase. The obtained data have been fitted to a model of linked micron scale surfactant-rich blocks, whose number, size and dimensionality of linkages vary systematically with the surfactant-oil interaction. The model results reveal that the compatibility of surfactant with oil is the major factor in the type, size and relative amounts of observed emulsion structures.

Synthesis and Characterisation of Novel Surfactants

J W White, J Zank and A J Scott

A plethora of novel surfactants for a potential application in high internal phase emulsion systems have been synthesised. Access to a large variety of monomers enabled us to prepare block oligomers with defined hydrophobic/hydrophilic building units and low polydispersity. The compounds have been characterised by Gel Permeation Chromatography (GPC) and Modulated Differential Scanning Calorimetry (MDSC). In order to understand and predict the behaviour of the surfactant molecules at the aqueous/oil interface the behaviour at the aqueous/air interface (Langmuir Trough) served as a model. The aim of our work is to investigate the stabilisation mechanism of these amphiphiles when used at lower concentration, for the preparation of high internal phase emulsions.

Denaturation of Proteins at Interfaces at the Nanometre Scale

J W White, A J Jackson, and M A Augustin (Food Science Australia)

Dried dairy ingredients are an important segment of the Australian dairy market. In the case of high protein content powders a loss of functionality (eg. solubility) is observed on drying. We are employing scattering techniques (neutron and X-ray) to examine the nanoscale structural changes that occur on dehydration. Our aim is to relate these changes to the observed loss of functionality and propose methods to restore that functionality.

Kinetics of Adsorption of Lysozyme at the Air-Water Interface

A W Perriman and J W White

The adsorption kinetics of Hen Egg White Lysozyme at the air-water interface has been studied using specular neutron reflectometry. Experiments were performed at a number of pH values to examine the effect of charge on the rate of protein adsorption. Solutions of Hen Egg White Lysozyme in Air Contrast Matched Water at 1 mg/mL were made. These allow direct determination of the surface excess of protein. High repetition experiments with short collection times were used to accurately determine only the surface excess, derived from the product of the film thickness and the scattering length density of the layer. The kinetic traces at pH values where the protein is charged are well fitted by a first order rate equation with two linear regions, where the change in the gradient occurs as the surface concentration reaches a steady state. This behaviour is characteristic of the transport and distortion of protein molecules, followed by rearrangement in the surface layer. The equilibrium concentration is a function of protein charge with steady state surface concentrations reaching 1.4 mg m⁻² at pH 4 and 3 mg m⁻² at pH 11. Protein charge is inversely related to the rate of adsorption. This dependency has been explored through use of thermodynamic analysis. For these experiments access to the SURF reflectometer at ISIS was essential.

SOLID STATE INORGANIC CHEMISTRY

Lead researcher: Professor Ray Withers, Australian National University

Overview

We aim to understand and exploit the factors (synthetic and processing conditions, strain, composition, electronic band structure, etc.) that determine structure and function in the crystalline solid state. Our interest is in the balance between local crystal chemistry and longer-range order in a wide range of compositionally and/or displacively flexible crystalline solids with important materials properties. The principal experimental research tools used include a wide range of solid state synthesis techniques, transmission and scanning electron microscopy in combination with powder and single crystal diffraction as well as physical properties measurements including resistivity as well as dielectric properties. On the theoretical side, group theory, lattice dynamical calculations and bond valence sum analysis are the principal techniques employed. Crystalline systems investigated include wide range non-stoichiometric solid solutions, displacively flexible framework structures, ferroic phases and phase transitions, solid electrolytes, dielectric materials and incommensurately modulated structures. Achievements over recent years include the first coherent view of the crystal chemistry underlying the phenomenon of ferroelectricity within the Aurivillius family of displacive ferroelectrics, the use of compositionally modulated structure formalism to understand “infinitely adaptive”, non-stoichiometric solid solutions, and the discovery and subsequent modelling of displacive flexibility and its consequences in the silica polymorphs and various zeotypic microporous molecular sieve materials.

Precise diffraction studies of temperature-dependent as well as composition induced structural phase transitions in the Ca_{1-x}Sr_xTiO₃ system

R Withers, CJ Howard [Australian Nuclear Science and Technology Organization], BJ Kennedy [U Sydney] and M Carpenter [U Cambridge, UK]

As part of an ongoing ARC-funded project involving precise diffraction studies of structural phase transitions in functional metal oxides, a coupled electron, synchrotron X-ray as well as neutron diffraction study of temperature-dependent as well as composition induced structural phase transitions in the Ca_{1-x}Sr_xTiO₃ system is under way. The mineral perovskite itself, CaTiO₃, is a major component of Synroc, a synthetic rock form designed for the immobilization of radioactive waste. Our interest in the Ca_{1-x}Sr_xTiO₃ system derives from the fact that the CaTiO₃ acts as a host for fission product Sr. It is therefore of some importance to precisely characterize the polymorphic and phase transition behaviour of this archetypal perovskite system. We are

concentrating on regions of the phase diagram where significant disagreements currently exist in the literature. Attention is currently focused on the $x = 0.70$ composition where diffraction studies have shown that the room temperature space group symmetry of $\text{Ca}_{0.3}\text{Sr}_{0.7}\text{TiO}_3$ is $I4/mcm$ rather than $Imma$ as recently claimed. In addition, it has been shown that only one polymorphic phase transition occurs above room temperature rather than the two claimed in previous literature. Work is also currently under way on the $x \sim 0.63$ composition where a novel anti-ferroelectric polymorphic form is being carefully investigated.

A Structure, Phase analysis and Dielectric Properties Investigation of 1:1 A_2InNbO_6 (A = Ba, Sr and Ca) and 1:2 $\text{Ba}_3\text{MnNb}_2\text{O}_9$ Complex Perovskites

R Withers, Y Liu, L Norén, V Ting, and J Fitz Gerald [Research School of Earth Sciences] and M James [Bragg Institute, Australian Nuclear Science and Technology Organisation]

The “1:1” $\text{A}_2\text{In}^{3+}\text{Nb}^{5+}\text{O}_6$ double perovskites have been the subject of recent interest due to their potential as visible light driven photocatalysts as well as for their microwave dielectric properties in the case of the A = Ba and Sr compounds. Likewise the 1:2 $\text{Ba}_3\text{Mn}^{2+}\text{Nb}^{5+}_2\text{O}_9$ triple perovskite is of interest for its dielectric properties. A careful investigation has therefore been carried out into the room temperature crystal structures of these complex perovskite materials as well as their temperature-dependent dielectric properties. A constrained modulation wave approach to Rietveld structure refinement of neutron powder diffraction data has been used to determine their room temperature crystal structures. In the case of the nominally “1:1” A = Ca compound, an extensive $\text{Ca}_2[(\text{Ca}_{2x/3}\text{In}_{1-x}\text{Nb}_{x/3})\text{Nb}]\text{O}_6$ ‘solid solution’ field spanning compositions virtually the whole way from $\text{Ca}_4\text{Nb}_2\text{O}_9$ to $\text{Ca}_2\text{InNbO}_6$ in the $\text{CaO-InO}_{3/2}\text{-NbO}_{5/2}$ ternary phase diagram has been shown to exist. In terms of the optimization of physical properties, the existence of B-site variable solid solutions fields such as this is of considerable interest as it raises the possibility of being able to continuously tune desired physical characteristics. In the case of the 1:2 $\text{Ba}_3\text{Mn}^{2+}\text{Nb}^{5+}_2\text{O}_9$ triple perovskite, stacking fault disorder appears to play a strong role in the dielectric loss properties of the material.

