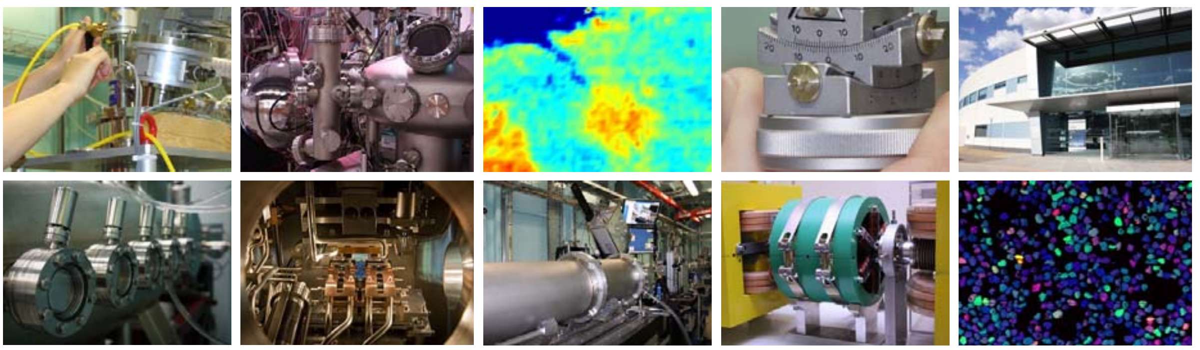
The Science Case for the Development of the Australian Synchrotron

June 2010



Australian Synchrotron Company Limited
ABN 52 126 531 271
800 Blackburn Road, Clayton Victoria 3168, Australia
p +613 8540 4100 **f** +613 8540 4200
e info@synchrotron.org.au **www.synchrotron.org.au**

Table of Contents

Australian Synchrotron

Executive Summary

In its short lifetime, the Australian Synchrotron has become one of Australia's premier pieces of scientific infrastructure. The Australian Synchrotron is a primary enabling tool that is already making active contributions to the national research and innovation system, providing research capabilities to researchers across Australia and New Zealand that allow them to compete on the international scientific stage and facilitating their ongoing contribution to the international scientific enterprise. This is not only of benefit to the scientific agenda but has immense potential to create positive social, economic and health benefits for the medium and long term.

Currently, the Australian Synchrotron supports user programs on eight world-class beamlines, covering a broad range of applications including health and biological sciences, earth and environmental sciences, advanced materials, engineering and manufacturing, energy and sustainability science, cultural heritage and archaeology as well as fundamental physics, chemistry and accelerator science. A ninth beamline, still under construction but already producing valuable results with 'expert' users, will be a world-leading facility for health and imaging sciences and will include a clinical research program.

In order to maintain the competitive position of the Australian Synchrotron in the many fields of science and engineering that it supports further growth and development is essential. This science case proposes a development plan based on broad consultation with the scientific community of current and potential users and international experts across all areas of synchrotron science. The science case presents a phased growth strategy, incorporating the following:

- ten new beamlines
- upgrades to the current accelerators
- major upgrades to the existing facility

The new beamlines are to be constructed in three phases. The proposed beamlines determined through the consultation process are:

Phase 1 beamlines (for immediate commencement in Year 1 of new funding)

- High Coherence Nanoprobe (HCN)
- Micro Materials Characterisation Beamline (MMC)
- Medium Energy XAS Beamline (MEX)

Phase 2 beamlines (for commencement in Year 2)

- Advanced Diffraction & Scattering Beamline (ADS)
- Small Angle Scattering Beamline for Structural Biology (SSB)
- Micro-Computed Tomography Beamline (MCT)

Phase 3 beamlines (for commencement in Year 3 or 4, with further development and scoping)

- Soft X-ray Materials Science Beamline (SXM)
- High Performance Macromolecular Crystallography Beamline (HMX)
- Advanced Infrared Beamline (AIR)
- Correlative Microscopy Beamline (CMB)

Acknowledgements

This document has been prepared by the Australian Synchrotron Co. Ltd, coordinated by Prof. Ian Gentle, Head of Science, and Dr Garry Foran, Science Case 2 Coordinator. The Australian Synchrotron gratefully acknowledges the assistance of many members of the Australian, New Zealand and international scientific communities in the preparation of this document.

The advice of the following committees has been of great assistance in this process:

Australian Synchrotron Scientific Advisory Committee

Prof. Ted Baker (Chair), Distinguished Professor of Structural Biology, University of Auckland, NZ
Prof. Mitchell Guss, Professor of Molecular and Microbial Biosciences, University of Sydney
Prof. Michael Hart, Emeritus Professor of Physics, University of Manchester, UK
Prof. Brendan Kennedy, Professor of Chemistry, The University of Sydney
Prof. Lisa Miller, National Synchrotron Light Source, Brookhaven National Laboratory, USA
Prof. Keith Nugent, Laureate Professor and ARC Federation Fellow, The University of Melbourne
Prof. Harald Reichert, Director of Research, European Synchrotron Radiation Facility (ESRF), Grenoble, France
Prof. Janet Smith, University of Michigan Medical School, Life Sciences Institute, USA
Prof. Soichi Wakatsuki, Director, Photon Factory Synchrotron Radiation Facility, Tsukuba, Japan
Prof. Hongjie Xu, Director of Shanghai Radiation Facility, Member Chinese Synchrotron Radiation Special Committee, China

Science Consultative Group

Dr Stephen Best, The University of Melbourne
Prof. Paul Dastoor, The University of Newcastle
Prof. Roland De Marco, Curtin University
Prof. John Drennan, The University of Queensland
Dr Richard Garrett, ANSTO
Prof. Andrea Gerson, University of South Australia
Dr Hugh Harris, The University of Adelaide
Dr Bridget Ingham, Industrial Research Ltd, NZ
Dr Kevin Jack, The University of Queensland
Prof. Erich Kisi, The University of Newcastle
Prof. Peter Lay, The University of Sydney
Prof. Jenny Martin, The University of Queensland
Prof. Jim Metson, The University of Auckland
Prof. Hugh O'Neill, The Australian National University
Prof. Michael Parker, St Vincent's Institute
Dr Andrew Peele, La Trobe University
Dr Mark Ridgway, The Australian National University
Dr Chris Ryan, CSIRO
Prof. Bill Skinner, Ian Wark Research Institute, University of South Australia
Prof. Geoff Taylor, The University of Melbourne
Prof. Bill Thomlinson, Monash University
Dr Jose Varghese, CSIRO
Prof. Matthew Wilce, Monash University

The **AS International Synchrotron Advisory Committee (ISAC)**, chaired by Prof. Keith Nugent.

The following people acted as spokespersons for the project proposals that were submitted on behalf of the respective scientific communities:

Accelerator Development Systems
Mr Greg Le Blanc, Australian Synchrotron

Advanced Diffraction & Scattering Beamline
Dr Matthew Rowles, CSIRO Process Science and Engineering

Medium Energy XAS Beamline
Prof. Peter Lay, The University of Sydney

High Coherence Nanoprobe
Assoc. Prof Andrew Peele, La Trobe University

High Performance Macromolecular Crystallography Beamline
Prof. Charlie Bond, University of Western Australia

Small Angle Scattering Beamline for Structural Biology
Assoc. Prof. Matthew Wilce, Monash University

Advanced Infrared Beamline
Prof. Donald McNaughton, Monash University

Micro-Computed Tomography Beamline
Dr Sherry Mayo, CSIRO Materials Science & Technology

Micro Materials Characterisation Beamline
Prof. Andrea Gerson, University of South Australia

Soft X-ray Materials Science Beamline
Prof. Paul Dastoor, University of Newcastle

Correlative Microscopy Beamline
Dr Marian Cholewa, Monash University

The following are the spokespersons for the Major Facility Upgrades projects:
David Paterson (Australian Synchrotron), Martin de Jonge (Australian Synchrotron), Hugh Harris (The University of Adelaide), Tom Caradoc-Davies (Australian Synchrotron), Nigel Kirby (Australian Synchrotron), Richard Farnsworth (Australian Synchrotron) and Greg Le Blanc (Australian Synchrotron).

Thanks are due to all those who have contributed to the development of the Science Case. The following staff members of the Australian Synchrotron are gratefully acknowledged: Tom Caradoc-Davies, Bruce Cowie, Chris Glover, Daniel Häusermann, Nigel Kirby, Martin de Jonge, Bernt Johannessen, David Paterson, Mark Tobin, Kia Wallwork, Nathan Cowieson, Mark Boland, Brad Mountford, David Cookson, Cathy Harland, Melodie Aitken, Brad Allen, Kerry Hayes, Nancy Mills, Lauren Green, Lyn Moorfoot and Samantha Chan. Special thanks to Chris Latif for help in production of the final document.

1. A Strategy for Development of the Australian Synchrotron

1.1 The Australian Synchrotron – Lighting up Australia

The Australian Synchrotron (AS) is a state-of-the-art, 3rd generation light source. It boasts performance that is competitive with contemporary facilities around the globe, including several that are still in the construction phase. As such, it provides leading-edge research and teaching opportunities on a scale that would be otherwise inaccessible to Australian and New Zealand researchers.

The AS is arguably Australia's premier piece of scientific infrastructure. It plays a pivotal role in the national and international research and innovation system, making world-class and, in some cases, world-leading capabilities available through a competitive, peer-reviewed process that prioritises high quality research.

The AS currently operates user programs on eight world-class beamlines with another under construction and delivers capabilities and scientific outcomes that are unique in Australasia. The scope of the existing beamlines is broad with applications spanning biosciences and health, earth and environmental science, advanced materials, engineering and manufacturing, energy and sustainability science, cultural heritage and archaeology as well as fundamental physics, chemistry and accelerator science. However, as only nine of a possible thirty-eight beamlines are operational, the scope for increasing the outcomes of this facility is significant.

The AS began user operations in July 2007 to international acclaim, not only for the speed and efficiency with which the project was delivered, but for the exceptional technical specifications and performance of the accelerators, beamlines and instrumentation that was realised.

In its short lifetime, the AS has already made a vital contribution to numerous high-profile research projects. In turn, this has raised the profile of Australian research on the global scientific stage and contributed to the reputation of the university and research sector in the region, whilst delivering gains in the economic and social welfare of Australia. The following section outlines a small selection of these early successes and their broad and positive impacts on the community. These early successes provide a rigorous and evidence-based framework for the positive outcomes that can be achieved through ongoing support of the AS and a rationale for continued development and expansion of the AS in the future to help achieve the full potential of this unique facility.

1.2 Science Highlights of the Australian Synchrotron

Stopping the malaria parasite in its tracks

Malaria is a major global disease and is responsible for over 2 million deaths each year. The symptoms of malaria are caused by the infection of red blood cells by a parasite called *Plasmodium falciparum*. This parasite uses red blood cells to feed and reproduce, destroying them in the process. This infection drives the debilitating and potentially deadly effects of malaria. With the rise of drug-resistant malarial parasites, new drug targets and potential therapeutics are urgently required for the development of new treatment strategies. In a recent study using synchrotron radiation at the AS, the molecular structure of a protein critical to the growth and development of the malaria parasite and its interaction with molecules that can inhibit their activity has been determined. These results lay the groundwork for the development of new anti-malarial drugs, focusing on targeting the proteins which the parasite uses to digest essential nutrients, in order to block the infection process. The progress of research in this area in Australia has been vastly accelerated by the availability of synchrotron science facilities in the country.

Roadmap to a new class of antibiotics

The rapid emergence of bacterial strains that are resistant to multiple forms of antibiotic is of growing global concern. This includes many lethal pathogens such as 'flesh eating' bacteria and 'golden staph'. The key to identifying novel ways to control infection by these microbes is a better understanding of their structure and function. Many bacterial pathogens that are harmful to human and animal health rely on *pili* to bind with each other (for reproduction) or with the cells targeted for infection. Pili are fibre-like structures that project from bacteria and are unique to different species. Therefore, developing a better understanding of pili structure and function is one potential key to the development of new anti-bacterial vaccines and treatments.

Using synchrotron radiation at the AS, the molecular structure of proteins that constitute bacterial pili has been studied, revealing that the interactions between the various proteins that constitute the pili resemble a string of pearls held together by special chemical bonds. Understanding the structure of the pilin proteins indicates that these molecules could be a very promising vaccine target. Moreover, it indicates that drugs that disrupt the bonds between them and interfere with pili formation could have great potential as a new class of antibiotics.

Further work at the synchrotron will be undertaken to study and better understand the pilin proteins, the bonds between them and how potential, novel compounds might interact with them to block the function of bacteria. Through such work, the facilities at the AS create novel areas of investigation far more rapidly and accurately than conventional means of scientific investigation.

Improving productivity and profitability in minerals processing

Small improvements in mineral extraction processes can dramatically increase both the productivity and profitability of the mining industry. As mining remains one of Australia's strongest areas of performance, this can have a significant impact on the local economy. Currently, alumina (Al_2O_3) is extracted from bauxite ore using the Bayer technique as part of the aluminium production process. However, this process is severely compromised by the accumulation of insoluble material or 'scale' on the walls of equipment. Scale build-up reduces the flow of materials through machinery and causes heat transfer, which results in the need for regular and costly maintenance and equipment replacement.

Scale formation is also a costly issue for other industrial processes, such as those involved in the purification of nickel, where silica and hematite scales are common and problematic. In cooling water systems and desalination plants, calcium carbonate scale can create problems, as can barium sulfate scale in offshore oil production process streams.

A better understanding of how scale formation occurs is critical to develop improvements in the mineral refinement process and provide ideas about how these costly issues can be overcome. Ideally, this requires an ability to study scale formation, as and where it happens (*in-situ*), because it allows for chemical reactions to be followed in real time, avoiding the unpredictable changes introduced when a sample is extracted from the processing environment.

In-situ X-ray diffraction experiments carried out at the AS have shed valuable light on the mechanism of scale formation in the alumina extraction process. These experiments used a custom-designed flow cell and mimicked Bayer processing conditions to pinpoint how scale forms and to provide information about how this process might be controlled. This information includes the mineralogy and crystallographic orientation of scale in the early stages of formation.

Such information will lead to the development of practical and cost-effective methods to prevent scale formation in the Bayer process and thereby has the potential to enhance the productivity and profitability of ore processing in the Australian mining industry.

Fuel storage materials for gas-powered vehicles

The ability to store and handle gases is a critical step in achieving new clean technology, such as hydrogen fuel cells. The development of this technology will require the development of novel materials, such as Metal Organic Frameworks (MOFs). MOFs are an exciting new class of hybrid materials that are very porous and have an extraordinarily large surface area per unit volume. These properties make MOFs extremely well-suited to the safe uptake, storage and release of gases, which would normally be hazardous and difficult to handle.

Cutting-edge research undertaken at the AS has helped scientists to understand the structural properties of various MOFs. This is critical in designing novel materials with optimal characteristics for use as gas handling materials. This work, which helps to understand the molecular structure of materials such as MOFs, could lead to applications in vehicular gas storage as a route to hydrogen and natural gas powered cars for the future.

1.3 The need for growth - new science enabled by the development plan

Around the world, synchrotron science continues to grow rapidly. This growth is manifested in the size and sophistication of user communities, the number of facilities in operation and under construction and developments in experimental techniques, instrumentation and associated technologies. The trends in Australian synchrotron science are no different.

Building on the outstanding success of projects previously funded by the Federal Government - the Australian National Beamline Facility (ANBF, Tsukuba, Japan, 1991-1995) and the Australian Synchrotron Research Program (1995-2008) – the AS has become the national hub for synchrotron radiation based research, building expertise and capability not only within the facility but fostering and promoting scientific and technical collaborations nationally and internationally.

