Australian Synchrotron

The National Science Case for the Initial Suite of Beamlines

Presented by
the Australian Synchrotron National Scientific Advisory Committee
on behalf of the Australian Science Community

DECEMBER 2003

This document has been prepared for submission to the Australian Government.

It was refined after consultation with Australian synchrotron users and after review by the National and International Scientific Advisory Committees.

Any enquiries about or comments on this document should be directed to:

Professor Frank Larkins
Chairman, National Scientific Advisory Committee to the Australian Synchrotron Project
c/o GPO Box 4509RR
Melbourne VIC 3001
Tel: +61 3 8344 1997
Email: f.larkins@unimelb.edu.au

Information about the Australian Synchrotron project, administered by the State Government of Victoria, can be found at the website: www.synchrotron.vic.gov.au

Information about the Australian Synchrotron Research Program, administered by ANSTO, can be found at the website: www.ansto.gov.au/natfac/index.html

Information about the Access to Major Research Facilities Program, administered by ANSTO, can be found at the website: www.ansto.gov.au/natfac/amrfp/

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Compiled by Dr Robert Hobbs, FTSE.
Edited by Stefanie Pearce.
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Cover: Detail of a synchrotron-generated x-ray diffraction pattern.
X-ray diffraction is the most widely used technique for 'imaging' molecules at atomic resolution and elucidating molecular structures ranging from several atoms to macromolecular assemblies. Particularly when illuminated by synchrotron light, x-ray diffraction is the method of choice for determining the three-dimensional crystal structure of metals and alloys, chemical compounds, minerals and complex molecules such as protein complexes, nucleic acids and viruses, essential for a wide range of applications in medical and other biological sciences.

Chairman’s Statement

AUSTRALIAN SYNCHROTRON – NATIONAL SCIENCE CASE FOR BEAMLINES

On behalf of the National Scientific Advisory Committee (NSAC) to the Australian Synchrotron, I am pleased to present a proposal entitled Australian Synchrotron: The National Science Case for the Initial Suite of Beamlines.

This proposal flows from extensive consultation with many members of the Australian and New Zealand synchrotron user community, whose contributions have been coordinated and evaluated by NSAC. Many helpful comments were received on the consultative draft that was issued in October 2003. This feedback was most useful in finalising the proposal. We are also grateful for advice and assistance provided by the Victorian Government, particularly in facilitating consultation through workshops for current and potential users.

We seek support for, and investment in, a balanced suite of beamlines to meet 95% of the anticipated needs of the Australian synchrotron research community for the first few years after the facility is commissioned in 2007. These initial beamlines represent vital enabling infrastructure for internationally competitive scientific and industrial research that will boost innovation. Convenient access to a synchrotron light source will promote frontier science in Australia and our region.

This National Science Case provides a framework to assist governments, research institutions and industries in deciding to help create the Australian Synchrotron as a truly national facility.

Yours faithfully

Frank P. Larkins

Frank P Larkins

Chair
National Scientific Advisory Committee
Australian Synchrotron Project

From the Minister for Innovation, State Government of Victoria

AUSTRALIAN SYNCHROTRON – NATIONAL SCIENCE CASE FOR BEAMLINES

To compete in the global innovation economy Australia needs world class science infrastructure. The Australian Synchrotron is an essential tool for new science. It will accelerate the innovations that create wealth and jobs for Australians.

Victoria is deeply committed to promoting Australian excellence in research and development. We are very proud to have provided $157 million – three-quarters of the capital cost – for the Australian Synchrotron. Although this is the largest ever investment by an Australian State Government in innovation infrastructure, we are determined that the Australian Synchrotron will serve universities, research organisations and industry throughout this nation.

The Australian Synchrotron will provide a world-leading technical capability, and the nucleus around which new science and industry networks will form as researchers interact at their own national facility. The synchrotron will deliver better and faster experimental techniques that will not only enhance current fundamental and applied research, but also open up new avenues of investigation to Australian science. This facility will promote the international collaboration now so important to leading-edge R&D, becoming a hub for research that will greatly benefit Australia and our regional neighbours.

Australia already punches above its weight in science, and the Australian Synchrotron will further enhance this nation's global competitiveness. Accelerating development of the intellectual property that drives commercial spinoffs, this powerful new tool will help deliver innovations that create the industries of the future.