Structurally frustrated relaxor ferroelectric behaviour in $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$

R Withers and Y Liu, L Norén

Ever since $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ (CCTO) was first reported in 2000 to have a giant dielectric constant at 1 kHz of $\sim 12,000$ that was nearly constant from room temperature up to ~ 600 K but which dropped rapidly to less than 100 below 100K, a huge amount of interest and work has been carried out in an attempt to understand the origin of these remarkable and potentially very useful dielectric properties. Both extrinsic (microstructural) as well as intrinsic mechanisms for the observed dielectric properties have been proposed. Dielectric constants greater than 1000 have traditionally been associated with intrinsic ferroelectric or relaxor ferroelectric (RF) behaviour. We have recently observed a reversible ferroelectric effect in CCTO as well as found direct diffraction evidence for structurally frustrated RF behaviour in the form of 1-d correlated, off-centre displacements of Ti ions within the TiO_6 octahedra of CCTO. That this incipient ferroelectric behaviour is only correlated along 1-d columns of TiO_6 octahedra in the absence of an applied electric field offers a crucial insight into the underlying nature of CCTO and suggests the existence of a unique new class of structurally frustrated, ferroelectric relaxors. As part of a just funded ARC grant, the correlation between composition, synthesis conditions, structure (both local as well as microstructural) and dielectric properties (dielectric constant as well as dielectric loss) will be carefully investigated in CCTO and related materials.

The refinement of minor components in twin-disorder Crystal Structures

R Withers and A.D. Rae

The structure determination and refinement of many crystal structures using diffraction techniques is complicated by the presence of minor components of the scattering density that

compromise the accuracy obtainable for the features of major chemical interest. It is necessary to use a limited number of independent variables to describe these minor components and a number of strategies are available. The program *RAELS* is currently being rewritten to simplify processes of model development and comparative refinement. A recent paper has clearly shown that refinement can be very pathway dependent, especially when twinning occurs, reducing the correlation between symmetrised components of a pseudo symmetric structure (Rae, Mossin & Sørensen, 2005). The concept of symmetrisation is to describe a structure in terms of a number of coexisting components of different space group symmetry using irreducible representation theory. Each space group has the true symmetry as a subgroup and is itself a subgroup of an idealised parent group. This becomes useful when this process reveals symmetrised components with limited contribution to the overall intensity of a crystal diffraction pattern. These components can be poorly defined if standard refinement procedures are used and mechanisms for stacking faults and twinning are not recognised. There is no correlation between symmetrised components if powder diffraction data is used. A pseudo symmetry operation can be defined as a symmetry operation that is a symmetry element of the parent group but not the true space group. This operation can be used to either disorder an ideally ordered structure or to create twin related orientations of a structure producing a twin related overlap of diffraction patterns. Sometimes a combination of both processes occurs and the diffraction pattern is the result of independent mosaic blocks with different orientation and disorder parameters. Sometimes the distinction between twinning and disorder is not well defined. The program *RAELS* allows the use of a structure factor algebra to combine the structure factors from pseudo-equivalent reflection of an ideally ordered prototype structure to simulate the diffraction pattern. This allows a limited number of global parameters to describe the structure. Two recent structures have shown that robust geometrical parameters can be obtained using this concept.

IN-SITU STUDIES OF HYDROGEN IN METALS AND PSEUDO METALS

Lead Researcher: Associate Professor Evan Gray, Griffith University

Overview

Gray and colleagues use neutron scattering, particularly neutron powder diffraction, to study the crystal structures and microstructures formed when materials absorb hydrogen. The ingress of H atoms at hydrogen-to-host atomic ratios up to one profoundly affects the structure and properties of the host. The metal-H interaction is the basis of the enormously successful nickel-metal-hydride battery technology, yet hardly anything about a metal-H system can be calculated from first principles, showing that our fundamental understanding remains in a fairly primitive state. Better understanding of the interaction of H with potential absorbers is vital for the development of new hydrogen storage systems with energy density sufficient for automotive use. Neutron, synchrotron x-ray and muon beams are used at several centres for both fundamental and applied studies of hydrogen uptake by materials including metals and alloys, nanostructures carbons and, most recently, metal complexes. Powder diffraction is the principal tool, but other techniques are also used at ISIS, including muon spin relaxation and deep-inelastic scattering, neither of which will be available at OPAL.

Access to ISIS has been and is expected to continue to be essential because our work is increasingly performed under quite high pressures of hydrogen gas, routinely up to 2000 bar in the case of powder diffraction. Above pressure of 100 bar or so, the walls of the sample cell become so thick that they dominate the diffraction pattern, so a fixed-angle time-of-flight technique with neutron absorbing masks is necessary. This technique cannot be used at OPAL.

Hydrogen absorption by nanostructured carbons

Assoc. Prof. E. MacA. Gray, Prof. J.F. Dobson, Dr T.P. Blach, Prof. J.W. White (ANU)

This project was supported by ARC funds for 2003-2005. Carbon-based materials show great promise for clean energy storage through the absorption and desorption of hydrogen. The project aims to use powerful theoretical and experimental methods to resolve the controversy that surrounds reports of massive hydrogen absorption by nanostructured carbons, by understanding why particular structures should or should not absorb hydrogen atoms or molecules. We have concentrated on intercalated graphites but have also studied carbon nanotubes made in Australia.

Neutron scattering techniques and muon spin relaxation are absolutely essential for the conduct of the project because of the lack of knowledge as to the location and environment of H atoms/ molecules reportedly absorbed by these materials. MuSR was used at ISIS to show that C₂₄K is the composition most likely to absorb hydrogen. Two in-situ neutron powder diffraction studies were performed under high pressure of hydrogen. A large uptake of hydrogen by C₂₄K was observed in the first experiment and, in the second experiment, the structural modifications caused by hydrogen ingress were followed.

Fundamental aspects of hydrogen in metals

Assoc. Prof. E. MacA. Gray, Assoc. Prof. E.H. Kisi (Newcastle), Prof. K. Yvon (Université de Genève), Dr Mark Pitt (Institute for Energy Technology, Norway), Dr T.P. Blach, Mr K.G. McLennan – *Note Swiss and Norwegian collaborations*

The important features of a metal-hydrogen (or carbon-hydrogen) system, such as ultimate hydrogen capacity, phase diagram and degree of absorption-desorption hysteresis cannot be predicted except in the most approximate way at present. The very origin of hysteresis in H-H interactions or energy loss mechanisms such as dislocation generation remains controversial after nearly 70 years of study. Having spent several years in developing first-class apparatus for in-situ neutron diffraction studies in particular, we now apply our technical expertise to obtaining authoritative data on metal-H systems, which are not hydrogen storage candidates, but are well-accepted models and test-beds for theory, such as LaNi₅ and Pd.