The Australian Synchrotron user community has grown dramatically and over 1800 researchers and students are currently registered with the facility. A noteworthy feature of this rapidly growing community of users is its geographic, institutional and scientific diversity. The AS user community includes scientists from every state and mainland territory, New Zealand and other nations. It encompasses almost every national research institution and 34 of Australia's 38 universities. In addition, the AS hosts a number of partnerships with the private sector and a number of industrial users have accessed the facilities through commercial arrangements for the purposes of proprietary research. Accordingly, demand for access to the existing beamlines far outstrips time available by an average of approximately 53%. At the current level of saturation, the AS hosts over 2800 user visits per year and also supports access to overseas light sources by *ca.* 70 Australian research teams per year. Clearly, further development of the facility is required.

Even before the opening of the Australian Synchrotron, the need for continued growth was recognised. Strategic planning was begun with a joint committee of the Australian Synchrotron Project and the Australian Synchrotron Research Program, publishing the "Synchrotron Strategic Plan 2007-2017", an important resource that has informed the development of this plan.

In order to maintain the global position of Australian research, it is crucial that scientists in the region are provided with the tools required to compete on the world stage and perform breakthrough research. Moreover, as new fields of research emerge and current research evolves, it is becoming clear that Australian scientists require access to a broader suite of technologies and techniques than those currently available at the AS.

Further urgency for the development of expanded capabilities at the AS is brought about by the imminent closure of the Australian National Beamline Facility. The ANBF was for many years the backbone of Australian synchrotron science and continues to operate with the support of our Japanese partners (Photon Factory, KEK) and an ARC LIEF Grant. In FY2009, the ANBF hosted 29 Australian research teams (75 user visits) utilising 97 days of beamtime primarily for X-ray absorption experiments. The impending cessation of operations at the ANBF at the end of 2010 will, therefore, significantly affect the ability of Australian research teams to access XAS capabilities and put critical demand stress on the XAS beamline at the AS.

It should be noted that the XAS user community is one of the largest single groups of synchrotron radiation exponents and is world-competitive in terms of the range and sophistication of the science outcomes it produces. The loss of the ANBF will be severely felt by this important part of the community.

The development plan aims to address these needs by proposing new leading-edge capabilities that will increase research and innovation capacity at the AS. The new beamlines will provide new capabilities and enhance existing ones in a manner that is complementary to those currently available and build on the proven track record of excellence at the AS. The proposed development plan will make possible new fields of research endeavour and promises increasing high-impact scientific outcomes, examples of which are summarised in Parts 3 and 4 of this document.

Through this development plan, the Australian Synchrotron has an opportunity to build on the existing infrastructure and expertise developed both within the AS and in the broader Australasian scientific community. Exploitation of this opportunity will maintain and build Australia's position in this rapidly growing area of technical and research growth and deliver health, economic and social benefits and therefore enhance Australia's international competitiveness within science and more broadly.

The ten beamlines proposed in the development plan have extensive scientific scope and application and are consistent with the goal of making world-class facilities and capabilities available to Australian and New Zealand researchers and their students. Similarly, they address directly the science and innovation priorities of Australia and the demands of the scientific community.

Support for an integrated and ambitious development plan at the AS will have a strong impact on the quality of science undertaken in the region. This will be seen through an increase in the number of Australian research groups performing at a world-class level and publishing in high quality journals, a boost in the quality and quantity of world-competitive researchers graduating from our universities and being retained within the domestic research community, and a reduction in the number of Australian researchers leaving to work at overseas facilities.

Synchrotron science is inherently collaborative, multidisciplinary and international. Ongoing investment in key research infrastructure at the AS will inevitably result in the continued development, growth and productivity of local and international research collaborations and networks. This international collaboration is aligned with national research priorities and will help to maintain Australia's leading position in the research sector.

The development plan addresses several growth areas in synchrotron-based research, including:

- Health and medical imaging
- Structural biology
- Pharmaceuticals and drug design
- Cellular imaging
- Engineering science
- Manufacturing technology
- Environmental science
- Materials science Including nano- & nanobiotechnology
- Energy science and sustainability
- Extreme conditions science
- Textile science
- Geological science
- Minerals processing
- Ultra-fast science
- Measurement trends
  Including ultra-fast, ultra-sensitive and ultra-small measurements

These target areas comprise a combination of fundamental and applied science, with a broad array of areas of vital interest and importance to the economic and social development of Australia.

1.4 Scientific Vision and Core Competencies of the Australian Synchrotron

The continued high performance of the AS in the future will rely on a clear scientific vision and on having clearly identified the core competencies required to achieve this. A key consideration in reviewing our vision and core competencies is the fact that the operation of the Australian Synchrotron must be transparent and accountable not only to stakeholders and users of the facility but also to the broader research community and general public of Australia. Accordingly, the activities of the AS must address identified and prescribed national priorities.

The vision of the AS is stated as:

"At the Australian Synchrotron, our vision is to be the catalyst for the best scientific research and innovation in Australasia."

In order to achieve the vision, management has developed a mission statement as follows:

"At the Australian Synchrotron our mission is to develop a world-class synchrotron facility, maximising the quality, breadth and impact of scientific output."

In other words, the AS aims to be a globally-competitive and recognised centre of excellence in synchrotron science and its applications. The AS will achieve this by enabling, supporting and promoting outstanding scientific research carried out by a broad user community and its own staff.

The core scientific competencies that will enable the realisation of this mission include:

- **Operations:** To construct and operate a reliable world-class national synchrotron radiation facility including:
  - SR storage ring and the associated accelerators
  - State-of-the-art beamlines and experimental stations
  - High-quality and extensive supporting research infrastructure

- **User Program**: To make available these facilities through a well-organised program to support the research activities of user groups from Australia, New Zealand and overseas. As part of its user program and in the interests of enhancing SR science and expertise, the AS also supports access to overseas SR facilities for experiments that cannot be performed at the AS.
- **SR Leadership**: To be a centre and to foster the development of synchrotron radiation and accelerator science expertise in Australia.
- **Research and Development**: To carry out world-class research and development and promote innovation by fostering a conducive, collaborative and multidisciplinary environment and encouraging the research aspirations of AS staff.
- **Skills Development**: To foster the development of technological expertise through the support of internal development programs and training with the goal of increasing the skills base of the AS and Australia generally.
- **Education and Outreach**: To be a national educational resource in leading-edge science and innovation and in this role actively engage with universities and schools, scientific organisations, industry, government agencies and the wider community

  In a broader sense, the AS has active collaborations and leadership roles in:

  - South East Melbourne Innovation Precinct (SEMIP)
  - Victorian Platform Technology Network (VPTN)
  - AusBiotech
  - BioMelbourne Network
  - Plastics & Chemicals Industries Association (PACIA)
  - Australasian Industrial Research Group (AIRG)
  - Future Materials Network
  - Australian Nanotechnology Alliance
  - Small Technologies Cluster
  - Australian Collaboration for Accelerator Science (ACAS)

Additionally, the AS has Memoranda of Understanding with 11 other synchrotron radiation laboratories, which are aimed at promoting collaboration and technology sharing with peer facilities around the world.

1.5 Scientific Strategy

The process of collating this development plan involved broad engagement and dialogue with the scientific community. This interaction is essential to achieve the best possible outcomes from future investment in the facility. To ensure that this dialogue is as constructive as possible, it is essential that the AS provides the scientific community with a clear indication of the scientific strategy that underpins this development plan. The vision has been described in general terms above. This has been used to prioritise and select the new beamlines and beamline enhancements according to the following principles:

I. International competitiveness

It is appropriate and informative that in the process of determining a strategy for the future the AS considers international trends in synchrotron science. The aim of this is not to simply copy the development of other facilities, but rather to learn from the experience and insights of others and apply this knowledge to the Australian context. From this analysis, it is clear that other existing facilities and those currently under construction have focused their development on features and capabilities where synchrotron radiation is known to provide superior scientific outcomes. Primarily these are techniques that provide higher resolution in space, time and energy and ever increasing sensitivity. Therefore, most developments of synchrotron facilities are focused on the ultra-small (microscopy and imaging), ultra-fast (time-resolved and high throughput), very high resolution spectroscopy and extreme environment experiments (temperature, pressure and magnetic field).

Additional specific trends in synchrotron science that have been identified include:

- Ultrafast dynamics and mechanisms
- Interfaces in complex systems
- Imaging & coherence
- Structural & functional biology and soft matter
- Protein dynamics and living systems
- Nanoscience & nanotechnology
- Hierarchical structures - studying materials on length scales from metres to nanometres and on to the atomic scale
- Studying chemical reactions, physical and biological processes and structure-function relationships at atomic time and length scales

II. Building on existing strengths

a. What projects are well-suited to the technical specifications of the AS?

It is essential that any new beamline or accelerator project be considered in the context of the technical performance and potential of the accelerators and feasible light sources at the AS. That is to say, no project should be supported, regardless of the potential scientific benefits, if it could not be adequately supported by the existing light source and facilities to ensure optimal outcomes. This is of particular concern when projects could excel at another light source.

b. How might we support high quality research outcomes?

Beyond the technical capabilities of the storage ring and the beamlines, there are many factors that contribute to successful research outcomes. These include sufficient and relevant human resources and the availability of supporting infrastructure such as laboratories, high-performance computing facilities and other enabling facilities. Throughout this development plan, significant consideration has been given to the supporting resources required for adequate operation and to ensure quality scientific outcomes.

c. In what areas do we have a track-record of excellence to build on?

Looking both within the AS and beyond to the wider scientific community, there are obvious advantages in identifying existing areas of experience and expertise where excellence has been demonstrated and which the AS can foster and build on via targeted development.

III. Existing demand for synchrotron science in the region

The current beamlines available at the AS maintain strong subscription rates, some with demand many times greater than the available beamtime. One aim of the development plan is to relieve demand 'pressure points' through a range of strategies including:

- Construction of new beamlines with capabilities that alleviate the existing strong demand for particular techniques and facilities
- Optimisation of existing facilities to maximise throughput and streamline experimental operations

Currently, we do not favour the approach of duplicating existing beamlines to cater for this growing demand, as this would represent a significant investment which would be to the detriment of enhancing existing beamlines or building new and much-needed beamlines. Rather, our approach is to build, specialise and optimise in a complementary fashion, to deliver a suite of facilities that operate efficiently and without compromise to deliver data of the highest quality.

IV. *Compatibility, complementarity and cohesion*

It is only natural that inspiration for growth at a facility such as the AS is born at least in part from the experience gained and success achieved with existing capabilities. It follows that this development plan should also consider compatibility with existing resources by selecting new beamlines that will complement and enhance the existing suite of beamlines at the AS. This principle also extends to considering each project for alignment with the over-arching scientific goals and research priorities of the AS.

From a scientific standpoint, several research themes have emerged over the first two years of operation of the AS that derive from factors including global and domestic research trends, user demand, targeted technical proficiency and the expertise and experience of in-house staff. These themes have been considered as priority research areas for the AS and will continue to be supported in the growth plan for the facility.

- Medical and Life Sciences
  - Medical imaging and therapies
  - Structural biology
  - Cellular imaging and biochemistry
- Advanced Materials and Engineering Science
  - Polymers, semiconductors, ceramics and composite materials
  - Magneto, optical and molecular electronics
  - Nanoscale materials
- Earth and Environmental Sciences
  - Mining technology and mineralogy
  - Energy technologies
  - Waste remediation and biotoxicity

As these are emerging areas of strength and need in the local synchrotron science community, the AS will focus its development with the aim of building capacity and capability in these areas. This strategic focus on concentrating on existing and emerging research themes where the facility can enable high quality research outcomes has the best potential to produce world-class outcomes.

1.6 Other Considerations

Scientific Excellence

The pursuit of research excellence is the highest scientific priority. A commitment to quality must be an overriding consideration to ensure we give local industry a competitive advantage and help to attract and retain the best scientific talent in this region. Maintaining a competitive edge internationally also requires a balance of fundamental and applied research and development, covering basic research, strategic research programs, tactical research, experimental development and short-term problem-solving.

Responsiveness to National Priorities

Synchrotron technology has long been a major contributor to all four of Australia's National Research Priorities (NRPs), namely:

- An Environmentally Sustainable Australia

  Transforming the way we utilise our land, water, mineral and energy resources through a better understanding of human and environmental systems and the use of new technologies.

- Promoting and Maintaining Good Health

  Promoting good health and well being for all Australians.

- Frontier Technologies for Building and Transforming Australian Industries

  Transforming Australian Industries

  Stimulating the growth of world-class Australian industries using innovative technologies developed from cutting-edge research.

- Safeguarding Australia

  Safeguarding Australia from terrorism, crime, invasive diseases and pests; strengthening our understanding of Australia's place in the region and the world; and securing our infrastructure, particularly with respect to our digital systems.

Similarly, the growth of the AS must incorporate and be consistent with the objectives of the National Innovation Priorities, specifically:

- Enhanced innovation capacity
- Invigorated growth of Australia's research capabilities and
- Enhanced international competitiveness

Previous Studies

The "Synchrotron Strategic Plan 2007-2017", completed in 2006, was an important document for the synchrotron science community, identifying the priorities for this area of science over the following decade. Many of the recommendations in that plan have already come to fruition. For example, the current beamlines at the AS have been completed to world class standards, investment in e-research has been put in place, the international access program is being operated successfully through the AS and resources for travel and accommodation for AS users are provided.

However, it was recognised in the document itself that there would be a need to constantly review and re-evaluate priorities in response to the changing community in Australasia and internationally. The current process achieves just that outcome, and there are some significant changes as a result of the greatly increased size and experience of the community. This is seen as a healthy process. Similarly, the beamlines identified as Phase 3 will require further consideration and planning over the life of this plan.

Industrial Impact

The Australian Synchrotron is already developing a targeted approach to engage industry with synchrotron science and the facility. The objective is to build an industry engagement program with rapid access for industry, protection of intellectual property, varying levels of service, and with a focus on industries best suited to Australian Synchrotron capabilities. Accordingly, strategies for future growth must address these objectives and strive to maximise industrial engagement and impact.

2. Australian Synchrotron Development Plan

2.1 Description of the process

In establishing the process to map the future of the AS, some fundamental principles were established. These were:

- Future development must be considered in the context of, and must complement, the existing accelerators and beamlines. For this reason, the terminology of 'projects' was used, to encompass beamlines, upgrades to beamlines and facilities and upgrades to accelerators.
- Two important drivers of growth and development are the need to satisfy strong demand from the scientific community in specific areas of synchrotron-related science and the need to identify areas in which the AS can be considered 'world leading'. Balancing these was considered to be extremely important.
- Each of the final projects chosen must be considered 'world class', recognising that this definition is necessarily imprecise.

From the outset the process was intended to be open and consultative and, most importantly, to be driven by the scientific community. The stated aims of the Australian Synchrotron Development Plan process were:

- To rationalise and justify future funding for the Australian Synchrotron on a sound scientific basis
- To identify the most effective combination of projects going forward, in order to maximise benefit to, and satisfy identified demand in, the Australian and New Zealand scientific communities
- To identify leading edge projects in which local scientists can become, or continue to be, world leading
- To effectively engage the scientific community in the process of moving forward

This process was based on an open, web-based submission system that followed a series of workshops held around Australia and New Zealand. Details of the workshops are given in the Appendix 2. While submissions were open, mailing lists were created and draft versions of the proposals made available on the website, with the intention of allowing interested members of the scientific community to contribute towards the development of the final proposal. The mailing lists were also a useful indicator of the level of support for the proposals.

By the closing deadline a total of 24 proposals had been submitted for consideration. A period of consolidation and moderation by AS management in collaboration with the proponents of the proposals ensued, and a final list of 12 resulted. This list included a range of smaller projects that were grouped in a category known as Major Facility Upgrades.