The Victorian Government is therefore proud to endorse the National Science Case for the Initial Suite of Beamlines, and urges universities, governments and industry to commit to partnership in developing the Australian Synchrotron.

JOHN BRUMBY MP
Minister for Innovation

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This document has been prepared by the Australian Synchrotron National Scientific Advisory Committee, with the assistance of the Australian scientific community. In particular, the following have made, or coordinated, particular contributions to the preparation of this document:

Executive Summary

Professor Frank Larkins AM FAA FTSE
The University of Melbourne

Overview, Introduction & Science Case

Dr Robert Hobbs FTSE

Dr Gerard Roe
Australian Synchrotron Project

Technical specification of the machine and beamline designs

Professor John Boldeman FTSE

Dr Richard Garrett
Australian Synchrotron Research Program, ANSTO

Dr Tony Warwick
Lawrence Berkeley Laboratory, Berkeley, California.

Dr David Cookson
Australian Synchrotron Research Program
Advanced Photon Source, Chicago, Illinois.

Dr Gary Foran
Australian Synchrotron Research Program, ANBF, Japan

Beamlines 1 & 2

Dr Jose Varghese
CSIRO Health Sciences & Nutrition

Professor Colin Raston
The University of Western Australia

Beamline 3

Assoc Professor Brendan Kennedy
The University of Sydney

Beamline 4

Assoc Professor Ian Gentle
The University of Queensland

Beamline 5

Dr Mark Ridgway
The Australian National University

Beamline 6

Professor Alan Buckley
The University of New South Wales

Beamline 7

Professor Robert Leckey
La Trobe University

Professor Jim F Williams FAA
The University of Western Australia

Beamline 8

Professor Dudley Creagh
University of Canberra

Dr Don McNaughton
Monash University

Beamline 9

Professor David Cohen
ANSTO

Beamline 10

Professor Rob Lewis
Monash University

Dr Steve Wilkins
CSIRO Manufacturing & Infrastructure Technology

Beamline 11

Assoc Professor Andrea Gerson
Ian Wark Institute, The University of South Australia

Beamline 12

Dr Mibel Aguilar
Monash University

Beamline 13

Professor Erol Harvey
Swinburne University of Technology and MiniFAB

Advisory Committees

National Scientific Advisory Committee

Professor Frank Larkins AM FAA FTSE (Chair)
Deputy Vice Chancellor (Research)
The University of Melbourne

Professor David Cohen
Senior Principal Research Scientist
Physics Division, Australian Nuclear Science
and Technology Organisation

Professor Dudley Creagh
Professor of Physics, Division of Health, Design and Science
University of Canberra

Assoc Professor Ian Gentle
Director, Brisbane Surface Analysis Facility
Department of Chemistry, The University of Queensland

Assoc Professor Andrea Gerson
Senior Research Fellow
Ian Wark Institute, The University of South Australia

Professor Erol Harvey
Deputy Director
Industrial Research Institute Swinburne/
CEO MiniFAB

Assoc Professor Brendan Kennedy
Assoc Professor
School of Chemistry, The University of Sydney

Professor Robert Lamb
Head
School of Chemistry, The University of New South Wales

Professor Robert Leckey
School of Physics, La Trobe University

Professor Robert Lewis
Professor of X-Ray and Synchrotron Physics
School of Physics and Materials Engineering, Monash University

Assoc Professor Jenny Martin
Group Leader
Institute for Molecular Bioscience, The University of Queensland

Assoc Professor James Metson
Light Metals Research Centre, The University of Auckland

Professor Keith Nugent
ARC Federation Fellow
School of Physics, The University of Melbourne

Emeritus Professor Brian O'Connor
Emeritus Professor of Physics
Department of Applied Physics, Curtin University of Technology

Professor Colin Raston
Professor of Chemistry
School of Biomedical & Chemical Sciences,
The University of Western Australia

Dr Mark Ridgway
Senior Fellow
Department of Electronic Materials Engineering,
The Australian National University

Dr Jose Varghese
Head
Structural Biology, CSIRO Health Sciences & Nutrition

Professor John White CMG FAA FRS
Professor of Physical and Theoretical Chemistry
Research School of Chemistry, The Australian National University

Dr Steve Wilkins
Research Area Leader, X-Ray & Synchrotron Science
CSIRO Manufacturing Science & Technology