The use of high gas pressures to force H atoms into interstitial sites not occupied under ordinary conditions is a way of investigating metal-H structures and of better understanding the metal-H interaction. An example is the recently gained knowledge that tetrahedral sites in palladium are occupied at high pressure, even at room temperature. When combined with band structure calculations, this result is expected to lead to a better understanding of the H absorption properties of Pd.

Powder diffraction at the highest possible resolution has been an essential tool for elucidating the mechanisms of the phase transformations that accompany hydrogen uptake. Data from HRPD at ISIS were essential components in PhD theses recently completed by Mark Pitt on hydrogen in LaNi₅ (2003) and by Keith McLennan on hydrogen in Pd (2005).

Hydrogen storage in light-metal complexes

Assoc. Prof. E. MacA. Gray, Assoc. Prof. C.E. Buckley (Curtin), Prof. A. Züttel (Université de Fribourg), Prof. B. Hauback and Dr Mark Pitt (Institute for Energy Technology, Norway), Dr T.P. Blach – *Note Swiss and Norwegian collaborations*

Recent international emphasis on energy security has added urgency to the development of commercially viable solid-state systems for storing hydrogen automotive fuel. The US

Department of Energy has set targets for hydrogen content by mass and volume that are very challenging. Pressurised gas cannot meet the volume density targets for 2010 and 2015, using the best-known structural materials. Therefore storage in solids or liquids will be necessary. Gray heads the hydrogen storage research stream in the new National Hydrogen Materials Alliance, funded by CSIRO and universities. The aim of the storage stream is to develop one or more materials meeting the density DoE criteria. Materials based on complexes of the light metals Li, B, Mg, Al plus nitrogen are now being investigated. Preliminary measurements on Li_3N and its amide and imide have already been carried out at ISIS. Again, ISIS is essential for much of this work, as it involves measurement under extremes of pressure and temperature.

NEUTRON REFLECTIVITY STUDIES OF INTERFACIAL PROCESSES

Lead Researcher: Dr Ian Gentle, University of Queensland

Overview

The Surface Chemistry Group in the School of Molecular and Microbial Sciences is engaged in several areas of research where neutron reflectivity measurements at the ISIS facility make an important contribution. The films of interest are either on an air/water interface or on an air/solid interface. Reflectivity provides information about the structure of ultra-thin films (as thin as a single molecule, known as a monolayer) on a surface, and is most powerful when the results are used in conjunction with those from other methods. Some examples of complementary methods routinely used by this group are grazing incidence X-ray diffraction and X-ray reflectivity. Each method provides unique information, and the neutron data are extremely valuable in that only neutrons provide the ability to vary contrast by isotopic substitution.

The Formation of Phospholipid Films from Dispersed Structures

A/Prof. I.R. Gentle, Dr W.K. Fullagar (Lund), Dr G.T. Barnes, Dr S.A. Holt (ISIS), Dr J.L. Ruggles

The transfer of lipid molecules from a dispersed phase to an air/water interface resulting in the formation of a monomolecular film is a fundamental step in certain biological processes such as those at the alveolar interface. Natural lung surfactant (NLS) plays an essential role in the respiratory function of the lung by lowering the alveolar surface tension. The absence of NLS in premature infants is a major cause of mortality and morbidity, yet the behaviour of NLS is not well understood. Fundamental studies of the interactions between the components of NLS, and of the nature of the dispersed structures involved in supplying the alveolar monolayer, are imperative in the search for satisfactory surfactant replacement therapies.

NLS is composed of saturated and unsaturated phospholipids (80-90%), neutral lipids (2%), proteins (10%), carbohydrates (2%) and other substances (2%). The majority of studies of NLS components at the air/water interface have examined the interaction between species in binary/ternary mixtures. The films have been formed in the conventional way by spreading from solvent followed by compression. Such studies ignore the important interactions between the film and film material in the subphase. In the lung, monolayers are formed by the supply of lipid molecules from the alveolar hypophase and monolayers that are isolated from such a source may not exist. We have shown that the properties of solvent-spread monolayers differ significantly from those formed from dispersions.

The process of film formation at the alveolar interface involves the presence of tubular myelin structures in the alveolar hypophase. Investigation of the unravelling of these structures to form the interfacial film will provide a key to understanding and mimicking surfactant behaviour. Much interest has centred on the role of the hydrophobic surfactant proteins SP-B and SP-C as they have been identified as promoting rapid respreading of the lipid film at the interface after collapse. The mechanisms of these self-assembly processes require further study, using conditions that are more physiologically relevant than many of those which have been used to date.

Our group has made use of ISIS facilities several times in the past to determine the structures of films formed at the air/water interface from components of lung surfactant. In particular, the interactions of natural and synthetic SP-B with phospholipids have been a major focus. The recent addition of a Brewster Angle Microscope to the neutron reflectivity facilities SURF and CRISP has been particularly beneficial for our work. It is becoming increasingly apparent that, in order to obtain unequivocal data from reflectivity, the combination of several contrasts from neutrons and X-rays is necessary. The ISIS reflectometers are the only facilities in the world that can provide the needed neutron reflectometry data on a timescale to be useful for work on these systems, and continued access is crucial for the continued success of this program of research.

Highly ordered monolayers of porphyrins

A/Prof. I.R. Gentle, Dr G.J. Foran (ANSTO), Dr J.L. Ruggles,

The assembly of functional molecules into supramolecular architectures is expected to yield electronic and other devices that act at the molecular level. In most cases, these devices involve the two-dimensional assembly of materials on surfaces. Some of the most useful molecules for such applications are porphyrins, which offer desirable properties from an electronic and structural point of view. The aim of this project is to develop ways of forming controlled two-dimensional patterned arrays of porphyrin-based materials on surfaces.

It has been established that such physical properties as electrical conductivity, magnetic behaviour and electro- and non-linear optical phenomena depend critically on the arrangement of the functional molecules from which these properties derive. In order to take advantage of the unique properties of the molecules, or to design a structure with particular properties, it is highly desirable to incorporate the functional molecules into well-ordered monolayers. An integral part of the challenge is to develop the ability observe the structural details at a molecular level, and to this end, neutron reflectivity at ISIS is particularly important. By revealing the details of the layered structure to extremely high resolution, we are able to determine the effectiveness of the various strategies being employed to achieve our goal. An additional benefit is that the use of contrast variation is highly effective with mixed films, which many of our materials are.