The final selection and prioritisation presented in this document has been done in consultation with:

International Peer Reviewers

Each of the final proposals was sent to 3 scientists for peer review. The selected reviewers were international experts in the relevant field, and were asked to provide comments on the following:

1. **Scientific Potential**
   What is the potential for the project to produce or enable high-quality and high-impact scientific outcomes?
2. **International Benchmarking**
   How does the project compare with international trends in the relevant field and synchrotron radiation science in general? Is the project consistent with international standards of technological sophistication, performance and experimental capability?
3. **Project Scope**
   Is the scope of the project as proposed reasonable? Should the objectives of the project be expanded or reduced in order to realise an optimal outcome?
4. **Technical Feasibility**
   Is the project as proposed technically feasible? What are the potential difficulties or risks that will need to be managed? Are there any enabling technologies that will need to be developed to realise the project?
5. **Design and Procurement**
   Is the project within the expertise and/or experience of commercial suppliers to design and supply to the required standard? If not, what component(s) would need to be designed and/or procured as 'specialty' items?

Science Consultative Group

The Science Consultative Group (SCG) is a group of prominent and highly respected Australian and New Zealand scientists who are also experienced synchrotron users. This group was brought together to provide a "local" perspective on the current and emerging needs of Australasian synchrotron users. This group met twice, and provided a report that helped shape the development plan. The list of members is given in the Acknowledgements.

Scientific Advisory Committee

The Scientific Advisory Committee (SAC) of the AS is an international committee that provides expert advice to the AS on a regular basis and last met in May 2010. The development plan was a major focus of the most recent meeting of the SAC. The feedback and deliberations of the SAC were another important influence in shaping the development plan presented here. Current members of SAC are listed in the Acknowledgements.

SAC provided a detailed report on the proposals, taking into account the international peer reviews, the SCG report and their own considerable experience.

Further important information was provided by the **International Program Advisory Committee** (IPAC), advising on the demand for access to international facilities by Australian research teams.

2.2 Outcomes of the Consultation Process

The culmination of this lengthy consultation and peer review process was the development plan described here, which outlines ten new beamlines, significant upgrades related to the accelerators and other major facility upgrades that are considered optimal and urgent. Any plan of smaller scope would leave the AS seriously hampered in its mission to remain at the cutting edge of global research and unable to provide the enabling and facilitating resources to support high quality research throughout Australasia. This development plan also includes a phased implementation approach, which is necessary for a number of reasons. These include the availability of resources, the need to minimise downtime of existing facilities and the importance of allowing time for further study and planning of the detailed technical aspects of some projects to ensure their successful implementation. The following plan is consistent with the Investment Case prepared by LEK Consulting, which recommends the commencement of 3 beamlines in Year 1, three beamlines in Year 2, two beamlines in Year 3 and two beamlines in Year 4. One of the outcomes of the development plan process has been to allocate to each of the final beamline proposals a status of Phase 1 (to begin in Year 1), Phase 2 (to begin in Year 2) or Phase 3 (to be reviewed and developed, then commenced in either Year 3 or 4).

The following phasing has been determined, based on the considerations above:

Phase 1 Beamlines

- High Coherence Nanoprobe (HCN)
- Micro Materials Characterisation Beamline (MMC)
- Medium Energy XAS Beamline (MEX)

Phase 2 Beamlines

- Advanced Diffraction & Scattering Beamline (ADS)
- Small Angle Scattering Beamline for Structural Biology (SSB)
- Micro-Computed Tomography Beamline (MCT)

Phase 3 Beamlines

- Soft X-ray Materials Science Beamline (SXM)
- High Performance Macromolecular Crystallography Beamline (HMX)
- Advanced Infrared Beamline (AIR)
- Correlative Microscopy Beamline (CMB)

Accelerator Development

Ongoing development of the accelerators is critical to the future performance of the Australian Synchrotron and the science that it supports. In particular, the move to 'top-up mode' must have the highest priority as it underpins all other developments. Without it, the AS will not be a competitive 3rd generation light source and the full potential of the proposed beamline projects will not be realised. This development will also foster the research interests of the accelerator physicists, helping to achieve the scientific strategy and more far-reaching goals of the facility, such as those related to capacity building and education. For these reasons this plan proposes an immediate start on the sub-projects that will enable the transition to routine operation of the storage ring in top-up mode as soon as possible. Accordingly, this project is given priority equivalent to the Phase 1 beamline projects above.

The development of a THz photocathode electron gun for THz radiation production is also seen as important for the next five-year development period. The THz source project is ranked equivalent to the Phase 2 beamline projects.

Major Facility Upgrades

Consistent with the goals of the Development Plan and in recognition of constantly advancing technologies and experimental demands, the suite of Major Facility Upgrades are all considered important to fulfilling the scientific mission of the AS. In some cases the proposed projects are integral to the beamline projects and where these affinities are present, recommendations have been made accordingly (See MFU project summaries in Section 4).

2.3 Costing of the Projects

Final costing of the individual components of the Development Plan will be completed after detailed conceptual designs have been prepared. More information on the projected funding requirements to implement this plan is given in the Investment Case, and in summary the overall projected costs are:

Item	Total Cost
Beamlines	$86.5M
Accelerator Development and Major Facility Upgrades	$15M

3. Beamline summaries

3.1 Phase 1 Beamlines

3.1.1 High Coherence Nanoprobe (HCN)

Introduction

The ability to image biological, geological and materials samples at very high resolution has improved dramatically in recent years due to advances in synchrotron optics and technology. Australian groups are world leading in this area of science and the current X-ray fluorescence beamline at the Australian Synchrotron is one of the most heavily oversubscribed of the facility. The proposed High Coherence Nanoprobe is a further development of this technique that has the potential to revolutionise our understanding of processes that occur in healthy human cells and those challenged by disease or disease treatment. This beamline would also have other applications outside health and medical research, in particular to advance nanoelectronics and nanofabrication, to improve the ability to extract metals from ores and to understand the detailed structure and chemistry of soils. This beamline would therefore represent a significant enhancement to the current facilities of the Australian Synchrotron.

Expected Scientific Outcomes

A nanoprobe is a device that produces images with very high resolution, in this case of less than 30 nm. The proposed design is a unique combination of two techniques, one of which involves the scanning of a sample with a focussed X-ray beam and the other in which the entire sample is illuminated by the beam and takes advantage of the unique coherence of the beam from the synchrotron. Such a device has a large number of applications across a range of fields of science.

Biological and health sciences

High resolution imaging of single cells has been a cornerstone of recent fundamental research related to the normal metabolic functions of cells. Such techniques are also critical to understanding the subtle changes that occur during the normal development of cells and tissues, during the ageing process and as a result of disease. This requires the study of the cell, as a whole, of the nucleus which houses the DNA of the cell and of the tiny organs within cells, called organelles. Although the nucleus can be seen with current technology, it is very difficult to identify individual organelles with the resolution achievable at current facilities. The improved resolution of the nanoprobe beamline would be of great benefit in the study of the architecture of cells and help to answer critical questions about the process of disease, development and cellular change outlined above. In particular, the study of mitochondria, the powerhouses of the cell, which provide the energy essential to every function of the body, will support rapid advancement in many areas of health and medical research.

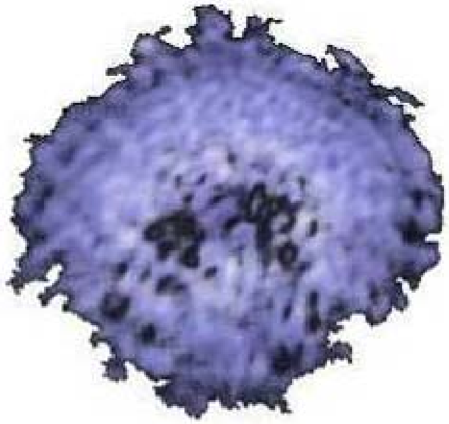


Figure 3.1 A malaria parasite within a red blood cell

An important example of how the nanoprobe might advance the study of sub-cellular structures is research related to the malaria parasite, *P. falciparum* (Figure 3.1). Malaria leads to more than two million deaths per year, mainly in the young. The malarial parasite spends part of its lifecycle inside human red blood cells, where it establishes a system of membranes within the host cell and causes changes in the membranes that surround the infected blood cells. These changes are critical to the processes by which the malarial parasite causes disease. X-ray wavelengths allow imaging at high spatial resolution of the inside of red blood cells infected with *P. falciparum* that will assist in the study of the development of the parasite and in the response of cells to different treatments.

In addition to the study of how parasites, viruses and bacteria cause disease in humans this beamline will help to enhance our understanding of other disease processes and help develop or improve current medical therapies. For example, the ability to study the localisation and associations of heavy elements (such as chromium and iron) in mitochondria and other organs within cells (such as lysozymes) is limited by the resolution available using the technology at current Australian facilities. The improved resolution of the new nanoprobe proposed for the Australian Synchrotron would allow the study of the efficacy and toxicity of metal-based anti-cancer and anti-diabetic drugs and fundamental biochemical processes involved in damage of cardiac and brain cells as a result of strokes, degenerative brain diseases such as Alzheimer's, heart disease and a number of other processes.

An extraordinarily powerful capability of the nanoprobe will be X-ray fluorescence tomography, in which 3-dimensional representations of the distribution of individual cellular components can be studied at very high resolution within a single cell. An example shown in Figure 3.2 (obtained in the US at much lower resolution than would be available on the new instrument) is of a diatom, *C. mehinghiania*, caught in the process of cell division. Diatoms produce 18 to 20 billion metric tons of organic carbon each year and their effect on global carbon cycling is estimated to be of similar magnitude as all rainforests combined, so this research is of enormous potential importance for the environment.

Apart from the specific examples given above, the application of this tool to health and medical research is very broad. Other such applications include

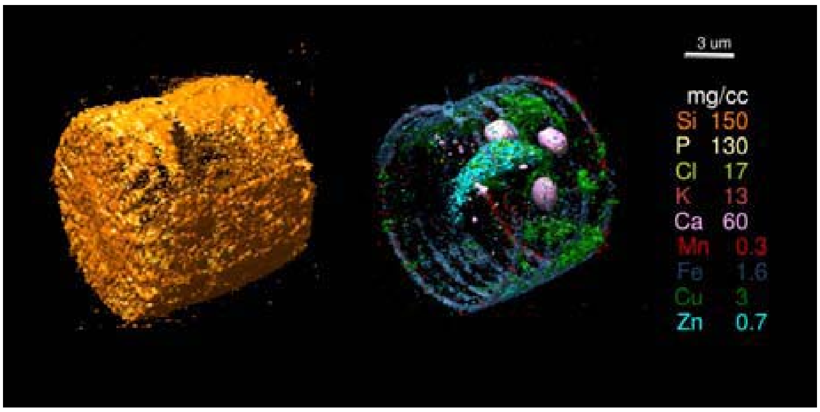


Figure 3.2 Fluorescence tomography of *C. Meninghiania* with an estimated spatial resolution of 300 nm.

formation of aggregates and distortion of cellular architecture in neurodegenerative diseases such as Alzheimer's disease and Parkinson's disease, the role of metals in pathogenic bacteria, the toxicity of nanoparticles, understanding the nanostructure of teeth and bone and many others.

Environmental and earth sciences

There are fundamental unanswered questions in environmental and earth sciences that could be directly addressed by the proposed nanoprobe. As this instrument has the ability to generate high resolution maps of heavy metals, it can therefore be used to examine the fate of toxic metals in soils, plants and microbes with great precision and in real time. For example, the transfer of metals from the inorganic (soils) to the organic (living tissue) can be understood using this tool. Current synchrotron approaches to studying micronutrients and contaminants in plants are conducted only at tissue level, with little information available at the sub-cellular level. This nanoprobe would provide unprecedented detail that would help to accelerate our learning in this area. A further feature of the proposed nanoprobe is the ability to accept frozen hydrated tissues, which is essential to progress this field of research.

As nanomaterials become more prevalent in consumer products, there are significant concerns about the effects of these substances on the environment and the potential that the components of such materials may become hazardous pollutants in the future. Nanomaterial behaviour in soils and sediments is poorly characterised and an understanding of the uptake and toxicity of these materials relies on the ability to map and define the state of the elements in nanoparticles in both soils and living materials, such as plants. Such interactions will be easily studied using the nanoprobe.

Materials science

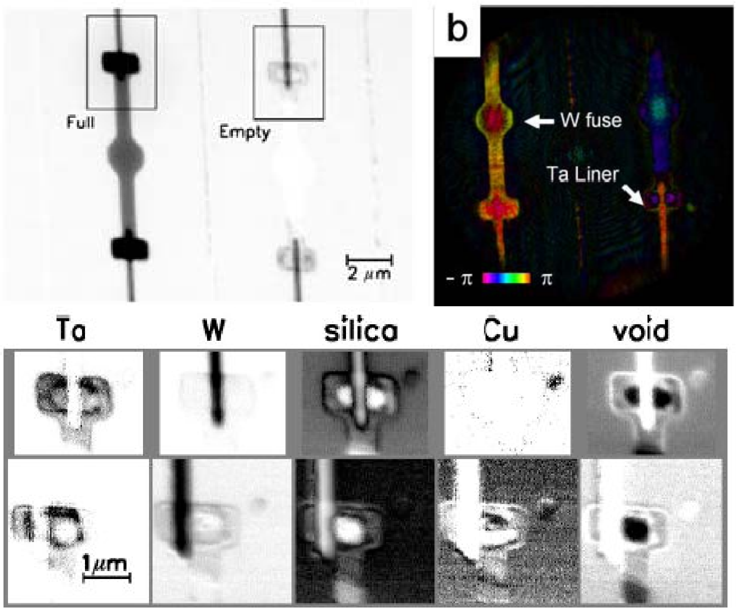


Figure 3.3 Scanning Transmission X-ray microscopy showing high resolution spectroscopic information on a fuse section of an integrated circuit

The integrated circuit industry is already able to create devices with features of a size beyond the imaging ability of current X-ray focussing technology and also beyond the ability of other imaging methods such as electron microscopy. These available technologies are particularly limited by the need to image in three dimensions. The proposed nanoprobe can close this gap in capability and become an important diagnostic tool for the microelectronics industry. As further miniaturisation becomes possible in the industry, this ability becomes even more necessary.

The Melbourne Centre for Nanofabrication (MCN) is located on the same site as the Australian Synchrotron, and with $45M of initial funding from the Australian Government through NCRIS, the Victorian State Government and partner institutions is set to become a national leader in nano-scale applications. While the centre is well equipped for fabrication and characterisation by electron microscopy, the nanoprobe beamline will greatly boost the capabilities of the centre and become a key characterisation tool for MCN.

Multi-component electronic devices based on functional organic materials with intrinsically nanoscale dimensions form a new class of materials that are finding application in what are known as organic electronic devices – devices such as light emitting diodes and photovoltaic solar cells that use organic materials as the active components. Understanding fundamental properties such as charge transport and recombination in these materials helps explain how highly efficient devices can already be fabricated based on this technology platform and will lead to whole new avenues of research into ever more efficient and durable components that will have direct application in consumer electronics. The nanoprobe is an essential tool for this research.

Potential User Community

There is already a thriving community using the current fluorescence microscope drawn from all states in Australia, as well as New Zealand and other countries – this includes users from both the academic/scientific and the industrial sector. It is the most heavily oversubscribed beamline of the Australian Synchrotron such that in some rounds only a quarter of submitted proposals are allocated time. With the new capabilities of the proposed nanoprobe and taking into account the wide applicability of the methods, this community is expected to continue to grow rapidly. Australasian leadership in this area is demonstrated by the ARC Centre of Excellence for Coherent X-ray Science based in Melbourne, the world leading detector system developed for the existing microscope in part by CSIRO researchers and the large number of research groups involved in imaging and microspectroscopy.