Professor Jim Williams FAA
Co-Director, Centre for Atomic, Molecular & Surface Physics
Physics Department, The University of Western Australia

International Scientific Advisory Committee

Professor Frank Larkins AM FAA FTSE (Chair)
Deputy Vice Chancellor (Research)
The University of Melbourne

Professor Mike Bancroft
Director of Research
Canadian Light Source, Canada

Professor Hiromichi Kamitsubo
Vice-Chairman
Japan Synchrotron Radiation Research Institute

Professor Tadashi Matsushita
Deputy Director
KEK, Institute of Material Structure Science, Japan

Professor Herbert Moser
Director & Professor (Research)
Singapore Synchrotron Light Source

Professor Volker Saile
Director
Forschungszentrum Karlsruhe,
Institute for Microstructure Technology, Germany

Dr Gopal Shenoy
Senior Scientific Advisor
Advanced Photon Source, USA

Dr Neville Smith
Scientific Director
Advanced Light Source, USA

Professor Emeritus Herman Winick
Assistant Director
Stanford Synchrotron Radiation Laboratory, USA

Professor Albin Wrulich
Director
Swiss Light Source, Villigen, Switzerland

International Machine Advisory Committee

Dr Stephen Milton (Chair)
ANL Linac Coherent Light Source Project Director
Argonne National Laboratory, USA

Professor John Boldeman
Science Adviser
Australian Synchrotron Project, Department of Innovation, Industry
& Regional Development, Australia

Dr Jeff Corbett
Group Leader
SPEAR 3 Accelerator Physics
Stanford Synchrotron Radiation Laboratory, USA

Professor Dieter Einfeld
Director
SESAME-UNESCO, Germany

Dr Dieter Kraemer
Head Accelerator Group
BESSY II, Berlin, Germany

Dr Annick Ropert
Assistant to the Machine Director (Future Developments)
European Synchrotron Radiation Facility, Grenoble, France

Table of Contents

Appendices

Volume 2

List of Tables

Appendix 1

Appendix 2

List of Figures

Appendix 2

EXECUTIVE SUMMARY

Executive summary

Science and Economic Context

In an increasingly competitive world, the scientific and technological innovations that fuel economic, social and environmental progress for 21st century knowledge-based economies require world class scientific infrastructure.

Scientific techniques and infrastructure are continuously improving, but occasionally breakthroughs occur that enable rapid advances in certain fields. The radio telescope revolutionised astronomy, and the electron microscope and microprobe dramatically transformed research in materials science and geology. Synchrotron technology is having a similar effect, but across many areas of science.

Synchrotron technology is advancing research and development in fields as diverse as:

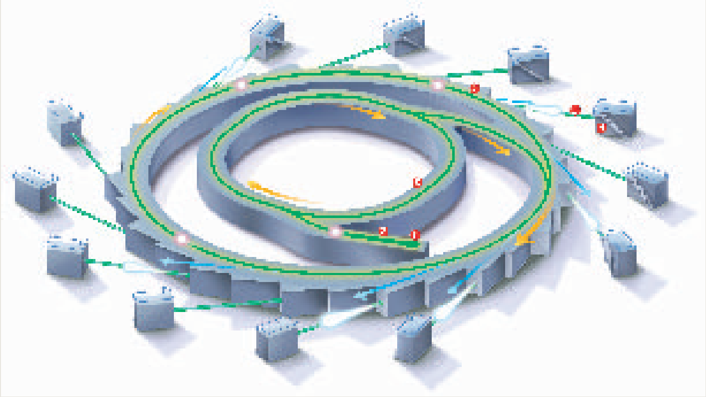
- biosciences (protein crystallography and cell biology)
- medical research (microbiology, disease mechanisms, high resolution imaging and cancer radiation therapy)
- environmental sciences (toxicology, atmospheric research, clean combustion and cleaner industrial production technologies)
- agriculture (plant genomics, soil studies, animal and plant imaging)
- minerals exploration (rapid analysis of drill core samples, comprehensive characterisation of ores for ease of mineral processing)
- advanced materials (nanostructured materials, intelligent polymers, ceramics, light metals and alloys, electronic and magnetic materials)
- engineering (imaging of industrial processes in real time, high resolution imaging of cracks and defects in structures, the operation of catalysts in large chemical engineering processes)
- forensics (identification of suspects from extremely small and dilute samples).