Greatly Improved Rectification by Molecular Diodes

A/Prof. I.R. Gentle, Prof. G.J. Ashwell (Cranfield), Dr G.J. Foran (ANSTO), Dr J.L. Ruggles, Ms K. Ford (PhD student)

Single molecule electronics represents the ultimate challenge in device miniaturisation. The molecular diode is the smallest active component in the molecular electronics toolkit, and to date only six active organic chromophores have been reported. Current rectification ratios are too small to be of practical use, although very significant improvements have been made in recent years. This research aims to dramatically improve the rectification ratio available from molecular diodes using a combination of advanced synthesis, film fabrication and characterisation, in order to mimic the current-voltage characteristics of macroscopic p-n devices by single molecules and molecular layers. The outcome will be the first molecular diode, based on an organic monolayer, with performance equivalent to current macroscopic devices.

Detailed film characterisation is an essential part of this process, and neutron reflectometry is the tool of choice for determining the structure of films at the molecular level. Our expertise in the use of neutron reflectometry is one of the reasons that this collaboration with Prof. Ashwell of Cranfield University has been successful.

STRUCTURAL STUDIES OF TECHNOLOGICALLY IMPORTANT MATERIALS

Lead researcher: Professor Brian O'Connor, Curtin University of Technology

The Co-existence of Cubic and Tetragonal Polymorphs of Gamma Alumina During Gibbsite Calcination

Professor B.H. O'Connor, Dr D.Y. Li, Dr C.E. Buckley, Mr S. Pratapa (PhD student)

Research conducted at Curtin University by Dr Bee Gan and supervisors (O'Connor and Li), as part of her PhD studies, revealed that gamma alumina co-exists as two phases during the calcination of gibbsite. Subsequent research by O'Connor and Li has confirmed the co-existence of the two phases, and shown that the cubic phase develops at the expense of the tetragonal phase as the calcination temperature increases.

We now wish to examine the co-existence of these phases from a fundamental perspective. In particular we intend to use theoretical modelling to describe the formation of the two co-existing phases on a *priori* basis, and to understand how temperature and pressure may be used to systematically influence the relative levels of each phase in this industrially important process.

We have performed static experiments on the transformation phenomenon using reactor-based neutron diffraction. We now wish to study the influence of temperature and pressure on the transformation of gibbsite to gamma alumina from a phase diagram perspective. The unmatched combination of instrument speed and resolution of HRPD at ISIS will permit us to follow the evolution of system under non-equilibrium conditions. The project has been discussed with Professor Bill David of ISIS who has expressed enthusiasm for the scientific merit of the proposal.

STRUCTURAL AND DYNAMICAL STUDIES OF MAGNETIC MATERIALS

Lead researcher: Professor Stewart Campbell, University of NSW (ADFA)

Overview

Today's technologically driven society relies on magnetic materials to an extent unimaginable even as recently as 20 years ago. Their usefulness and applications range from the trivial but useful refrigerator magnets to the ubiquitous computer (with its unlimited scope for application), recording media, mobile telephones and superconducting magnets with life-saving potential in scanning and imaging devices. These spectacular developments and achievements have been achieved as a result of research investigations into several thousand materials [1]. Critical appraisals of the evolution of magnetic materials in the 20th century have demonstrated that this progress has resulted from a synergetic combination of the systematic search for new materials and a desire to understand their properties, along with the need to optimise the magnetic performance of materials. This in turn has led to the best possible performance of known magnetic materials for technological applications. The study of rare-earth (R) transition-metal (T) compounds has become established in recent decades as one of the most important topics in magnetism. Their significance can be readily appreciated by the outstanding intrinsic magnetic properties exhibited by the binary RCo_5 and ternary $\text{R}_2\text{Fe}_{14}\text{B}$ series. For example SmCo_5 exhibits the largest known uniaxial anisotropy at room temperature (17.2 MJ m^{-3}) with $\text{Nd}_2\text{Fe}_{14}\text{B}$ displaying the largest energy product (445 kJ m^{-3}) [1]. The microstructure of these materials can then be controlled by suitable treatments leading to optimal extrinsic magnetic behaviour for technological applications. Despite the impressive technological and commercial developments of rare-earth magnetism there remain numerous aspects that remain to be developed and resolved.

EuMn_2Ge_2 and EuMn_2Si_2 - Magnetic Structures and Valence Transitions

The ternary EuT_2M_2 series (T = transition metal; M = Si, Ge, P) have attracted particular attention

as such tetragonal 1-2-2 compounds form readily across wide concentration ranges of the T and M elements; this provides model systems for systematic investigations of the interplay between structure, magnetic interactions and valence transitions. While the temperature-induced valence transitions in EuT_2M_2 systems have been investigated by a variety of techniques and the main factors governing the magnetic ordering and structures documented [e.g 1, 2], the magnetic structures of EuMn_2M_2 compounds mostly remain unknown as a result of the prohibitively large neutron absorption of natural Eu. By careful sample preparations using the ^{153}Eu isotope of relatively low neutron absorption and with access to the high intensity and resolution available at the GEM diffractometer ($\sim 1.8\text{-}723\text{ K}$), ISIS for two days, we have been able to both determine the magnetic structures of $^{153}\text{EuMn}_2\text{Ge}_2$ and $^{153}\text{EuMn}_2\text{Si}_2$ and analyse the valence-induced volume changes in EuMn_2Si_2 [3].

The Mn sublattices of both EuMn_2Ge_2 and EuMn_2Si_2 order antiferromagnetically ($T_N = 667(9)\text{ K}$; space group $I4'/m'm'm$ and $T_N = 391(5)\text{ K}$; space group $I_p4/m'm'm'$ respectively) with no evidence for ordering of the Eu^{+2} ions in EuMn_2Ge_2 down to 1.5 K . EuMn_2Si_2 exhibits a thermally driven valence transition around $T_v \sim 527\text{ K}$ with a pronounced increase in the unit cell volume of $\sim 7\%$ from the Eu^{3+} state at low temperatures ($T < \sim 150\text{ K}$) to an average valence state of ~ 2.5 at high temperatures ($T > \sim 600\text{ K}$). As indicated by the volume fit in Fig 1, we have analysed the valence-induced volume changes for the first time in terms of the interconfigurational fluctuation model [4] with occupation probabilities for the Eu^{2+} state in EuMn_2Si_2 and the average Eu^{val} values found to agree well with our re-analysis of earlier $^{151}\text{EuMn}_2\text{Si}_2$ isomer shift data [5]. This agreement demonstrates the applicability of the interconfigurational fluctuation model in enabling valence changes induced by volume changes in Eu and related compounds to be determined. Our analysis also demonstrates that the strength of the magnetic interaction for antiferromagnetic ordering of the Mn sublattice is decreased by $\sim 10\text{-}15\%$ as a result of the change in electronic configuration of EuMn_2Si_2 .

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152. Insight and Understanding in Rare-Earth Magnetism

J M Cadogan, UNSW and S J Campbell, UNSW@ADFA, Dr M Hofmann Tech Univ München, Prof D Ryan, McGill Univ, Canada, Prof O Moze, Univ of Modena, Italy – note international collaborations.