The experience of the International Synchrotron Access Program, administered by the Australian Synchrotron, has shown that a large proportion of applications for funding have been to use imaging techniques, representing the second highest demand after absorption spectroscopy. This reflects the fact that the Australasian imaging community is large and vibrant. While the current fluorescence microprobe is considered by many to be world leading, there is already demand for ever more challenging capabilities such as those provided by the nanoprobe. It is certain that this instrument would be in heavy demand from the time of commissioning.

Description of the Proposed Beamline

The conceptual design of the nanoprobe will use lessons learned from recent nanoprobe designs worldwide. It is proposed to provide a unique combination of two modes of operation that can be readily interchanged. The main design features are:

- Combined scanning X-ray microscopy (SXM) and full field coherent diffractive imaging (CDI)
- Diffractive optics (zone plates or multilayer Laue lenses)
- Resolution of 25 nm (SXM) and 5 nm (CDI)
- Energy range of 2-22 keV

- Cryo-capability for biological samples
- Fast scanning stages
- Maia detector for SXM and CCD detector for CDI (to be reviewed as this field is progressing rapidly)
- Long beamline (~100 m) to maximise coherent flux
- In-vacuum undulator insertion device

3.1.2 Micro Materials Characterisation Beamline (MMC)

Introduction

Although it is not always obvious, the world is heterogeneous – that is, on a small enough scale materials generally lack uniformity. When the probe used for analysis of structure is very small, for example of submicron dimensions (less than one millionth of a metre) it becomes possible to study the heterogeneity in composition and structure of a sample in a completely new way. The proposed Micro Materials Characterisation (MMC) beamline offers the ability to simultaneously measure diffraction and fluorescence with submicron resolution, creating completely new scientific opportunities. This method has implications for the study of materials in a wide range of fields, such as solar cells, high-temperature and nuclear energy materials, pollutants in the environment, mining and mineral recovery processes and can even provide new information on biological materials.

Expected Scientific Outcomes

By using an extremely finely focussed beam, combined with the ability to measure simultaneously structure (by diffraction) and composition (by absorption) the MMC beamline will be a world-leading facility. Traditional synchrotron X-ray microprobes use an X-ray beam composed of the narrowest energy distribution achievable - a 'monochromatic' beam. For heterogeneous materials, however, the size of the crystallites may be larger than the beam, so that little or no diffraction information may be measurable and hence vital information may be overlooked (Figure 3.4).

The proposed MMC beamline will use a broad energy bandpass to avoid this problem and collect structural information that is spatially resolved on the smallest possible length scale. Another extremely valuable benefit of this technique is that diffraction patterns generated from high energy broad bandpass synchrotron radiation may be produced from deep within a sample. Deconvolution of these data as a function of depth can be carried out using a technique developed by scientists at Oak Ridge National Laboratory (USA) to give 3-dimensional structural information.

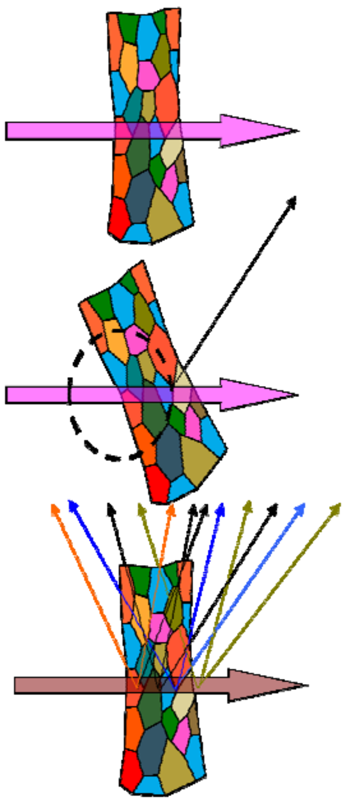


Figure 3.4 The principle of using a 3D microscope to study polycrystalline materials

This powerful tool has applications across a broad range of science.

Minerals exploration, mining and the environment

The MMC beamline will provide new opportunities and critical information for a large number of existing projects at several institutions in Australian and New Zealand, leading to increased mineral processing recovery and benefits to the environment. Applications include investigating the deportment of valuable metals in various mineralogical sites in both the mineral exploration and mineral processing context, improved ability to cross correlate mineral phase with high value trace elements such as uranium and increased understanding of deep earth materials and processes. For example, the ability to trace the flow of gold through processing circuits has the potential to impact on the world's major gold producers. Whether the gold occurs as fine inclusions or intimately mixed in minerals is an important question that can be answered by the proposed beamline (Figure 3.5). The answer will determine to what degree it will be possible to increase gold recovery through the application of fine grinding technology followed by either flotation or cyanide leaching.

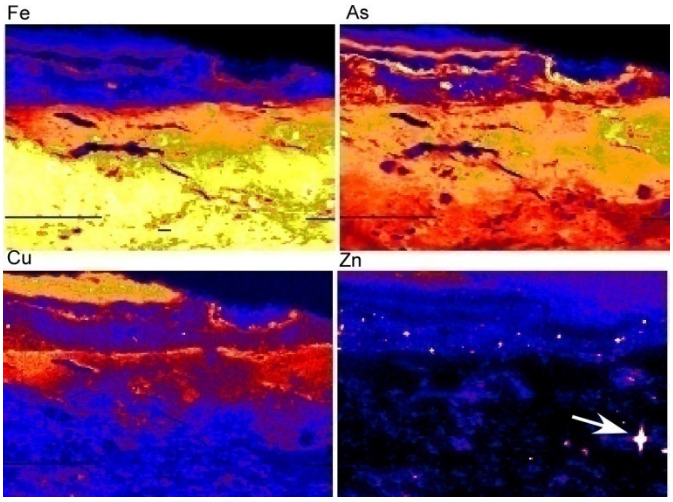


Figure 3.5 Synchrotron XRF of metal distribution in an exploration regolith sample from above a gold prospect.

Projects that offer direct benefits to the environment include environmental remediation of degraded acid sulfate soil landscapes and the transport and speciation of hazardous metals within estuarine and river environments. Adequate examination of the clay sized minerals that mediate and control the geochemistry in these environments requires the advanced capabilities afforded by the proposed facility. This knowledge will underpin the formulation of management techniques for such landscapes.

Soils, their salinity and acidity are critical environmental issues for Australia. The MMC beamline is well suited to the study of geochemical changes in soils on weathering, their interactions with groundwater and understanding porosity in soils.

Materials science

Advanced materials development frequently requires a detailed understanding of the 3-dimensional nature of heterogeneous structure, particularly in composite nanostructured materials. Light weight metal alloys are very important in a number of industries such as transport. The ability to study the development of hexagonal close packed (hcp) structures of, for example, titanium and magnesium to produce lightweight alloys will be greatly assisted by the MMC beamline. The micron-scale thermo-mechanical properties of alloys and the micro-crystallinity and spatial distribution of grains in glass-ceramic waste form materials are also able to be studied in this way. The latter has important implications for the long-term storage of intractable hazardous waste.

Biological sciences

Many of the biological applications of the proposed facility relate to plants and plant-derived products. For example, the organisation and order of large protein complexes and protein assemblies arranged in polycrystalline states in biological membranes is very difficult to study by traditional methods. The ability to create descriptions of structural and functional relationships of plant transporters will create opportunities for basic and applied research that could improve crop yields and quality, and the environment sustainability of crops in low input agricultural production systems.

A range of applications exists in the health sciences, such as porous silicon scaffolds for tissue engineering, optimised addition of silicon to orthopaedic materials for enhanced bone growth, nanoparticles for cancer diagnosis and understanding the role of metals in disease processes and their treatment by mapping of healthy and diseased tissue.

Microdiffraction will be of great help in research projects on the structure of membrane proteins in particular receptors associated with the brain, like dopamine and serotonin receptors. The fluorescence capabilities of the MMC beamline would be of considerable aid with the study of the redox chemistry of proteins involved in Alzheimer's disease, currently being undertaken within a CSIRO Flagship initiative on neurodegenerative diseases.

Potential User Community

Four specific groups of users have been identified that would benefit greatly from the availability of the MMC Beamline:

a) the considerable section of the scientific community that specifically requires microdiffraction either by itself or in conjunction with X-ray absorption spectroscopy (XAS) and X-ray fluorescence microscopy (XFM). Currently there are no microdiffraction facilities at the Australian Synchrotron.
b) the already well-defined scientific community that currently applies to use the XFM beamline (*i.e.* requires XAS and XFM) that requires spatial resolution in the order of 1 µm. The XFM beamline is currently heavily oversubscribed, with many worthwhile studies being rejected or being delayed due to lack of access.
c) PD users: a considerable number of studies being undertaken on the PD beamline would also benefit from microdiffraction where the samples being studies are heterogeneous and the phase of interest is a minor component and not resolvable by a bulk analysis *e.g.* the examination of uranium containing ores.
d) XFM users: the microdiffraction line would also address the requirements for higher energy XFM. A wavelength-shifter light source will enable examination of excitations (either XRF or XAS) in the high energy range not accessible to the undulator based XFM beamline.

Description of the Proposed Beamline

The design of, and technical requirements for, the MMC Beamline are well advanced and have been developed in collaboration with an international team from Oak Ridge National Laboratory (Gene Ice), NSLSII (Ruben Reininger), Advanced Photon Source/University of Chicago (Mark Rivers)and the Canadian Light Source (Renfei Feng, Emil Hamil, Stewart McIntyre).

Major design features of the beamline are:

- Bending magnet or possibly wavelength shifter source
- Minimum beam size of 1x1 µm
- Energy range of 5-40 keV
- The ability to use white light, or selectable energy bandpass with the ability to vary while sampling the same volume
- Fast CCD detector for diffraction measurements and MAIA detector for XRF mapping

3.1.3 Medium Energy XAS Beamline (MEX)

Introduction

X-ray absorption spectroscopy (XAS) is a sensitive and element-specific technique that can provide detailed information on the structural and chemical state of the element under investigation in a wide range of materials and physical environments. Accordingly, XAS measurements have the power to transform our understanding of many important problems that impact on such areas as human and animal health, environmental and agricultural processes, the development and production of new materials, understanding mineral formation and extraction and the optimisation of and mediation of problems in industrial processes.

The current XAS beamline at the Australian Synchrotron is a world-class instrument catering for measurements of the heavier metallic elements. However, the elements silicon (Si), phosphorus (P), sulfur (S), chlorine (Cl), potassium (K) and calcium (Ca) are of critical importance and research interest in the biological, environmental, earth and materials sciences, but are not readily studied on the current beamline. Australian groups are producing world-leading XAS research in this elemental range but are currently seriously hampered by very limited access to overseas facilities that cater to the required energy range. The full potential and benefit of these techniques to Australia could be realised, however, by the construction of a beamline designed to access this medium energy range at the Australian Synchrotron.

The productivity of the Australian XAS user community is further hampered by a general high level of oversubscription to the XAS beamline at the AS and Australian National Beamline Facility (ANBF) which continues to operate at the Photon Factory in Japan. This problem will be exacerbated to a critical status when the ANBF program finishes at the end of 2010 or by mid-2012 at the latest depending on pending grant applications. The proposed beamline will both maintain current levels of access once the ANBF ceases and greatly enhance Australia's capability and standing in producing world-class XAS research.

Expected Scientific Outcomes

Biological and medical sciences

Approximately 40% of the human proteome consists of metalloproteins. Commonly known metalloproteins include haemoglobin and myoglobin, which are iron-containing proteins that store and transport oxygen throughout the body. Understanding the molecular-scale structure, function and mechanism of such proteins is essential in determining their role in biochemistry and the origins of many diseases caused by protein dysfunction e.g. sickle-cell anaemia and the group of porphyria disorders. Using XAS, the structures of the active sites of metalloproteins can be determined at higher accuracy and precision and with less light-induced damage than can be determined by complementary protein crystallography and provide vital information in the investigation and treatment of a range of pathologies.

The energy range proposed for this beamline covers the absorption edges of most of the inorganic elements of interest to biology and medicine. The distribution of the lighter elements (S, P, Cl, Ca, K) and their chemical forms are crucial to understanding many biological processes, including diseases and their treatment. The oxidative stress in cells can be quantified by determining the chemical ratio of thiols and tholates - sulfur-containing molecules - and their distributions within cells are crucial in many biological samples. The same sulfur compounds are also implicated in the development of resistance responses to anti-cancer drugs. The chemical state and distribution of phosphorus is key to understanding energy production and storage, chromosome interactions as well as the structure and well-being of bone and teeth. Similarly, Cl is an essential component of a whole class of heavy-metal anti-cancer drugs (e.g. *cis*-platin). Understanding the release of Cl^{-} from these chemotherapy agents can be monitored as a function of time, space and environment, which is very important to resolving their biological activity. Finally, the Si K-edge XAS has the potential to provide unique insight into the structure and formation mechanisms of biominerals, an understanding of which has direct significance to more cost and energy effective manufacture of ceramics.

Thus, this new capability will greatly enhance the strength of Australian research that uses XAS to improve drug design, understand fundamental processes involved in diseases at the molecular level, and determine normal physiological processes in biology and medicine.

Environmental and earth sciences.

There are many fundamental aspects of these sciences that remain unaddressed owing to the lack of a beamline delivering the necessary energy range at the AS. Similar issues as those mentioned for biological samples can be investigated in environmental samples, *e.g.*, redox status and speciation from S K-edge, distributions and speciation of inorganic and organophosphate pollutants and their breakdown; speciation of organochlorine pollutants and their breakdown to inorganic Cl, etc. An example is the use of Cl K-edge XAS to study the fate of NaCl in coal in order to determine temperature thresholds for the formation of organochlorine species – highly undesirable by-products of coal combustion.

In soils and minerals, silicates, phosphates, sulfur and chloride ions are common and the absorption spectra of these ions are sensitive to the nature of the metal to which they are bound and the environment. When combined with the metal XAS on the same samples, superior speciation and spatial distributions will be possible than relying on a metal K-edge alone. Such information is invaluable to the study of plant growth, micro-nutrient transport and soil salination.

With controlled environment cells, information can also be obtained on speciation of complexes under hydrothermal conditions leading to a better understanding of how precious metals are transported and deposited in the earth's crust. An example is the use of S K-edge XAS characterization of acid sulfate soils. The S K-edge XAS will be used to identify reactive intermediates in reduced S sediments in order to characterize biotic versus abiotic reaction chemistry, as well as key chemical differences between different acid sulfate soil environments.

A fundamental understanding of all of the above problems will provide the information required for proper management and control of many significant environmental problems including soil acidity, salinity and the degradation of waterways due to pollutant run off. Improve mineral exploration and metal extraction practices will be developed and superior farming practices will result. All of these are of high economic and social significance to Australia and New Zealand.

Advanced materials

The target energy range of the medium-energy XAS beamline will open up numerous avenues of research in the field of advanced materials. Silicon is the backbone of the electronics industry and more exotic semiconductors such as indium phosphide are emerging for specialist applications. The ability to characterise these materials post modification reveals structural details such as the degree of crystallinity or amorphisation and strain forces in the material that impact directly on their performance and suitability for applications in electronic components.

Many emerging materials technologies such as amorphous and micro-crystalline materials, nano-particles and composite materials employ elements in the target range of this beamline. Silicon, in particular, also has multiple industrial and engineering applications. A better understanding of the structure of amorphous phases of Si and Si oxides is critical to the development of mass-production methodologies for solar cells – an area of technological development in which Australia is world-competitive and which has potential to significantly change Australia's energy source mix.