Synchrotron science is advancing rapidly. All major OECD countries have now invested or are investing in synchrotron facilities[1]. Without a world class national synchrotron facility Australia will fall quickly behind its competitors in the capacity to perform leading edge medical, scientific and industrial research.

National Science Case

This document presents the national science case for the initial suite of beamlines that will enable researchers to use light created by the Australian Synchrotron. It is presented by the National Scientific Advisory Committee to the Australian Synchrotron. It aims to provide a framework for consideration by governments, research institutions and industries to support and invest in the establishment of the initial suite of beamlines, which should meet 95% of the anticipated needs of the Australian industrial, scientific and medical research community. This suite of beamlines is essential to undertake the range of experiments critical for achieving economic and social benefits in Australia and in our geopolitical region.

1 Electron Gun **2** Linac **3** Booster Ring
4 Storage Ring **5** Beamlines **6** Experimental Stations



What is a Synchrotron?

A synchrotron is a large machine (about the size of a football field) that accelerates electrons to almost the speed of light, where they have a very high energy level. As the electrons are deflected around the storage ring they give off beams of extremely intense radiation (light) that run tangentially from the machine. These beams are captured in specially designed beamlines and are then used to perform many different types of experiments simultaneously.

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[1] Lists of world's synchrotron facilities at http://www.spring8.or.jp/ENGLISH/other_sr and at http://www-ssrl.slac.stanford_edu/SR_SOURCES.html

Current Status

The Victorian Government is funding, at a cost of $157.2 million, the construction of the synchrotron machine as the light source required to generate the photons (light) for scientific experimentation, and the building that will house the machine and associated laboratories. In parallel, the National Scientific Advisory Committee has developed the national science case for the initial suite of beamlines. These beamlines are intended to form the experimental hub of the facility.

An International Machine Advisory Committee has been established (see Acknowledgments, page vi) to advise on the design of the machine, and an expert team has been assembled to oversee its construction.

Building work has started and a construction timetable has been established (see chapter 8), with the target date of March 2007 for commencement of operations. The Australian Synchrotron will be a state of the art machine with an energy of 3 GeV and a capacity to provide photons from the infrared region (0.001 eV) to the hard x-ray region (120,000 eV).

The Victorian Government, with the advice of the Australian scientific community, has established broad-based expert National (NSAC) and International (ISAC) Scientific Advisory Committees (see page vi) to the Australian Synchrotron project. These committees have identified the needs of the medical, scientific and industrial research communities and guided the development of this case for an initial suite of beamlines. The aim is to service the majority of Australian synchrotron researchers and their collaborators across a broad range of disciplines, where Australians either currently undertake internationally competitive research or have the potential to do so once a national facility is available. Extensive consultations over the past two years have included an Australian Synchrotron workshop for potential users in January 2003, sponsored by the Victorian Government, and a wide range of workshops and conference sessions, culminating in the preparation of this National Science Case. Australian scientists have received generous expert assistance from their international colleagues in the preparation of this proposal.

The Australian Synchrotron initiative builds on progress already made through the Australian Synchrotron Research Program. This program has been funded since 1996 as part of the Australian Government's Major National Research Facilities Program. The impact of the ASRP on Australia's science and technology has been considerable. The synchrotron user community has experienced major growth (see chapter 5), so much so that limited overseas access is hampering the development of Australian science in several national priority areas. With demand for beam time outstripping supply worldwide, it will become increasingly difficult to meet the needs of Australian research and development using overseas facilities. Furthermore, because of quarantine restrictions, work such as soil science studies and small animal investigations is very difficult to pursue, while the fragile and transient nature of some samples makes long distance travel to other major facilities (all of which are in the northern hemisphere) impractical.

Benefits from Investment in Beamlines

At full capacity, the Australian Synchrotron will be able to accommodate more than 30 beamlines, operating simultaneously and engaging hundreds of scientific and medical researchers, engineers and technologists in the pursuit of scientific discovery and understanding across a broad range of disciplines.

It will be a focal point for interaction among these communities and for enhanced international collaboration. There is an increasing international trend towards large-scale, formalised collaborations, particularly to explore complex medical and biological challenges. These collaborations combine the strengths of major laboratories through research networks, such as the US National Institutes of Health, and Canadian and European equivalents. The Australian Synchrotron will place Australian scientists in a globally competitive position to participate in such large-scale collaborative ventures.