Our systematic approach to unravelling the behaviour of such systems is exemplified by our recent comprehensive studies of the complex magnetic interactions that occur in the 1-2-2 series of $\text{La}_{1-x}\text{Y}_x\text{Mn}_2\text{Si}_2$ compounds [6, 7]. As shown by Figure 1, the antiferromagnetism of YMn_2Si_2 gives way to the predominant ferromagnetism of LaMn_2Si_2 with increasing La concentration. Consistent with the mixed magnetic states, the compounds were found to exhibit coexisting canted ferromagnetic and antiferromagnetic structures around the critical concentration $x_c \sim 0.2$ [6, see also 8]. A related aim is to establish the magnetic structures and account for the magnetic and valence transitions, which, from previous magnetisation and Mössbauer studies, are known to occur in the $\text{YbMn}_2\text{Si}_{2-x}\text{Ge}_x$ and $\text{EuMn}_2\text{Si}_{2-x}\text{Ge}_x$ series.

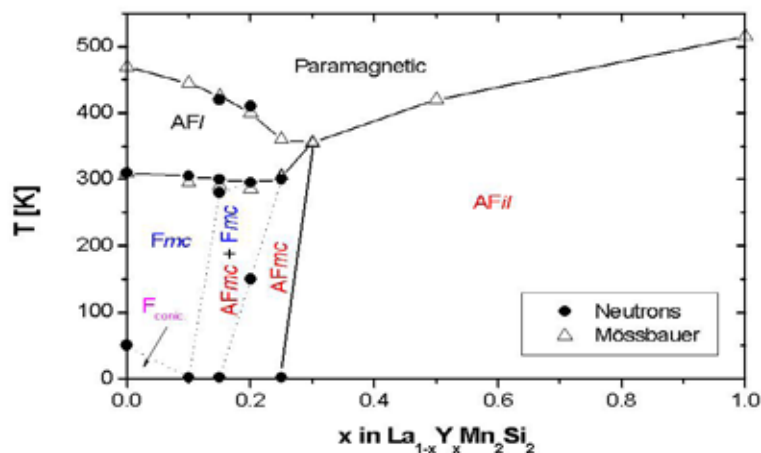


Figure 21. The magnetic phase diagram of $\text{La}_{1-x}\text{Y}_x\text{Mn}_2\text{Si}_2$ [6, 8].

Scope to undertake neutron diffraction studies of these materials is central to the success of our project. Besides enabling the crystallographic and magnetic structures of the intermetallic compounds to be determined by Rietveld refinement, neutron scattering probes the entire sample and provides a sensitive check on sample quality and the possible presence of low level (~ 1-2 %) impurity phases. This is particularly important in the investigation of new materials where small fractions of strongly magnetic phases can mask the intrinsic magnetic behaviour of the prime phase of interest.

Similarly we shall apply muon spin relaxation/rotation (μSR) techniques to study the magnetism of selected crystalline rare-earth intermetallics. Muon spin relaxation/rotation experiments provide microscopic information about the local atomic environment in the region of the muon probe. Microscopic information is also obtained from Mössbauer spectroscopy and NMR for the probe atoms located at specific crystallographic sites. Muon measurements will thus complement the insight gained from both Mössbauer spectroscopy and NMR on the same samples, providing unique, detailed insight to the behaviour of the selected intermetallic compounds.

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Novel Insight in Spin Crossover Phenomena in Fe(II) Compounds

P Gütllich (University of Mainz, Germany), S J Campbell (UNSW@ADFA, Australia), V

Ksenofontov and Y Garcia (University of Mainz, Germany) – note German Collaboration.

The Mainz Group continues to make a leading contribution to the European Community's research programme into the Thermal and Optical Switching of molecular Spin States (TOSS; <http://ak-guetlich.chemie.uni-mainz.de/toss/index.html>) and have investigated the response of a number of spin crossover (SC) compounds subjected to external perturbations [e.g. 1]. The dramatic changes in the magnetic and optical properties that accompany the spin state transition have led to extensive exploration of these compounds with technical applications in mind [2].

Muons provide an ideal micromagnetometer to probe the spin states in a wide range of compounds. Following a period of study leave by Stewart Campbell with Professor Gütllich at Mainz in 2000, we have applied MuSR techniques to further delineate the microscopic behaviour of selected SC compounds. We are continuing a systematic investigation of muon spin relaxation in dinuclear compounds to gain novel insight to the magnetic properties and the local structural environment, as well as to the mechanisms causing these spin transitions. Our current applications of muons centre on two new aspects - firstly the overall behaviour of the spin transition curve and secondly identification of the magnetic entities, which occur in the transition from the HS to the LS states for a family of dinuclear compounds.

In Iron (II) spin crossover molecular materials the spin state can be modified from high-spin (HS, $S = 2$) to low-spin (LS, $S = 0$) by temperature, pressure or light [1]. The initial set of MuSR measurements which we carried out at ISIS (February 2001 and December 2001) on a series of well characterised Fe(II) SC compounds have enabled us to delineate the temperature dependence of the asymmetry parameters in a spin transition for the first time [3] and to establish that the behaviour of the asymmetry parameter correlates well with the nature of the spin transitions, whether continuous or discontinuous. These novel findings have also been presented at recent international conferences (TOSS2001, France; ICAME2001, UK; TOSS2002, Germany; Seeheim Mössbauer Workshop, Germany 2002).

We shall shortly extend our studies by investigation of the MuSR behaviour of the paramagnetic compound $[\text{Fe}(\text{hyetrz})_3](4\text{-Br-ps})_2$ and the antiferromagnetically coupled Fe(II) dinuclear complexes $[\text{Fe}(\text{bpym})(\text{NCSe})_2]_2\text{bpym}$ and $[\text{Fe}(\text{bt})(\text{NCS})_2]_2\text{bpm}$. These muon spin relaxation measurements ($\sim 10\text{-}350\text{ K}$; January /February 2003) will provide new insight about the behaviour of the magnetic entities during the spin transition. Our continuing systematic investigation of SC materials with potential technological applications will enable us to develop fully the understanding of the processes and magnetic entities responsible for these changes in spin state.

[1] P. Gütllich, A. Hauser, H. Spiering, *Angew. Chem. Int. Ed. Engl.*, 33 (1994) 2024.

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IN-SITU STUDIES OF MATERIALS IN SIMULATED SERVICE OR SYNTHESIS ENVIRONMENTS

Lead researcher: Associate Professor Erich Kisi, The University of Newcastle

Overview

This program of research aims to understand the behaviour of a broad range of materials via *in-situ* neutron diffraction studies on samples at high temperature, high pressure, applied electric

field or in simulated service or processing environments. The need for neutron diffraction comes from a need to study bulk specimens in realistic stress and thermal environments for which we rely on the low absorption of neutrons by most engineering materials. Most of the ceramics studied are oxides or carbides and their neutron diffraction patterns are very sensitive to the light element positions in the structure. Structural work on these materials is hence sounder than with X-rays, and closely related phases are more easily distinguished and their relative proportions quantified.