Cultural heritage and archaeology

Many pigments used in artworks and that are prevalent in archaeological artefacts contain metals as well as sulfurous, chloride and phosphate ions. XAS measurements of such items will assist greatly in the identification of pigments and their aging and weathering processes. Such studies, when related to historical records of the use of pigments, are important in establishing provenance and provide vital background information to support curatorial practices and restoration projects including dating of samples, and trade associated with the use of pigments. As such they are important in understanding many aspects of the development of civilization and the preservation of cultural heritage worldwide.

Potential User Community

There is already a thriving community using the XAS beamline of the Australian Synchrotron and the ANBF. In addition, the largest number of applications to the International Synchrotron Access Program for any technique is for XAS for applicants who have gained access at highly competitive international beamlines. With access to the ANBF ending in 2010 or at the latest mid-2012, there is a very large unmet demand drawn from all states in Australia, as well as New Zealand and other countries. Australasian leadership in this area is demonstrated by the large number of XAS experiments that gain access to highly competitive international beamlines. The current demand at the XAS beamlines does not cover the energy range of 1.8-5 keV and the importance of this region discussed above will increase the user base and range of experiments enormously.

Description of the Proposed Beamline

A common difficulty faced by researchers studying biological materials is photo-damage to the samples caused by the X-ray beam from the synchrotron. For this reason, a bending magnet beamline optimised for XAS over the desired energy range is well-suited to studies of materials containing elements particularly sensitive to photo-reduction.

The conceptual design of the medium energy XAS beamline will use lessons learned from similar designs worldwide for both the XAS capability and added KB-mirror X-ray microprobe capability, which will be readily interchangeable. The main design features are:

- Bending magnet source to reduce photo-damage and produce superior transmission data
- Microprobe mode with KB mirrors: spatial resolution of 1-2 μm
- Energy range of 1.8-14 keV (InSb 111, 1750 to 3750 keV and Si 111, up to Se edge).
- Cryo-capability for biological samples, both stages and He cryostat
- Ion chambers for transmission experiments and energy calibration; a four-element Si-drift detector (optimized for ~2-5 keV); ultimately a Si-drift Maia detector optimized for this energy range; and an electron-yield vacuum cell for measurements conducted under moderate vacuum conditions.

Furthermore, the micro-focus optics of the beamline form part of an integrated approach of complementary micro/nano probe capabilities described in this Development Plan to meet the demand for such high spatial resolution capabilities at the AS.

Australian Synchrotron

3.2 Phase 2 Beamlines

3.2.1 Advanced Diffraction and Scattering Beamline (ADS)

Introduction

The strong and growing community of scientists working in the field of materials engineering in Australia and New Zealand has not been particularly well serviced by the facilities currently available at the Australian Synchrotron. The biggest gap in support to science and development endeavours in this area is the provision of high energy X-rays, which are able to penetrate thick materials. An Advanced Diffraction & Scattering Beamline is proposed to fill this need, providing X-rays covering a wide energy range and featuring ancillary facilities to cater to applied, fundamental and industrial researchers from diverse backgrounds including materials science and engineering, earth sciences, chemistry and biology. This beamline will be highly complementary with the facilities at the OPAL Research Reactor at Lucas Heights and will eliminate the need for scientists to use overseas facilities for high energy diffraction experiments.

Expected Scientific Outcomes

The proposed Advanced Diffraction & Scattering (ADS) Beamline will be designed for analysis of bulk materials, optimised for real-world samples of relevance to industry including the automotive and aeronautical sectors. The science to be undertaken will have implications for energy production and storage, the environment, functional materials development and improvements to the mining and manufacturing sectors. It will compare well with beamlines at overseas synchrotron facilities such as ESRF (Grenoble, France), APS (Chicago, USA) and a planned beamline at NSLS-II (Brookhaven, USA). Apart from the opportunities presented to materials scientists and engineers, this beamline is likely to attract strong commercial interest, potentially greater than any existing beamline available at the Australian Synchrotron. Matched with a well experienced and growing user community, this beamline could provide significant social and economic gains for the community.

In many applications - particularly in the fields of engineering and materials processing - high-energy X-ray methods can be considered to be complementary to neutron-based experiments such as those now possible at the OPAL research reactor at ANSTO. Indeed, many of the Australian exponents of high-energy X-ray techniques are also users of OPAL and other neutron sources. This is because in spite of similar areas of application, the two types of techniques “see” very different things and extract different information from ostensibly similar experiments.

Both methods have the advantage of deep penetration and are therefore useful for bulk sampling of heavy and/or large samples or in-situ processes. There are however significant differences. For example, neutron beams are typically spatially large compared to synchrotron X-rays, leading to good spatial averaging. X-rays provide high spatial resolution, which is often very important for heterogeneous samples. Another key difference is that the brilliance of a synchrotron-based high-energy X-ray source enables much faster data collection rates than even the highest-flux neutron sources making accessible a time-domain that cannot be studied by neutrons. With the recent opening of the AS and OPAL, researchers in engineering and materials science have a unique opportunity to access these highly synergistic techniques.

Materials science and engineering

A wide range of problems in materials science, including many that are relevant to industrial processes and design, can be solved using a high-energy diffraction facility. An important example is research and development related to mixed ionic conductors, that is, the materials used in fuel cells, batteries, electrodes and sensors. Understanding the function of such materials requires the ability to study their behaviour under conditions encountered during fuel cell operation, including high humidity and moderate temperature (up to approximately 600°C), as water uptake is critical to the function of these materials. The ability to study these materials in situations that are relevant to their normal function requires cells with walls that are too thick for lower energy X-rays to penetrate. Therefore, it is not possible to perform this work on the existing powder diffraction beamline at the AS. However, solving these issues is critical to achieving significant and important advances in this area, such as the development of clean technologies.

For example, hydrogen storage is a pressing engineering and materials science issue, as the storage of hydrogen fuel is one of the prime barriers to the widespread use of hydrogen fuel cell powered vehicles. Hydrogen fuel cells could hold the key to achieving significant reductions in carbon output and solving the looming global energy crisis created by a shortage of fossil fuels combined with a rapidly growing population. However, the study of potential hydrogen storage materials requires the ability to place the sample in an environment of very high hydrogen pressure (up to 700 bar) and temperatures of around 600°C. This can only be done with high energy X-rays. Development of research capacity in this area in Australia is essential if we are to maintain leadership in the clean technology area on the global stage.

A further example of the application of high energy X-ray technology at a synchrotron is the study of thermal barrier coatings (TBC). These are thin coatings applied to components that are exposed to hot combustion gases within gas turbine and piston aircraft engines in order to thermally insulate the components. They are typically composed of a 0.3 mm layer of partially stabilised zirconia over a bond coat of 0.2 mm of a nickel-cobalt-chromium alloy applied to a metal substrate. While TBCs are widely used, their lifetime cannot be reliably predicted, resulting in costly failures that cause significant disruptions and loss of income. The ability to predict TBC lifetimes would enable a greater utilisation of these materials in diverse applications. However, this requires a detailed understanding of their failure mechanism. In research being undertaken by scientists from the Defence Science & Technology Organisation (DSTO) at overseas facilities, the use of high energy X-rays has allowed the mapping of phase composition, texture and structure. Observation of out-of-plane tensile strains has suggested a proposed mechanism of TBC failure based on localised swelling of the material underlying the zirconia.

Low density, high specific strength, high oxidation resistance and good creep properties at elevated temperatures make γ-TiAl based alloys excellent candidates as structural materials for advanced jet and automotive engines as well as future hypersonic vehicles. The mechanical properties depend strongly on composition, thermo-mechanical processing and subsequent heat treatment. While the processes occurring during heat treatment are complex and difficult to study directly, high energy X-rays can penetrate centimetres into light and medium density materials as studied here. Encouraging results have been obtained by a group of ANSTO researchers working at the ESRF, characterising *in-situ* phase transitions, recrystallisation behaviour and phase evolution in an intermetallic alloy up to 1400°C. It would be of great benefit to be able to carry out work like this in Australia and once again, the industrial applications of such work would be extensive.

Chemistry

Intense high energy X-rays provide sufficient transmission and diffraction intensities to directly measure the rates of chemical reactions. Using time-resolved diffraction, optimisation of novel material synthesis has been demonstrated in a non-destructive manner. This has led to significant reductions in the cost of developing novel materials, allowed for improvement of the efficiency of industrial processes and provided direct observation of previously unknown phenomena. Therefore, this technique has added to both the development of both basic and applied scientific research. Until now, research in this area has relied on neutron diffraction, as it provides sufficient penetration of samples and ancillary equipment to allow routine measurement of reaction kinetics. However, the proposed synchrotron beamline X-rays will have several distinct advantages over the available technology, such as the ability to achieve greater spatial resolution and chemical selectivity using absorption edge contrast.

Other applications

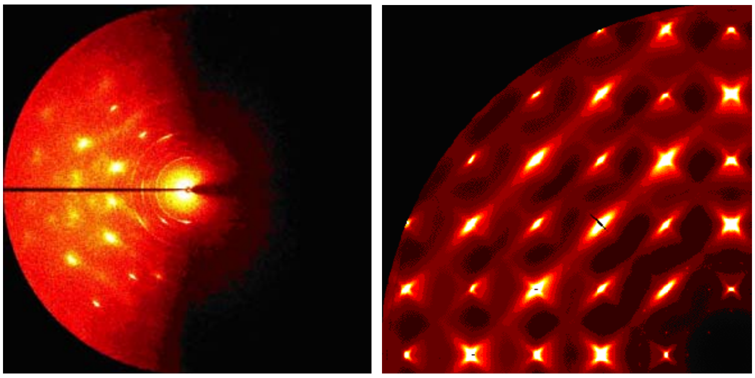


Figure 3.6 Diffraction data of ferroelectric material known as PZN-PT collected with 25 keV X-rays

The proposed Advanced Diffraction & Scattering beamline has a significant level of versatility that will enable a broad range of potential applications. For example, in addition to the case studies provided above, this beamline will have applications in structural biology, where the radiation damage generated during synchrotron experiments can cause experiments to fail and significantly hinder research advances. Early research indicates that high energy X-rays could potentially solve this problem facilitating significant progress in these areas. Other materials science applications include structural studies of ferroelectric materials with piezoelectric properties that are promising candidates for the next generation of solid-state actuators and transducers. Conventional crystallography often cannot give structural details about the small local deviations that can give these materials their unique properties. Therefore, this beamline will facilitate significant advances in this area.

Potential User Community

There is strong demand for the techniques that would be enabled by the ADS beamline. This would include current users of the powder diffraction beamline currently available at the Australian Synchrotron. The ADS beamline would support them to extend their work to take advantage of the unique properties of a high energy X-ray source. However, it would also open the Australian Synchrotron to a new community of potential users, who currently access similar resources at OPAL or are forced to use overseas synchrotrons to meet their needs in engineering and materials science. Many of the potential users are employed by Government-funded organisations such as ANSTO, DSTO and CSIRO as well as universities in the region.

It is also expected that this beamline would attract strong interest from industry, given its application to a wide range of applications. Comparable overseas facilities have seen strong use from the commercial manufacturing and engineering sectors, as has been found for example at ID-15 at ESRF which has generated commercial income averaging €75k per year over the past decade.

Description of the Proposed Beamline

The main conceptual design aspects of the ADS beamline are high energy, flexible sample environment for industrial and engineering samples and the ability to provide either monochromatic or polychromatic radiation. Such a design will present challenges such as dealing with high heat loads; however, these have already been faced with the Imaging and Medical Beamline. Experience gained in implementing that beamline will be very useful. The following features will be included:

- Superconducting multipole wiggler, to provide X-rays of energy 30-120 keV
- Monochromatic radiation using large area detectors for ultrafast powder diffraction, PDF analysis, single crystal studies and rapid texture analysis/2D materials mapping
- Polychromatic radiation for energy dispersive and Laue diffraction studies
- Spot size of 20 x 100 µm
- 2D detector such as Pilatus for rapid, real-time data acquisition
- High resolution energy-resolving detector system for energy-dispersive diffraction studies
- Variety of sample stages and sample environment ancillaries for *in-situ* experimentation

3.2.2 Small Angle Scattering Beamline for Structural Biology (SSB)

Introduction

Small angle X-ray scattering (SAXS) has become an important method for understanding proteins and their interactions and therefore developing a better understanding of many fundamental biological processes. This knowledge has profound and wide-ranging implications for public health, disease diagnosis and treatment and vaccine development. The Small Angle Scattering Beamline for Structural Biology (SSB) couples sophisticated sample handling infrastructure and an instrument highly optimised for measuring biological macromolecules. The beamline will be aimed at the life science and biotechnology community and will complement the current SAXS/WAXS and macromolecular crystallography beamlines. Biological samples currently comprise around 50% of the total use of the existing, more general purpose SAXS beamline at the AS and the need for SAXS in the life sciences community is growing rapidly. A high performance, dedicated beamline with a high level of automation will enable applications and outcomes far beyond what is possible with existing facilities.

Expected Scientific Outcomes

The proposed SAXS beamline will have the greatest impact in the field of structural biology, that is, the study of the structure of the larger molecules involved in the critical functions of human cells, such as proteins and the nucleic acids that compose the genetic material within cells. Traditionally, structural biology has involved the solution of a high-resolution structure of a protein or nucleic acid sample by crystallography or NMR spectroscopy. Both of these methods require relatively large amounts of purified protein. To be amenable to analysis by NMR spectroscopy requires a sample that will deliver well dispersed peaks in a two-dimensional NMR experiment. In a protein crystallography experiment, the sample must form diffracting crystals to provide usable data. However, the process by which proteins are purified and crystallised is highly demanding, and it is not always possible to produce sufficient samples in terms of quality or quantity. Moreover, current trends in structural biology are towards more challenging protein targets such as membrane proteins and large complexes, which are notoriously difficult to purify for such analysis. For this reason, there are a large number of important proteins, including many that are known to be involved in disease processes that have remained intractable to analysis by these methods. The ability to elucidate the structure of these proteins could rapidly accelerate the study of the biological processes and diseases in which they are involved and potentially lead to rapid advances in health and medical research and development.

The need for the proposed SAXS beamline has been further heightened by an emerging imperative to construct a far broader picture of protein structure and function. Important problems now faced often require developing an understanding of the structure of biological molecules that exist in the form of large aggregates, changes in molecular shape and the study of other dynamic behaviour. Such work is nearly impossible with existing technology, and what progress has been made has required significant levels of supposition, rather than firm experimental evidence. Successful experiments in this area have a high level of novelty and the potential to make significant breakthroughs in a broad range of research areas. This will lead to high impact publications and ultimately to a far more profound understanding of biology. Some specific examples of relevance to the research context in Australian and New Zealand are given below.

Life Sciences

Examples of disease processes that are currently being studied using SAXS in Australia include assembly of proteins central to HIV infection, formation of amyloid plaques in Alzheimer's disease, degradation of collagen in arthritis, antigen/antibody interactions during pathogenic infection and emergence of antibiotic resistance in bacterial diseases.

The design of new drugs to help overcome significant public health issues such as antibiotic resistance is one important area that will benefit from the proposed beamline. In recent years, Monash University scientists have used SAXS in combination with crystallography to characterise medically important protein and nucleic-acid samples. One such example is the Biotin Protein Ligase protein from *Staphylococcus aureus* (SaBPL). Antibiotic resistance is a serious problem to human health and *S. aureus* is one of the most problematic pathogens that has developed resistance to front line antibiotics leading to severe disease states and even death. SaBPL is an attractive target for antibiotic drug design and the SAXS method has played an important role in directing efforts to develop these proteins as drug targets.

The use of SAXS analysis has also had proven success in the study of complex proteins. For example, Retromer is a protein complex that associates with membranes and which, in mammals, plays a critical role in a broad range of developmental and pathological processes. It exists as a complex with three different proteins forming a trimeric core, with a dimer of proteins that help it associate with the membrane. Knowledge of the structural and biochemical characteristics of Retromer is crucial to understanding a variety of processes within the secretory and endocytic systems of the human cell, but it is very difficult to study. The proposed SSB beamline would play an important role in this study.