The work is supported by a number of ARC funded research projects including the following:

- a) *Combustion synthesis of ternary carbides*, E.H. Kisi and S.J. Kennedy, ARC Discovery Grants Scheme (2002-2004);
- b) *Neutron diffraction studies of the giant piezoelectric effect in relaxor ferroelectrics*, E.H. Kisi, ARC small grants scheme;
- c) *Nanocrystalline processing of polycrystalline ceramics exhibiting the giant piezoelectric effect*, E.H. Kisi and J.S. Forrester, ARC Discovery Grants Scheme (requested 2003-2005);
- d) *Understanding the stress-strain state in polycrystalline materials*, E.H. Kisi, ARC large grants scheme, (2000-2002).
- e) Structural basis of the giant piezoelectric effect, Kisi, Forrester and Howard, \$230k, ARC DP, 2006-2008.

155. The Synthesis Of Ternary Carbide Ceramics (Ti_3SiC_2 And Related Compounds)

Mr D.P. Riley, Dr E.Wu (China), Dr R.I. Smith (ISIS), Dr T.C. Hansen (ILL, France), Dr A.W. Hewat (ILL, France), A/Professor E.H. Kisi

Ti_3SiC_2 is the archetypal compound of a family of ternary ceramics with a very unusual mix of properties. It has the refractory and high temperature properties normally associated with ceramics, combined with the electrical and thermal conductivity of a metal. In addition, the material exhibits ductility due to shearing of the layered structure that enables it to be readily machined with ordinary machine tools. Other mechanical properties include excellent thermal shock resistance, reasonable fracture toughness, a high Young's Modulus and good high temperature strength. There is universal agreement that this set of properties can lead to an exceedingly wide range of applications. The primary difficulty in realising these diverse applications is that Ti_3SiC_2 has proven difficult to synthesize without unwanted extra phases. The reactions between the starting materials (typically $3Ti+SiC+C$ or $3Ti+Si+2C$) occur over widely varying time scales depending on the heating rate. This group has conducted *in-situ* neutron diffraction studies over a very wide range of time resolution from 18 minutes per diffraction pattern at ANSTO to 0.38 seconds per pattern on D20 at the ILL. The reactions change dramatically within this range from conventional reactive sintering, involving two intermediate phases slowly reacting, to violent combustion synthesis where a single intermediate phase forms in 0.5s and then precipitates the final phase in the next 35s. The combustion synthesis is a very promising method as the heat generated by the reactions is the primary energy source for the synthesis.

Whilst the most rapid data collection can only be conducted at the ILL, the ISIS instruments (GEM and POLARIS) are required for data collection in the range 30s to 15 minutes as we study the transition between the two types of behaviour. This is essential for optimisation of the process.

156. Polycrystalline ceramics exhibiting the giant piezoelectric effect

Ms. J.S. Forrester, Dr R.O. Piltz (ANSTO), Dr G. McIntyre (ILL) and A/Prof E.H. Kisi

Piezoelectric materials interconvert electric and mechanical energy. They have been incorporated into a wide range of industrial, medical and domestic applications. The newest, known as PZN-PTs, are only available as single crystals. They have ten times the response of conventional piezoelectric materials, however they are expensive, mechanically fragile and have shape limitations. This project will tailor nanostructured intermediate states that will allow the production of stronger, more versatile polycrystalline PZN-PT ceramics. It will develop scientific results on nanocrystalline processing applicable to many materials and allow deeper insight into the mechanism of the anomalous piezoelectric response of these materials. Of particular importance here is the ability of the ISIS instrument HRPD to resolve pseudo-symmetric structures. All of the current theories of the large piezo-response of PZN-PT materials involve very minor departures from cubic symmetry that nonetheless have a profound influence on properties. HRPD is the highest resolution neutron diffractometer in the world.

STRUCTURAL AND DYNAMICAL STUDIES OF MAGNETIC MATERIALS

Lead researcher: Professor Stewart Campbell, University of NSW (ADFA)

Overview

Today's technologically driven society relies on magnetic materials to an extent unimaginable even as recently as 20 years ago. Their usefulness and applications range from the trivial but useful refrigerator magnets to the ubiquitous computer (with its unlimited scope for application), recording media, mobile telephones and superconducting magnets with life-saving potential in scanning and imaging devices.

These spectacular developments and achievements have been achieved as a result of research investigations into several thousand materials [1]. Critical appraisals of the evolution of magnetic materials in the 20th century have demonstrated that this progress has resulted from a synergetic combination of the systematic search for new materials and a desire to understand their properties, along with the need to optimise the magnetic performance of materials. This in turn has led to the best possible performance of known magnetic materials for technological applications.

The study of rare-earth (R) transition-metal (T) compounds has become established in recent decades as one of the most important topics in magnetism. Their significance can be readily appreciated by the outstanding intrinsic magnetic properties exhibited by the binary RCo_5 and ternary $\text{R}_2\text{Fe}_{14}\text{B}$ series. For example SmCo_5 exhibits the largest known uniaxial anisotropy at room temperature (17.2 MJ m^{-3}) with $\text{Nd}_2\text{Fe}_{14}\text{B}$ displaying the largest energy product (445 kJ m^{-3}) [1]. The microstructure of these materials can then be controlled by suitable treatments leading to optimal extrinsic magnetic behaviour for technological applications. Despite the impressive technological and commercial developments of rare-earth magnetism there remain numerous aspects that remain to be developed and resolved.

Our contributions have centred on enhancing the knowledge and understanding of rare-earth compounds while also pursuing the search for new materials. As examples we discovered a new series of compounds based on R_3T_{29} [2, 3] and, more recently, a series of novel quaternary compounds $\text{R}_3\text{T}_{29}\text{Si}_4\text{B}_{10}$ ($\text{T} = \text{Co, Ni}$; $\text{R} = \text{rare-earth elements La to Lu}$) [4, 5]. Intermetallic compounds containing both R and T elements provide a unique environment in which to study the complex fundamental interactions of the localised (R) and de-localised (T) electrons and the associated magnetic moments, not only with each other, but also with their surroundings. The key aims of our current research are to understand the critical interplay between the R and T sublattices in ternary compounds and to explore our recently discovered set of quaternary

intermetallic compounds. The ternary compounds of interest are based on R-T-X combinations in the ratios 1-10-2, 1-6-6, 1-4-2 and 1-2-2 all of which show interesting, and at times puzzling, magnetic behaviours.

158. Insight and Understanding in Rare-Earth Magnetism (international Collaborations)

J M Cadogan, UNSW and S J Campbell, UNSW@ADFA, Dr M Hofmann Tech Univ München, Prof D Ryan, McGill Univ, Canada, Prof O Moze, Univ of Modena, Italy)

Our systematic approach to unravelling the behaviour of such systems is exemplified by our recent comprehensive studies of the complex magnetic interactions that occur in the 1-2-2 series of $\text{La}_{1-x}\text{Y}_x\text{Mn}_2\text{Si}_2$ compounds [6, 7]. As shown by Figure 23, the antiferromagnetism of YMn_2Si_2 gives way to the predominant ferromagnetism of LaMn_2Si_2 with increasing La concentration. Consistent with the mixed magnetic states, the compounds were found to exhibit coexisting canted ferromagnetic and antiferromagnetic structures around the critical concentration $x_c \sim 0.2$ [6, see also 8]. A related aim is to establish the magnetic structures and account for the magnetic and valence transitions, which, from previous magnetisation and Mössbauer studies, are known to occur in the $\text{YbMn}_2\text{Si}_{2-x}\text{Ge}_x$ and $\text{EuMn}_2\text{Si}_{2-x}\text{Ge}_x$ series.

Scope to undertake neutron diffraction studies of these materials is central to the success of our project. Besides enabling the crystallographic and magnetic structures of the intermetallic compounds to be determined by Rietveld refinement, neutron scattering probes the entire sample and provides a sensitive check on sample quality and the possible presence of low level ($\sim 1-2\%$) impurity phases. This is particularly important in the investigation of new materials where small fractions of strongly magnetic phases can mask the intrinsic magnetic behaviour of the prime phase of interest.

Similarly we have applied muon spin relaxation/rotation (μSR) techniques to study the magnetism of selected crystalline rare-earth intermetallics [ISIS, July 2005]. Muon spin relaxation/rotation experiments provide microscopic information about the local atomic environment in the region of the muon probe. μSR thus complements the microscopic information obtained from our Mössbauer spectroscopy studies of the same compounds.

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Novel Insight in Spin Crossover Phenomena in Fe(II) Compounds (international collaborations)

Y Garcia (Université catholique de Louvain, Belgium) S J Campbell (UNSW@ADFA, Australia), V Ksenofontov, P Gütllich (University of Mainz, Germany), J Lord ISIS

Our project stems from the very successful leading contribution that the Mainz Group has made to the European Community's research programme into the Thermal and Optical Switching of molecular Spin States (TOSS; <http://ak-guetlich.chemie.uni-mainz.de/toss/index.html>). In

particular TOSS investigated the response of a number of spin crossover (SC) compounds subjected to external perturbations [e.g. 1]. The dramatic changes in the magnetic and optical properties that accompany the spin state transition have led to extensive exploration of these compounds with technical applications in mind [2].

Muons provide an ideal micromagnetometer to probe the spin states in a wide range of compounds. Following a period of study leave by Stewart Campbell at Mainz in 2000, we have applied MuSR techniques to further delineate the microscopic behaviour of selected SC compounds. We are continuing a systematic investigation of muon spin relaxation in di-nuclear compounds to gain novel insight to the magnetic properties and the local structural environment, as well as to the mechanisms causing these spin transitions. Our current applications of muons centre on two new aspects - firstly the overall behaviour of the spin transition curve and secondly identification of the magnetic entities that occur in the transition from the HS to the LS states for a family of di-nuclear compounds.

In Iron (II) spin crossover molecular materials the spin state can be modified from high-spin (HS, $S = 2$) to low-spin (LS, $S = 0$) by temperature, pressure or light [1]. The initial set of MuSR measurements which we carried out at ISIS on a series of well characterised Fe(II) SC compounds have enabled us to delineate the temperature dependence of the asymmetry parameters in a spin transition for the first time [3] and to establish that the behaviour of the asymmetry parameter correlates well with the nature of the spin transitions, whether continuous or discontinuous. These novel findings have also been presented at several international conferences (TOSS2001 France; ICAME2001 UK; TOSS2002 Germany; Seeheim Mössbauer Workshop Germany 2002; MuSR2005 UK).

We have recently extended our studies by investigation of the MuSR behaviour of the paramagnetic compound $[\text{Fe}(\text{hyetrz})_3](4\text{-Br-ps})_2$ and the antiferromagnetically coupled Fe(II) dinuclear complexes $[\text{Fe}(\text{bpym})(\text{NCSe})_2]_2\text{bpym}$ and $[\text{Fe}(\text{bt})(\text{NCS})_2]_2\text{bpm}$. These muon spin relaxation measurements have provide new insight about the behaviour of the magnetic entities during the spin transition. Our continuing systematic investigation of SC materials with potential technological applications will enable us to develop fully the understanding of the processes and magnetic entities responsible for these changes in spin state.

[1] P. Gütllich, A. Hauser, H. Spiering, *Angew. Chem. Int. Ed. Engl.*, **33** (1994) 2024.

[2] O. Kahn, C. Jay-Martinez, *Science*, **279** (1998) 44.

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Crystallography of Perovskites

Dr B Kennedy, University of Sydney

This group in the School of Chemistry concentrates on the crystallography of technologically interesting materials, including perovskites, pyrochlores and cements. Structures in the perovskite family have held the interest of crystallographers over many years, and continue to attract a wider interest because of their fascinating properties, including high-temperature superconductivity and colossal magnetoresistance, both of great technological importance. Nevertheless, there remain unanswered questions about the various structural phase transitions that occur as the temperature is altered and how these affect their electronic and magnetic properties.

Our work is currently focussing fundamental studies of structural phase transitions in perovskite type oxides. Our emphasis is on establishing the nature of the phase transitions, first order, continuous, tricritical etc and identifying the spontaneous strains associated with

these transitions. We are particularly interested in the study of materials where the structural transition is associated with an electronic instability as occurs in PrAlO_3 – see the diagram below.

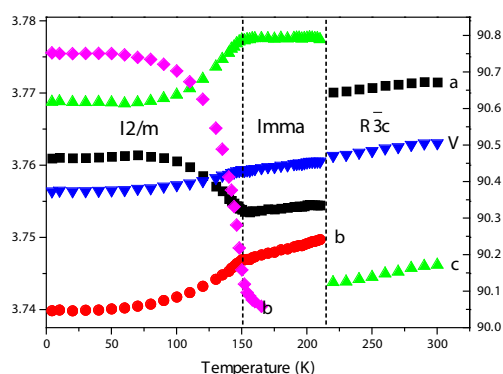


Figure 22. Lattice parameters for PrAlO_3 , suitably scaled, as a function of temperature. The cube root of the volume per formula unit is shown on the same plot

A comparable study has been completed on the ordered double perovskites $\text{Ba}_2\text{Bi}^{\text{III}}\text{Bi}^{\text{V}}\text{O}_6$ and $\text{Ba}_2\text{Bi}^{\text{III}}\text{Sb}^{\text{V}}\text{O}_6$. These studies have revealed a number of similarities and more importantly differences between the chemically and charge ordered systems. Using the ISIS HRPD we should for the first time the existence of a primitive monoclinic structure at low temperatures and the structure was refined in SG $P2_1/n$.

Isis provides access to many more state-of-the-art instruments than will OPAL. In the area of powder diffraction the High Resolution Diffractometer at ISIS is unique in that its resolution function is both extremely high and constant across the entire d-space range. This feature is critical for much of our work on Phase Transitions. Further, the q-range available on GEM cannot be matched by any of the instruments currently under construction at GEM. It is our view that the majority of powder diffraction will be done at OPAL and /or the Australian Synchrotron but regular use will be made of the unique features at the ISIS diffractometers. Further, ISIS also provides MUONS – something not possible at OPAL.