Potential User Community

The potential users of the beamline will be:

- Structural biology and biochemistry groups that produce soluble protein samples for crystallography, NMR or functional assays. There are several dozen of these laboratories in Australia and New Zealand, in every major university as well as numerous high-profile research institutions such as the Walter and Elisa Hall Institute, bio21, the Peter MacCallum Cancer Centre or the Maurice Wilkins Centre for Molecular Biodiscovery.
- Biotech clients such as Biota, Avexa and CSIRO taking advantage of the ease of setup, reliability and high degree of automation for commercial research and development.

The beamline will give information about sample quality as well as structural information. There will be several access modes for users such as provision for remote access and potentially rapid access modes and sample queuing systems. Some access may also be awarded in block to centralised facilities such as crystallization and proteomics facilities and this will further increase the user base.

The user group of the existing SAXS/WAXS beamline has been steadily increasing and is oversubscribed by more than 200% in the first cycle of 2010. Around 50% of the users of the

SAXS/WAXS beamline are from the life science community and it is estimated that 80-90% of these experiments will be suitable for the proposed SSB beamline. Moving between biological and material science samples is a significant source of dead time on the existing SAXS/WAXS beamline and dedicating the SSB beamline to biological samples will reduce dead time and increase the productivity of both the SSB and SAXS/WAXS beamlines.

Description of the Proposed Beamline

The conceptual design of the SSB Beamline will utilise the numerous developments made on the Australian SAXS/WAXS Beamline and other recent designs worldwide. The beamline will be highly optimised for solution analysis of biological molecules over a wide size range, supporting analysis of ultra-weakly scattering samples, fast time-resolved analysis, on-line complementary techniques such as spectroscopy, chromatography and light scattering analysis, and emerging technologies such as microfluidics.

The sample environment of the SSB beamline is designed to optimise not just throughput but output of publication quality data. The beamline will include an integrated high-pressure liquid chromatography system that will be used to deliver the samples. This will allow samples to go through a final purification step directly before analysis and to be characterised prior to measurement and will allow the beamline to be highly automated. The HPLC will automatically load samples which then run through an analytical size exclusion column to separate the desired sample from unwanted aggregate. The sample will go through several analytical techniques to give crucial information on sample concentration, molecular weight and size in solution, before the sample is delivered into a capillary for SAXS measurement. Measuring sample parameters in-line with SAXS will remove uncertainties of data quality and provide cross-validation.

Automated validation and normalisation of SAXS data will allow automation of data analysis to an extent that has not previously been possible. This longer-term goal will involve working together with the molecular modelling and high-performance computing communities and create opportunities for new science throughout the lifetime of the beamline.

As well as being a primary method in structural biology the beamline will also drive development in protein crystallography by characterising the process of protein crystallisation, a major bottleneck in protein crystallography. The SSB beamline will be used by laboratories and national protein-crystallisation facilities to quantify parameters such as the compactness of proteins, their oligomeric state, monodispersity and aggregation as a tool to direct buffer optimisation.

The main design features are:

- An optical design optimised for solution scattering using a double multilayer monochromator and KB mirror system for advanced low-angle performance and extreme peak flux levels
- A world-leading instrument background intensity function through the design of the collimation system, lack of vacuum windows, in-vacuum sample cell, and noise-free diagnostics/control detectors
- A specialised endstation featuring automated sample handling, rapid camera length change capacity such as a SAXS camera with in-vacuum detector, online complementary

chromatography, spectroscopy and light scattering instrumentation, and automated data processing

- *q*-range from 0.001 to 2 $Å^{-1}$
- Large-area solid-state photon-counting detector (e.g. Pilatus 2M)
- In-vacuum undulator insertion device
- 8-15 keV energy range optimised for 12 keV, typically fixed energy operation

3.2.3 Micro-Computed Tomography Beamline (MCT)

Introduction

Micro-computed tomography (micro-CT) opens a window on the three-dimensional structure of a wide range of samples at the microscopic scale. This technology is relevant to a wide range of research, including life sciences, materials engineering, palaeontology and geology. The technique can reveal the detailed internal structure of delicate samples such as fossils in an incredibly detailed way without causing any damage to the samples. Australian palaeontologists are already making significant scientific breakthroughs on overseas synchrotrons using micro-CT to study fossils, allowing the reconstruction of soft tissues and growth patterns with accuracy never before realised, giving an unprecedented understanding of fossils and the evolutionary process. A host of other examples demonstrate the power of micro-CT for delivering outstanding scientific outcomes. These range from minerals discovery and extraction to the effects of medication on bone health and understanding tooth decay. The proposed expansion of the Australian Synchrotron to include a micro-CT beamline will complement the existing Imaging and Medical Beamline and cater for the existing and potential demand for access to this important method in addition to building increased expertise and capacity in Australia in this crucial area of scientific endeavour.

Expected Scientific Outcomes

Micro-CT measurements lead to three-dimensional (3D) images of the internal structure of samples (Figure 3.7). Scientists who are familiar with laboratory-based micro-CT are now turning to synchrotron micro-CT to enable research that requires high throughput, higher resolution images, the ability to use phase-contrast, techniques that give chemical information and high-speed data collection. This provides 3D observations of processes occurring in real time. The range of applications for this technology is extremely broad.

Biological and health sciences

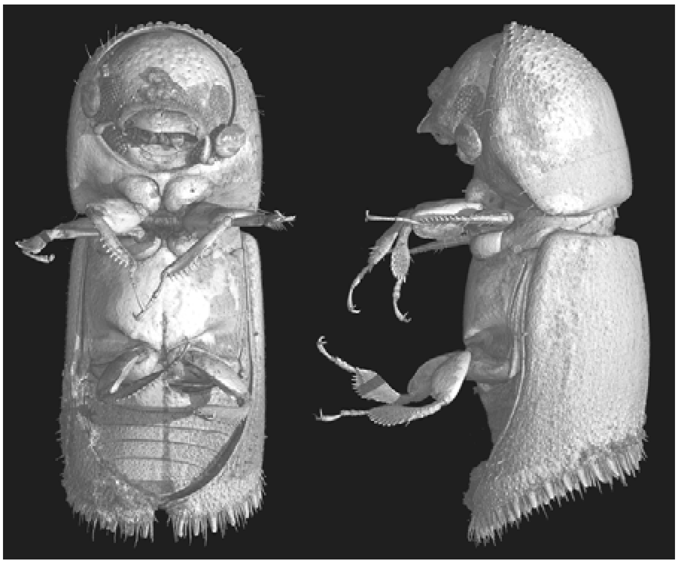


Figure 3.7 Miocene insect fossilised in opaque amber from Cape York (Paul Tafforeau, ESRF, Susan Hand, UNSW)

As the Australian population ages, bone diseases that largely afflict elderly patients, such as osteoporosis, are becoming increasingly important. Such health issues create a significant social and economic burden through the reduced mobility of the patient and as a result increased costs to the health system. To better understand and combat the fractures associated with osteoporosis, it is vital that a more complete understanding of the differences in bone architecture that exist between healthy adults and the elderly who are at risk of fracture is developed. Current research generally utilises clinical CT; however, this imaging technology cannot resolve the detail of internal pore structure of bones. This is problematic, as studying the processes that underlie bone formation and degeneration are crucial in increasing our understanding of osteoporosis and therefore developing new therapies and improving clinical practice. For a group working at the University of Melbourne, high-throughput synchrotron-CT can provide radically new information about these very functions in a relatively short period of time. This enables characterisation of age-dependent changes in bone architecture in the thigh bone and helps to unravel the relation of these changes to hip fracture. This could provide unparalleled insight into the processes underlying this prevalent disease of the elderly.

A related and highly significant health issue is the negative side-effects of medications that are currently used to treat epilepsy on bone growth and health. These side-effects cause significant problems for patients who take them that can endure throughout their lifetime. Once again, the cost of this issue is not just to the individuals afflicted with this disease, but the health system and society more broadly, in particular as the burden of this disease often peaks at a younger age. A number of researchers around Australia are using animal models to assess the effect of various medications on bone health. Micro-CT is one promising way to assess these effects accurately and, moreover, to determine ways to overcome these issues. Synchrotron studies would enable micro-CT of a large number of similar samples enabling researchers to amass high quality data at a level that provides statistically significant information to be obtained. Such studies could ultimately lead to better treatment regimes and result in improved quality of life for patients with chronic conditions.

Stem cells offer the potential for radical improvements for the treatment of disease by helping to stimulate the repair of damage to the human body. This includes healing of damage to the spinal cord, regeneration of lung cells and replacement or repair of parts of the human heart. Each of these therapeutic improvements offer hope to patients who currently face debilitating or life-threatening illness. One significant limitation of the development of stem cell technology for medical applications is the difficult process of locating and targeting stem cells. Locating stem cells within the body is a difficult task and reliable, non-invasive techniques for stem cell recovery are essential to fully achieving the full potential of stem cell technology. Synchrotron-CT offers this potential, which will be of great value to stem cell researchers such as the world-leading team at Monash Immunology and Stem Cell Laboratories and Monash Institute for Medical Research.

There are also several important implications for the use of synchrotron-CT to improve dental health – this is rapidly emerging as a key area of health and medical research. Tooth decay can lead to significant health problems, in particular if left untreated. This is a significant health challenge in developing countries and even in lower socio-economic areas of developed countries. Understanding the progression of demineralisation in tooth decay is of great importance if the goal of developing non-invasive treatments that can reverse the disease process is to be attained. The provision of synchrotron-CT at the AS will allow accurate mapping of the changes in the mineral density of teeth in three dimensions, which would significantly progress our knowledge of the tooth decay process and help with the development of a means of reversing it. The microstructure of teeth is also of importance in determination of age at death, which is essential to help identify deceased individuals, particularly under tragic circumstances such as war or an explosion. Existing methods require the preparation of thin sections and are known to be inaccurate or provide limited information that is insufficient to advance research in this area. These problems will be eliminated by the availability of synchrotron-CT.

Earth sciences

Micro-CT data is valuable in the fields of geosciences associated with minerals exploration and mining. For example, understanding the mechanical behaviour of materials under stress, the detection of fracture and clarification of pore saturation are all of practical importance in geophysics, civil engineering and geo-environmental sciences. Micro-CT and numerical simulations work hand-in-hand to allow scientists to understand and predict flow and diffusion, elastic wave propagation and many related processes. Related work includes imaging of fluid deposits and their spatial distribution within minerals such as calcite and quartz, real-time studies of thermal expansion and fluid-rock interactions in granites and studies of the 3-dimensional morphology of magmatic sulfides. Such work is expected to have a significant impact on oil and gas exploration and production, mineral ore grade identification and processing, subsurface pollutant transport and mitigation as well as underground storage and monitoring of CO_2.

Palaeontology

Dramatic results of 3-dimensional images of insects in amber with extraordinary detail have already been demonstrated by Australian scientists working at overseas synchrotrons (Figure 3.7). Study of translucent samples of amber indicates that 20% have multiple inclusions such as insects, spiders, feathers, hair, plants and fungi. Many of the samples are, however, opaque and cannot be studied using optical microscopy methods in Australia. Propagation-based micro-CT carried out at the European Synchrotron Radiation Facility (Grenoble, France) has revealed high quality preservation of these fossils and has provided vastly more detailed biological data on these specimens. In many cases this has created a unique gain to the fossil record, elaborating the evolutionary process and helping us to understand the biological history of modern day species.

The ability of micro-CT to reveal complex internal structure in a non-destructive manner (“virtual dissection”) is of great benefit for rare and fragile samples, such as the skulls of extinct leaf-nosed bats discovered in Oligocene and Miocene deposits in Riversleigh (north western Queensland). Such bats emit ultrasound to aid in hunting prey, and the internal structure and function of the narial chamber they use to achieve this is poorly understood even in modern bats. Micro-CT offers a unique opportunity to examine how the bats modulate sound, and could offer new insight into how animals have evolved innovative ways to use sound to better interpret their environments and compete more effectively for resources. Similarly, because of the unique ability of CT to image cavities, it can reveal details of the brain cavity, sinuses and the paths of vessels and nerves in fossils without destroying the fossil.

Teeth and jaws of fossils are an excellent source of insight into morphology and function in mammals, such as jaw and teeth movement during feeding. High resolution 3D reconstructions of teeth and jaws can also shed light on the evolutionary development of animals and have for example been used for palaeodietary reconstruction of Pleistocene mammals. This is not only an exciting technological and scientific advance, but an opportunity to generate excitement and interest in this area of research that helps drive the creation of a new generation of researchers in Australia.

Materials science

Examples of the usefulness of synchrotron-CT in the materials sciences abound. In particular, this technique is well suited to porous materials, and the detection and study of cracking and fractures. An important example of how this might be used is the study of corrosion in aluminium alloys used in aircraft and marine platforms. High-throughput micro-CT at the synchrotron would greatly facilitate the study of initiation and propagation of corrosion with respect to time and environmental factors, with implications for improved safety in air transport. Other examples of materials science enabled by this method include studies of wood microstructure, loading and wear of dental materials, fluid flow and distribution in microporous materials and particulate pharmaceuticals in tissues and airway surface layers.

Potential User Community

The potential user community for synchrotron micro-CT consists of a mixture of experienced scientists who already make use of overseas micro-CT beamlines and a growing number of scientists who have added micro-CT to their suite of characterisation tools and are finding that they have applications that cannot be satisfactorily carried out in the lab. Experience at overseas synchrotrons clearly indicates that micro-CT in all its forms is a rapidly growing area of activity worldwide.

Two well-attended national workshops have been held for micro-CT scientists in the past two years and over 90 scientists have expressed an interest in this proposal, indicating that there would be strong demand initially for this new capability and very large growth potential.

This area clearly has extensive application in the industrial arena – in particular in mining, defence and manufacturing, which aligns well with Australia's industrial assets.

Description of the Proposed Beamline

The beamline is envisaged to provide a complementary set of capabilities to the high energy, larger field-of-view capabilities of the Imaging and Medical Beamline, which is the only other beamline capable of full-field CT at the Australian Synchrotron. It will focus on applications requiring higher resolution and lower X-ray energies and will be particularly targeted at high-throughput and dynamic micro-CT applications.

Major design features include:

- Bending magnet or wavelength shifter source
- Energy range of 8-40 keV
- Capability for white/pink beam, high bandwidth quasi-monochromatic beam (multilayer mirror monochromator) and highly monochromatic beam (Si monochromator)
- Possibly located adjacent to IM beamline to take advantage of complementarity
- Collection times as short as sub-second using broad bandwidth beam
- Automated sample exchange

3.3 Phase 3 Beamlines

3.3.1 Soft X-ray Materials Science Beamline (SXM)

Introduction

'Soft' X-rays are low-energy X-rays that have limited penetration in materials and are particularly suited to studies of surfaces and light elements. In order to complement the current world-class soft X-ray beamline the development of a suite of capabilities in the soft X-ray field focussing on 'environmental' studies (eliminating the need for samples to be under ultra-high vacuum), full-field imaging (eliminating the need to scan the beam across the sample) and the potential for future development of an advanced imaging facility that combines X-ray imaging with scanning probe microscopy is proposed.

The proposed beamline has broad application in the development of new materials, plant science, minerals processing and environmental science to name a few.

Expected Scientific Outcomes

The main advantage of the proposed facility is the ability to image samples with high contrast even if they do not contain heavy elements, giving it very broad applicability. A small subset is described below.