Appendix 5 AINSE Strategy for ISIS Access

AINSE Mission Statement

AINSE will advance research, education and training in nuclear science and engineering and their applications within Australia by being, in particular, the key link between universities, ANSTO and major nuclear science and engineering and associated facilities.

AINSE Objectives

1. To provide a mechanism for users in member organisations of AINSE to have access to major nuclear science and engineering and associated facilities at ANSTO and other agreed sites for research purposes;
2. To facilitate graduate and undergraduate education and training experience utilising major nuclear science and technology facilities at ANSTO and other agreed sites;
3. To encourage collaboration and cooperation between member organisations of AINSE in areas primarily related to nuclear science and engineering and their applications; and
4. To sustain and support the development of major nuclear science and technology facilities at ANSTO and other agreed sites for shared use by member organisations of AINSE.

The value of ISIS to Australian Researchers

As a neutron spallation source ISIS is able to provide facilities that are complementary to those provided on HIFAR as well as to some of those to be available on the Replacement Research Reactor (RRR).

The RRR will have a neutron flux order of magnitude greater than HIFAR, and will allow “cold neutron” experiments done in Australia for the first time. ISIS range of instruments is very broad and will be further extended by the second target station. The strategic value of continuing both scientifically and technically will be great.

In addition, once the RRR is commissioned ISIS will still have relevance to Australian researchers by:

- 1 Providing a mechanism for international collaborative science
- 2 Providing facilities that do not exist in Australia eg time of flight high-resolution inelastic scattering.

History

The need for “suitcase science” access for Australians to major international facilities was recognised by the ASTEC report “Small Country – Big Science” subsequent to an extensive national survey in 1990. ANSTO facilitated access to ISIS until 1998 when it was decided that AINSE would be a more appropriate vehicle for this provision – as it is representative of most likely users of the facility – i.e. universities and ANSTO. It is noted that AINSE does not represent other research organisations nor does it represent industry.

Having taken over management of access to ISIS, AINSE then approached ARC for financial assistance through the RIEF Scheme.

Access to ISIS

Access to ISIS is provided for by the payment of an annual membership fee. Currently this is \$400k pa. The ARC provides about 65%, the remainder being contributed by selected universities, ANSTO and AINSE.

Strategies

- Liaison with the Director of ISIS
- Promotion of the benefits of ISIS
- Assistance with the proposal process
- Publication of successful proposals in the AINSE Annual Report
- Publication of highlights resulting from ISIS research in AINSE Annual Report

- Mentoring for new applicants at ISIS

Appendix 6 AINSE Strategic Plan (2003-2008)

AINSE's Mission

AINSE will advance research, education and training in the field of nuclear science and engineering and related fields within Australasia by being, in particular, the key link between universities, ANSTO, other member organisations and major nuclear science and associated facilities.

Strategic Plan 2003-2008

Vision

AINSE will be the facilitator of choice of excellent science at major nuclear science and engineering facilities by maintaining its philosophy of inclusiveness and financing. To achieve this vision AINSE will implement strategies in the following key areas:

- Access to major facilities
- Scientific outcomes
- Membership
- Networking

We will know that we have achieved this vision when the following goals are attained:

- Goal 1 By the end of 2008 members will have access to the Australian major nuclear and related research facilities and some overseas, through AINSE.
- Goal 2 By the end of 2008 the research performance of our scientific outcomes will have increased substantially.
- Goal 3 By end 2008 all universities in Australasia, the some sections of CSIRO, many major museums, many non teaching hospitals and a significant proportion of the scientific institutes in Australasia will be members of AINSE.
- Goal 4 By the end of 2008, we will have expanded AINSE's existing set of excellent scientific networks.

Access to Major Facilities

Goal 1 By the end of 2008 members will have access to the Australian major nuclear and related research facilities and some overseas, through AINSE.

It is clear from our analysis of the research landscape that major research facilities are increasingly important in science. Many of these facilities are based on nuclear or related science and engineering areas. AINSE's vision is to serve its membership through increasing their opportunities to use new these new facilities competitively. Some of these will be a part of ANSTO while others may fall under the control of other organisations, either nationally or internationally.

Strategies

1. AINSE will actively pursue the opportunity to promote and facilitate access to and to foster expanding utilisation of the replacement research reactor and complementary facilities overseas.
2. AINSE will lobby for the opportunity to facilitate access to Synchrotron Radiation

research, in particular the Australian Synchrotron. AINSE sees great benefits to users and the managing organisation of the Australian Synchrotron if its established networks and facilities are used in this way.

3. AINSE will open negotiations with other managing organisations in Australasia that are responsible for major research facilities that are related to nuclear science. This will be of benefit both to these managing organisations as well as to the members of AINSE.

4. AINSE will expand its role to leverage funds from granting agencies for new equipment and instruments at major facilities.

5. AINSE will study ways in which instruments based in Universities, which perform at an internationally competitive level of quality can be made accessible to AINSE members.

6. AINSE will lobby government to make certain that appropriate pricing policies are implemented that will ensure the sustainability and facilitate the growth of access to national facilities.

Scientific Outcomes

Goal 2 By the end of 2008 the research performance of our scientific outcomes will have increased substantially. AINSE's mission is to "advance research, education and training" and so a goal of any strategic plan must be to improve how we perform in this core area.

Strategies

1. AINSE will undertake a benchmarking exercise in 2004 to evaluate our current performance and will continue thereafter to monitor our progress towards this goal and will establish a set of performance targets.

2. AINSE will continue to develop its peer review processes with an emphasis on the quality of proposals and their outcomes.

3. AINSE will increase its level of funding available for student support.

4. AINSE will use its networks to increase the numbers of effective collaborations between universities and government science agencies to promote scientific outcomes.

5. Set targets for publications, and students.

Membership

Goal 3 By end 2008 all universities in Australasia, the some sections of CSIRO, many major museums, many non teaching hospitals and a significant proportion of the scientific institutes in Australasia will be members of AINSE. AINSE understands that much has changed in research and that there are now many more players that could benefit from the style of access to major facilities enjoyed by its current members. It will therefore pursue strategies that will increase the diversity of its membership group.

Strategies

1. AINSE will develop policy on subscriptions and governance in accommodating potential new members.

2. AINSE will approach a range of potential new users with an invitation to join.

3. AINSE will conduct a two year rolling survey to gauge its level of success in filling its member's needs.

Networking

Goal 4 By the end of 2008, we will have expanded AINSE's existing set of excellent

scientific networks. AINSE recognises that the scientific enterprise is enhanced through the networks that develop between its member institutions. It understands that such networks are important to give Australian researchers access to national and international scientific discourse. It undertakes to promote the growth of these interactions for the benefit of its members.

Strategies

1. To increase the range and number of conferences it supports.
2. To improve the ease of access to facilities under its control.
3. To establish working parties charged with informing the Council of new scientific and engineering fields needing access to the AINSE supported facilities.
4. To strengthen the networks and collaborative research amongst its members.