Materials and Energy Science

The development of organic photovoltaic (OPV) technology offers the prospect of inexpensive and flexible solar cells that can be fabricated over large areas. Such cells could be used on roofs or walls of buildings where current technologies cannot be used resulting in wastage of space that could be ideal for capture of UV energy. The performance of these materials is critically dependent on the nanoscale design or morphology of the polymer blends used in their construction. The microscopy techniques available on the proposed beamline would provide sufficient contrast for this purpose at the required resolution – something that is not possible with any other technology.

Further examples of the use of this beamline in the development of clean energy solutions abound. One of these, relating to the production of hydrogen by splitting water using the visible portion of the sun's radiation to provide sustainable, carbon-neutral green power in a convenient form for transport applications. This process requires a catalyst based on semiconductor nanoparticles captured within the pores of mesoporous materials. Imaging of the supported materials using the proposed beamline would provide essential data to enhance the information produced by electron microscopic studies and definitively establish the distribution of the nanoparticles in the mesoporous supports. This is critical in effectively characterising these materials to support commercial development and manufacture.

Mineral processing invariably begins with the grinding of ores. This creates fracture surfaces which may be dominated by internal, reacted layers and films at the interfaces between dissimilar phases, particularly where the ore contains a range of mineral types. Strategies for improving mineral processing practices can be improved with the help of imaging data giving the nature of these interlayers.

Plant Sciences

The proposed beamline will provide combined data of the chemistry and ultra-structure leading to a better understanding of the uptake and metabolism of toxic and nutrient metals in the environment. Some plants can accumulate extremely high concentrations of trace metals (hyperaccumulation) in specific cells (e.g. nickel in epidermis cells, manganese in mesophyll cells). The proposed beamline will allow the investigation of localisation of target elements with high spatial resolution, giving insight into the physiological mechanisms of heavy metal tolerance and hyperaccumulation in plants.

Safeguarding Australia

The development of safe, non-intrusive, rapid, portable and cost-effective sensing equipment that is more sensitive and selective for detecting traces of concealed explosives and narcotics would greatly enhance the 'dual-tasking' capability of law enforcers in controlling security (i.e. protection against threat of terrorism) and preventing drug trafficking at entrance portals and other domestic situations such as in buses, trains, buildings. Molecular imprinted polymers (MIPs) are stable, robust, re-usable and can be generated, in principle, for any type of target and, thus, have significant advantages over the widely used biosensors. The new beamline would provide the ability to characterise these polymer blends on the nanometre length scale.

Potential User Community

A large and growing community of scientists using soft X-ray techniques exists in Australia and New Zealand, working across the full range of science and technology disciplines. The area of greatest need identified by this community is the ability to provide quantitative chemical maps of surfaces with extremely high resolution. The proposed new beamline will meet this need. Further expansion of the community would occur with the ability to image samples under a range of pressure conditions, which would enable the expansion of soft X-ray techniques into the biological sciences.

Description of the Proposed Beamline

Further detailed development of the proposed beamline will be taking place. The concept is to construct:

- A bending magnet beamline to allow low energy spectroscopy, mid-energy X-ray absorption, environmental X-ray absorption spectroscopy and full-field imaging
- In a possible future development, to add an associated undulator beamline to focus on scanning transmission X-ray microscopy (STXM)

3.3.2 High Performance Macromolecular Crystallography Beamline (HMX)

Introduction

Macromolecular crystallography (MX) produces structures of proteins and protein complexes at the level of individual atoms. The current MX beamlines have been arguably the most productive of the current suite at the AS and have supported publications in very high impact journals. The MX beamlines are used extensively by a vibrant community of structural biologists and scientists in a number of related fields, such as immunology, cell biology and those studying specific disease processes. Of particular note is the use of the MX beamlines to undertake detailed analysis of specific proteins and their interaction with potential inhibitors, which is a critical step in drug development. This structure-based design of drugs is an area of outstanding achievement in Australia. Unfortunately, in many cases it is not possible to produce protein crystals of sufficient size and diffraction quality to use on conventional synchrotron beamlines. This prohibits utilisation of a rational drug design process for application in a number of areas where there is a significant burden of disease in the community, including chronic diseases such as diabetes and arthritis.

This proposal is to build a world's-best standard facility for solving the structures of very small and/or weakly diffracting macromolecular crystals, allowing research to be undertaken on smaller samples of lower quality. This could revolutionise this area of research in Australia, leading to medium and long term benefits that would have a direct impact on the community.

Expected Scientific Outcomes

This development plan includes the construction of a beamline designed to complement the current MX beamlines at the AS by offering a beam of particularly high intensity and an extremely small focus. This would enable science that cannot be currently performed at the AS, and for which users have to travel to overseas facilities.

Membrane protein/receptors

The proposed beamline would be particularly useful in advancing the study of proteins that are difficult to purify or have complex or changeable structures. For example, the HMX beamline could be used to study proteins that are located in or associated with membranes. Normally, such proteins present enormous challenges with respect to crystallisation and therefore structure determination. This is particularly true for receptors, which are present within membranes. Protein receptors are a crucial part of all cell signalling pathways, where dysfunction can lead to a range of diseases including many forms of cancer. Most membrane receptors exist as complexes of smaller proteins, called subunits, which can only be purified in very small quantities as microcrystals. These crystals cannot be studied on the current MX beamline available at the AS but could be analysed with the HMX.

A specific disease case study relates to Alzheimer's disease. This neurodegenerative disorder is characterised by the presence of extracellular amyloid plaques in the brain. In the quest for a cure for this condition, Australian scientists are studying precursor proteins that are responsible for the peptides that form the plaques and have been shown to be toxic to neurons. Only very small crystals of these targets have been produced, which are too small to study with the current AS beamlines.

Another example is the study of biological rotary motors. These are fascinating protein assemblies that are found in the body and which are inherently difficult to study due to their trans-membrane nature and size. Once again, facilitation of this study is critical as these structures are often implicated as the cause of diseases, such as heart disease. A high-brilliance microfocus beam, such as the HMX, allows scientists to expose only small parts of a crystal that might be better ordered than others. Currently Australian researchers from the Victor Chang Cardiac Research Institute have been forced to work at the Advanced Photon Source in the USA and the European Synchrotron Radiation Facility in France to undertake this work.

Virology

Viruses are responsible for a wide range of diseases in humans and other animals, ranging from the common cold to ebola, AIDS and even some types of cancer. Aspects of viral structure and behaviour have been studied using crystallography, but this normally involves small, weakly diffracting crystals which could be studied using the proposed beamline. For example, insect viruses can remain active for years in the environment using a type of armour formed of crystals called viral occlusion bodies. Understanding these bodies would have important implications for the development of new bio-insecticides and vaccines.

A wide range of other applications exists in the life sciences, and this need is increasing as scientists turn to the more challenging but potentially more significant health problems that this beamline will make possible.

Materials science

Scientists working in other fields will also find that this beamline could also be of great utility. A wide range of materials only form incredibly small crystals that cannot be studied using existing beamlines. Examples include microporous and mesoporous materials, hydrogen storage materials, novel metal oxides and ceramics, superconductors, minerals, 'smart' materials, piezoelectric materials, novel magnetic materials, photonic devices, information storage materials, molecular switches and sensors, biomimetic materials and pharmaceutical materials.

Potential User Community

It is anticipated that virtually all of the structural biology community in Australia and New Zealand, who are currently users of the existing macromolecular crystallography beamlines, would have applications for the HMX beamline. A large number of chemists and engineers who have a need to study small crystals of a range of materials can be added to this community.

Given the experience with the existing macromolecular crystallography beamlines, it would be an obvious choice to include remote access for this beamline. It would also be an ideal candidate for a "mail-in" service for users with small numbers of difficult samples. These would be run by AS staff and the results returned to the users, eliminating the need for travel of users to the facility and improving efficiency and throughput.

Description of the Proposed Beamline

- In-vacuum undulator source
- Microfocus using Kirkpatrick-Baez (KB) mirror pairs

- Beam size of 1x1 µm
- Pixel array detector (such as Pilatus 6M)
- Robotic sample changer
- Remote access capabilities
- Endstation designed for optimal thermal and vibration stability

3.3.3 Advanced Infrared Beamline (AIR)

Introduction

Infrared (IR) spectroscopy is a technique that is familiar to chemists and biologists, providing detailed information about the chemical nature of samples. Synchrotron IR spectroscopy offers significant advantages over laboratory-based IR techniques, particularly for imaging with high spatial resolution and very small samples. IR spectroscopy is already well established at the AS, with two beamlines operating in parallel. The Advanced Infrared (AIR) beamline will be a novel design, adding new capabilities including rapid time-resolved spectroscopy, new modes of imaging and spectroscopy under extreme conditions.

Expected scientific outcomes

The concept of the beamline is to make advances at the cutting edge of synchrotron infrared spectroscopy and provide a resource with unique capability. A major strength of the current IR microscopy beamline at the AS is the ability to record spectra at a single point with high resolution. To record high spatial resolution images with a high signal-to-noise ratio, which is a major desire of the majority of users, the sample must be scanned below the finely focussed beam. For even small samples this takes many hours. Instruments that operate in two dimensions however, such as IR focal plane array (FPA) imaging instruments can produce images in minutes.

An ability to rapidly identify and monitor disease before the onset of physical symptoms would be a major advance, and this is one of the strengths of IR spectroscopy.

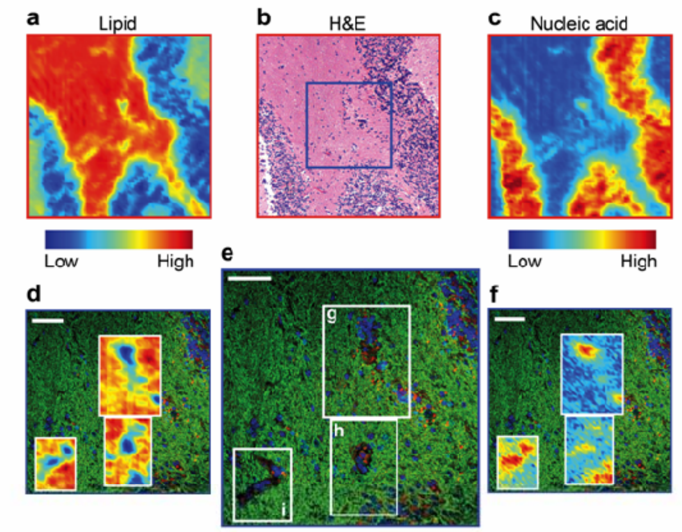


Figure 3.8 FPA images of small sections of brain tissue. With the synchrotron IR beamline lesions that are likely indicators of early onset of EAE can be discerned

A case study where this beamline would provide immense benefit is the location of early stages of Experimental Autoimmune Encephalomyelitis **(**EAE), an animal model of Multiple Sclerosis (MS – see Figure 3.8). With a rapid imaging system, full-scale maps could be obtained at the highest possible spatial resolution and microlesions could be rapidly located.

The same advantages apply in many other fields that require imaging to locate and identify and characterize micro-regions within complex matrices. Such fields include geology, forensics, semiconductors, polymers, materials science, cultural heritage and pharmaceuticals.

Potential User Community

The infrared community in Australian and New Zealand is widespread and committed to the present beamlines. There are many research problems that arise, however, that require facilities and techniques well beyond those currently available. This proposal will provide a beamline that will be driven by the community to provide cutting edge facilities. In addition to the community currently using the IR beamlines at the AS, a very large potential group of users exists around the country, as users of conventional IR spectroscopy become aware of the enormous increase in capability offered by the synchrotron beamlines.

Description of the Proposed Beamline

A second extraction port for IR already exists at the AS and it is envisaged that the same extraction optics that have been highly successful in the current IR beamlines will be employed on the new beamline. Two highly credentialed IR beamline scientists (Paul Dumas, Soleil; and Ulrich Schade, BESSY II) have assessed the feasibility of the ideas and availability of components for the proposed design, and are confident that it can be built successfully. The major design features are:

- Rapid imaging at high lateral resolution
- Near field spectroscopy (thermal and scattering AFM probes)
- Dispersive detection with linear and/or 2D array detectors.
- Long working length objectives for custom made experimental apparatus (high pressure cells, high temperature cells, cryostat cells)
- Pump-probe capabilities using a UV source
- Time resolved IR spectroscopy

3.3.4 Correlative Microscopy Beamline (CMB)

Introduction

The correlative microscopy beamline is a novel beamline, which combines X-ray, infrared and confocal fluorescence microscopy, aimed at the simultaneous measurement of sample properties using the three different techniques. Each adds important information, and when combined, this analysis could provide a powerful tool suited to a diverse range of user communities including biomedical, forensic science, materials science, nanofabrication and others.

Expected scientific outcomes

The proposed CMB beamline represents a new concept for a synchrotron facility. Therefore, many of the applications are yet to be envisaged. However, there is considerable advantage for the biomedical research community, where imaging of a single cell by transmission X-ray microscopy will be possible (Figure 3.9). This will allow the detailed study of individual cells without the need for fixatives or dyes, which can cause damage to cellular structures or create artefactual results as a result of the preservation process. When combined with infrared spectroscopic analysis, which will provide further data such as the secondary structure of proteins or the extent of saturation in lipids, this will be a powerful technology that could provide significant advances in health and medical research. The addition of the third technique of confocal microscopy would span the spatial resolution of the other two techniques, and add further information through use of imaging tools such as fluorescence.

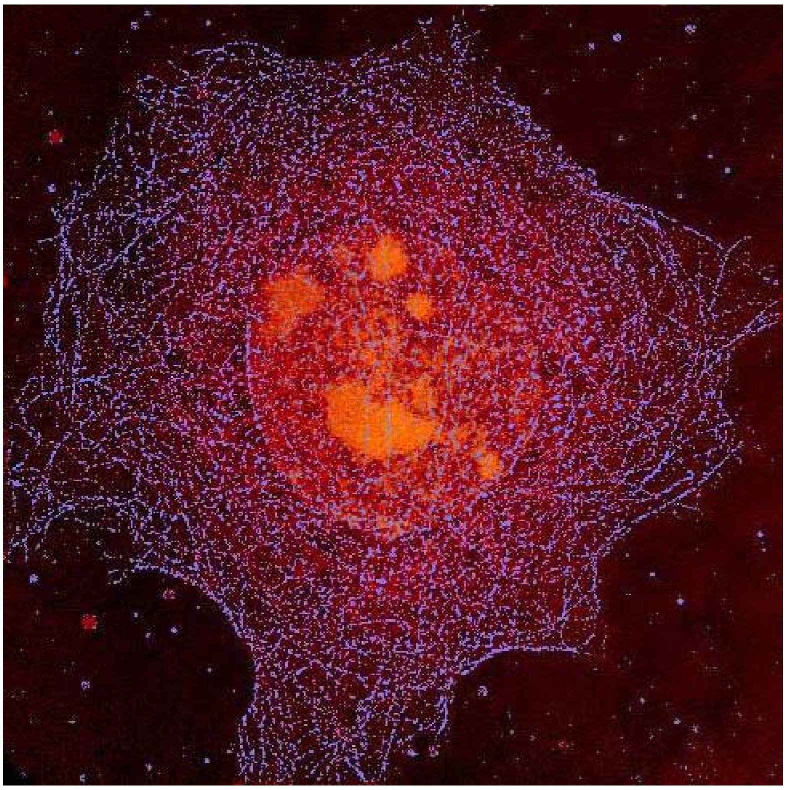


Figure 3.9 Transmission X-ray microscopy image of a whole, hydrated mouse mammary epithelial cell. The cell nucleus containing several nucleoli (orange) is in the centre of the cell.

Biomedical sciences

Another area of application for the proposed CMB beamline is regenerative medicine. This is a relatively new field of medicine, which aims to accelerate natural healing processes, or use special materials to regrow missing or damaged tissue. This would have significant applications in repairing damage caused by inherited diseases such as cystic fibrosis or congenital heart disease, as well as repairing acquired injuries such as trauma to the brain or spinal cord. For example, a specific cell type known as human amnion epithelial cells (hAEC) has attracted attention in recent years as a source of cells for such regenerative therapy. These cells share many characteristics with stem cells, in that they differentiate into different and highly specialised cell types, such as liver, pancreas, bone, fat and neural and glial cells. If these cells are derived from the person requiring the therapy (the host), they will have similar markings to other cells in the host, which will help minimise the effect of immune rejection. This is a significant limitation of many forms of stem cell therapy and other transplant-based cell therapies. Another benefit of amnion cells is that they do not require the sacrifice of embryos, as the amnion is usually discarded as medical waste along with the placenta following birth. The methods offered by this beamline would shed light on the process of differentiation of hAECs towards functional cells. Detailed study of living amnion cells individually and within living host tissue is essential to realising these potential regenerative therapies. Such study would be vastly improved by the use of the CMB beamline.

Such research would have application to a number of neurodegenerative diseases, including Huntington's disease (HD). HD is an incurable late-onset neurodegenerative disorder that affects approximately 1 in 10,000 individuals worldwide. Symptoms of the disease include uncontrolled movements and severe psychiatric problems including depression. HD ultimately results in death 10-15 years after onset. The genetic cause of HD results in expression of a mutant protein that accumulates in cells and progressively aggregates. Whether the aggregates are a cause or consequence of the disease is not known, but they are widespread throughout many tissues. This beamline will help scientists to observe the formation and nature of these aggregates, and in particular study their interaction with neurons in the region of the brain where the effect of the illness is first observed. Such research would be facilitated by the CMB beamline in a way that cannot be achieved using current techniques.

Environmental sciences

Coccolithophores are marine single-cell algae which, though tiny, can form vast blooms in the ocean. They form a fundamental part of the global carbon cycle in many ways. Notable for the intricate calcite structures which surround each cell, they represent the largest class of calcifying organisms on the planet. The formation of these cells is important for sedimentation of organic carbon in clouds known as "marine snow", and this understanding can be obtained using the microscopy techniques of the proposed CMB.

Many other applications exist, such as the imaging of nanostructures which are important in the field of materials science, analysis of small forensic samples, large proteins and their aggregates and many more.

Potential User Community

The initial user community for this beamline would be drawn from several existing communities who are currently users of X-ray microscopy and/or IR spectroscopy methods. Many of these researchers are already familiar with confocal microscopy, so the combined methods would readily find high demand. Many of the potential users from the biomedical community are not currently synchrotron users, but the power of this unique beamline would be a strong incentive to new users.

Brief Description of the Proposed Beamline

The unique feature of the proposed beamline is the ability to measure confocal fluorescence microscopy (CF), infrared spectroscopy (IR) and transmission X-ray microscopy (TXM) simultaneously. Major features are:

- Bending magnet source, with custom IR mirrors to simultaneously allow passage of soft X-rays
- Tomographic imaging to 20 nm spatial resolution
- Contrast via absorption, phase contrast or diffraction contrast

4.0 Accelerator Development and Major Facility Upgrade Projects

4.1 Accelerator Development Projects

4.1.1 Top-up Mode

'Top-up' is a mode of operation of a synchrotron that aims to maintain a steady current in the storage ring by periodically injecting small amounts of current. It produces a more stable beam by keeping the heat loads and signal strengths constant over long time periods in both the storage ring and on the beamlines. Most of the third-generation light sources, including the Australian Synchrotron, are designed to run in top-up mode. Presently the APS, SLS, SSRL, ALS, SSRF, SOLEIL, Diamond, Spring8 and TLS operate in top-up mode. ESRF, BESSY, ALBA, and NSLS-II plan to move to top-up operation in the future.

Top-up results in an increase in the number of photons on sample at the beamlines by maintaining the 200 mA stored beam current for long periods of time. This, combined with the increased stability from the constant heat load on optical elements is the motivation behind the majority of third generation light sources implementing top-up operations. The constant current also provides a constant signal level in the storage ring beam position monitor electronics and eliminates the current dependence of the orbit feedback system. The reduced dependence on electron beam lifetime will allow the storage ring to be run with a much reduced emittance coupling which reduces the vertical source size. Top-up also eliminates the need to normalize data to the current and allows long scan times with no interruptions.

4.1.2 Electron Gun and Tera Hertz Light Source

Electron gun development is an important area for pushing towards low emittance electron sources. An electron gun test stand is proposed to be built in the linear accelerator (linac) tunnel. This project would enhance the capabilities of the accelerator physics and engineering groups and would allow for extensive collaborations with other research institutes and university groups. The project would increase our in-house capabilities and increase local industry participation in the precise machining needed for producing the accelerating structures and integrated magnet systems.

This is the first stage in an accelerator development program which would lay the foundations for a THz radiation source. With an RF photocathode electron gun generating ultra-short pulses and a single bending magnet it will be possible to generate temporally and spatially coherent synchrotron radiation between 10 to 100 cm^{-1} (0.3 to 3 THz) with an intensity that is currently unavailable using conventional sources. With the addition of an accelerating section to accelerate the electrons to between 10 and 30 MeV the photon flux would increase due to relativistic effects that collimate the beam in the forward direction. Such a source would add to the capability of the high resolution far-IR beamline currently at the Australian Synchrotron, complement already existing laser sources in Australia and provide a test bed for the development of THz imaging technologies which are becoming increasingly important in security screening applications.

4.2 Major Facility Upgrade Projects

4.2.1 X-ray Fluorescence Microscopy Beamline Upgrade

As described above, the XFM beamline accommodates a diverse range of environmental, biological and materials science applications and is currently one of the most over-subscribed beamlines with extremely high demand for X-ray fluorescence elemental mapping.

Upgrades to the optics and scanning stages would simultaneously increase the sample throughput at the beamline – thus relieving user demand – and enhance capabilities.

A key component in the planned upgrade is a double multilayer monochromator (DMM). The estimated increase in X-ray flux at the sample position that would be derived by the incorporation of the DMM is 20-50 times that obtained using the existing double crystal monochromator. In combination with new fast-scanning sample stages, this increase in flux will make feasible fast fluorescence tomography of biological specimens yielding 3D elemental images with unprecedented detail and resolution.

4.2.2 Microscopy Enabling Facilities

Microscopy will form a major part of the scientific endeavour at the Australian Synchrotron in the long term. This proposal seeks to provide a range of onsite facilities to enable new approaches to microscopy experiments, and place Australasian scientists at the forefront of research in this area. Experimenters frequently encounter issues associated with sample preparation and transport that limit the extent of information available from their samples; the ability to prepare samples onsite will overcome these issues in a large number of cases. The coordination of sample mounting and handling across beamlines and energy regimes will extend these microscopy capabilities, providing further advantage.

4.2.3 Advanced X-ray Absorption Spectroscopy

The field of XAS experimentation continues to develop apace with new and more powerful experimental methods becoming increasingly prevalent. Specifically, time-resolved, quick-scanning XAS (QuEXAFS) opens up myriad possibilities for the study of rapidly-changing systems and inelastic scattering techniques (Resonant inelastic scattering and X-ray Raman spectroscopy) allow for the study of complex mixtures or systems otherwise inaccessible with increasing information content.

The XAS beamline at the AS (12ID) was designed and constructed to accommodate these flux intensive techniques and a plan has been developed to add QuEXAFS, RIXS, X-ray Raman and microfocus capabilities. The proposed upgrade will comprise the acquisition and installation of the components required for the beamline to perform at the level originally intended.

Components include:

- X-ray spectrometer and associated controls system
- QuEXAFS monochromators
- Fast data acquisition system
- 384-element MAIA detector system
- 250 mm Kirkpatrick-Baez mirror system
- Extreme-environment sample cells

4.2.4 Macromolecular Crystallography Expansion

As noted above the existing MX beamlines at the AS are utilised heavily and productively. However, further benefits could be realised through expansion of the existing facilities that would be aligned with the scientific strategy outlined here.

This project has four strategic objectives to extend the capabilities of the existing crystallographic infrastructure at the Australian Synchrotron (AS) in order to meet key areas of growth and development in the crystallographic community. These strategic objectives are:

- To increase the capabilities, capacity and performance of the MX beamlines at the AS
- To facilitate crystallography of membrane proteins, protein complexes and other challenging proteins
- To enable drug design by fragment-based screening
- To support synchrotron-based small-molecule crystallography (SMX).

In order to meet these strategic objectives three building projects are proposed:

- Upgrade of the existing high-throughput beamline (MX1) to greatly increase its capabilities, throughput and improve its functionality for the SMX community
- Upgrade the end-station and focusing optics of the existing microfocus beamline (MX2) to enhance flux, beam stability, performance and functionality for the SMX community
- A comprehensive lab upgrade to produce a working structural biology lab at the AS with a set of fragment libraries for users and staff to use for screening experiments in conjunction with crystallization facilities

4.2.5 Hyper Small Angle X-ray Scattering

The SAXS/WAXS beamline is a leading X-ray scattering facility serving a large user base performing challenging experiments across a diverse range of scientific applications. At a modest cost this upgrade will facilitate impressive improvements in performance and capability that are readily achievable and increasingly required by users pursuing the highest quality science. Upgrades needed include sample handling and environments, a double multilayer monochromator, extending the length of the beamline, a basic Bonse-Hart ultra-small angle X-ray scattering (USAXS) capability and detector and hardware upgrades. These investments capitalize on the very high quality of the current setup and allow the facility to remain highly competitive with advanced new storage rings coming online worldwide.

4.2.6 Petabyte Data Storage System

The Australian Synchrotron has a need to retain and archive data generated on all the beamlines and the accelerator for a lengthy period of time. This data should be stored in a secure and safe fashion allowing the original researcher and subsequent authorised researchers to access the data for any purpose, including original research, verification, data mining and further deeper data analysis. Currently this function is not able to be performed by the facility. Original data is kept for a short time, and only to the limit of the particular technology of the beamlines. The onus for data storage and curation is left to the user.

A petabyte storage array is the collective name for the various technologies used to facilitate such a safe and secure data storage system. It will consist of an array of disk, tape and networking technologies combined to give the facility the ability to retain the data for the long term.

Though the specific focus of the proposed petabyte storage proposal is different to the core objectives of the MASSIVE supercomputer collaboration, it is possible that such a large-volume data storage system could be incorporated into the scope of the MASSIVE project and benefit from the existing collaborative arrangements that have facilitated it.

4.2.7 Secure Remote Access System

There are many benefits to the AS and the scientific community arising from the ability to control beamlines from locations physically remote from the facility. Two of the main benefits are the ability for beamline scientists to be able to provide support at times when they cannot be present in the facility and meeting the increasing demand from users to control and monitor experiments remotely from their home institution.

The current relatively simplistic techniques used to achieve this suffer from serious limitations and cannot be sustained into the long term operations of the facility. The most serious of these limitations relate to access security, the possibility of multiple simultaneous remote access, making the systems “aware” that remote access has been invoked, the need to ensure the safety of personnel who may be in the vicinity of equipment under remote control and the need for a consistent facility-wide protocol that can be readily supported and audited.

This project aims to address these and other related issues resulting in safer and more efficient operation of facilities at the AS.

This proposal has obvious links to the VeRSI project and the considerable work undertaken to build the Virtual Beamline. The success of the VeRSI collaboration is acknowledged and the strong desirability of future collaboration on this project should be explored.

4.2.8 Diagnostic and Development Beamline

The primary benefits of constructing a Diagnostic and Development Beamline (DDB) at the Australian Synchrotron can be categorized under three main headings:

- Characterize and monitor the electron beam for user operations
- Provide a platform for accelerator development and optimization
- Provide a platform for developing techniques and concepts for future accelerator and beamline projects and upgrades in areas of science and engineering

Developing a DDB would have immediate benefits as it would enhance in-house capabilities of science and engineering staff and also provide a focal point for design collaboration with both national and international universities and facilities. Once in operation scientific and engineering development will continue by using the DDB to support beamline development in areas such as detectors, high heat load design, optics, shutters and slits etc. With the development of these sorts of projects not only would existing and new beamlines benefit from the newly developed technology but it will also potentially place the science and engineering teams involved in the work at the leading edge of their field.

Appendix 1 – Beamline Summary Table

		Light Source	Energy Range	Applications
Phase 1 Beamlines	High Coherence Nanoprobe (HCN)	In-vacuum undulator	2-22 keV	High-resolution X-ray microspectroscopy and elemental mapping, coherent diffraction imaging
	Micro Materials Characterisation Beamline (MMC)	Bending magnet or wavelength shifter	5-40 keV	Microdiffraction (mono and poly-chromatic), 3D phase and strain mapping, simultaneous XRF/XRD capability
	Medium Energy XAS Beamline (MEX)	Bending magnet	1.8 -14 keV	Tender-hard X-ray absorption spectroscopy, microspectroscopy capability
Phase 2 Beamlines	Advanced Diffraction and Scattering Beamline (ADS)	Superconducting multipole wiggler	30-120 keV	High energy diffraction, pair distribution function analysis, Laue diffraction, energy dispersive diffraction imaging, time-resolved and extreme environment powder diffraction
	Small Angle Scattering Beamline for Structural Biology (SSB)	In-vacuum undulator	8-15 keV	Small angle scattering structural characterisation of biomolecules (proteins, protein assemblies, viruses and hormones) using dedicated supporting infrastructure for high-throughput sampling.
	Micro-Computed Tomography Beamline (MCT)	Bending magnet or wavelength shifter	8-40 keV	High-resolution 3D imaging with applications in the biosciences, geomaterials, palaeontology and materials science
Phase 3 Beamlines	Soft X-ray Materials Science Beamline (SXM)	Bending magnet (2 branches) Possible future undulator	10-300 eV (VUV), 95-1600 eV (Soft X-ray)	General purpose soft X-ray spectroscopy of non-UHV compatible materials, VUV spectroscopy (toroidal analyser)
	High-performance Macromolecular Crystallography Beamline (HMX)	In-vacuum undulator	5-21 keV	Micro-focus macromolecular crystallography for small and/or poorly diffracting samples. Applications in membrane proteins and receptors, virology and materials science.
	Advanced Infrared Spectroscopy Beamline (AIR)	Bending magnet	Infrared	Fast and time-resolved IR mapping using dispersive optics/detectors, Ultra-high spatial resolution IR spectroscopy
	Correlative Microscopy Beamline (CMB)	Bending magnet	Soft X-ray and infrared	Transmission soft X-ray microscopy/imaging, infrared spectroscopy, confocal fluorescence microscopy

Australian Synchrotron Company Limited
ABN 52 126 531 271
800 Blackburn Road, Clayton Victoria 3168, Australia
p +613 8540 4100 **f** +613 8540 4200
e info@synchrotron.org.au **www.synchrotron.org.au**

Appendix 2 – Consultation Workshops

In order to begin the consultation process and engage as fully as possible with the Australasian science community, workshops were held in 2009, organised in collaboration with the Foundation Investor Groups. Each workshop was 3 hours long, and included presentations and an open discussion forum.

The dates and locations of the workshops were:

Date	Location	Venue
5/08/2009	Canberra	The Scarth Room at University House
6/08/2009	Brisbane	The Lady Thiess Room at Customs House
13/08/2009	Sydney	NSW Trade & Investment Centre Level 47 MLC Centre
14/08/2009	Lucas Heights	AINSE Council Room
20/08/2009	Adelaide	Equinox Room, Union House, University of Adelaide
21/08/2009	Perth	Meeting Room 2, Perth Convention & Exhibition Centre
24/08/2009	Hobart	The University Club, University of Tasmania
25/08/2009	Melbourne	RACV Club
4/09/2009	Wellington	Lecture Theatre, Royal Society of NZ