It will have a major impact on the education and research training of the next generation of graduate students, post-doctoral fellows and other emerging researchers in the physical, chemical, materials and biological sciences. Access to such a wide range of the highest quality, state of the art research techniques, together with the opportunity to work in a collaborative community of leading national and international scientists, will enhance the sophistication and breadth of their approach to research.

The Australian Synchrotron will open new opportunities for working across boundaries and in clusters that are linked internationally to world class science. It will assist with attracting and retaining the most talented people. Indeed this is already starting to happen, with lively interest being expressed by world-ranking international scientists, including a number of expatriate Australians.

National Research Priorities

Investment in the Australian Synchrotron beamlines will support the desired outcomes from the four National Research Priority Areas identified by the Australian Government, as outlined in chapter 1.

Synchrotron research will contribute towards building an environmentally sustainable Australia through supporting research in plants and crops, soil science, water and atmosphere pollution, industrial site remediation, mine wastes and fuel improvements.

Synchrotron research is vital to advancing modern medical research, in order to achieve the national priority for promoting and maintaining good health. The synchrotron is an essential tool for drug design, biological research, biotechnology, food sciences and medical imaging, and is showing exciting potential for medical therapy.

The synchrotron is particularly useful in enhancing fundamental research in the basic sciences that underpin the frontier technologies for building and transforming Australian industries. Australian synchrotron research is already contributing to advances in photonics, polymers, ceramics, metals and alloys, bio- and nano-materials, organic and inorganic chemistry, thin film technologies, and advanced manufacturing, particularly in the production of micro-devices.

With regard to safeguarding Australia, the Australian Defence Science and Technology Organisation currently uses synchrotron research for aviation materials testing, and is interested in developing sensor technology. Internationally, synchrotron methods are widely applied in forensic science, and in developing anti-toxins to biological weapons such as anthrax.

The national and international economic benefits of having an Australian facility are outlined in chapter 7.

Industry Engagement

Since its inception the Australian Synchrotron initiative has sought to involve industry and major government agencies such as departments of agriculture and primary industries in the planning of the facility. At the Users' Workshop in January 2003 the following industries and agencies were represented and contributed actively to the decision-making on the choice and specifications of beamlines for the initial suite:

- automotive – three companies
- advanced manufacturing – two companies and one consulting organisation
- scientific equipment – nine companies
- information and communication technology industry – two companies
- food manufacturing – one company and one major research agency
- mining and minerals – two companies
- defence – one company and two research organisations
- health – two pharmaceutical companies, one medical equipment company, two medical imaging and radiotherapy centres, five medical research institutes
- CSIRO – ten divisions.

Since then an active program of seminars and displays at conferences has been held to continue the process of engaging and increasing the number of these commercially oriented potential users. (see appendix 3)

Experience at overseas synchrotrons has been that industry usually accesses synchrotron techniques by collaborating with universities or expert research organisations such as the CSIRO, ANSTO, or DSTO, especially in the early stages while they gain experience and knowledge of the capability of a synchrotron. Accordingly the Victorian Government, in conjunction with ASRP, is sponsoring an industry engagement program with the purpose of ensuring that an active industry/major agency user community is in place when the Australian Synchrotron opens in 2007. Demonstration projects are being supported in the following areas:

- minerals exploration
- manufacturing
- agriculture
- medical science

The industry engagement program will be developed further leading up to the opening of the Australian Synchrotron in 2007. The proposals for industry focussed beamlines (beamline 11 – microdiffraction and fluorescence probe and beamline 13 – lithography) will be facilitated, and industry funding for protein crystallography infrastructure will be sought. The establishment of an x-ray detector centre, with products targeted for general laboratory as well as synchrotron applications, will be encouraged. The program to enable industry access to overseas synchrotron facilities will be expanded nationally, provided funding is made available.

Summary of Benefits

An Australian Synchrotron will assist economic and social development through:

- providing core enabling scientific infrastructure indispensable for building an innovation economy
- stimulating international collaborations and networks vital for the solution of multi-disciplinary globally oriented problems
- facilitating the development of high level scientific and technical skills for the Australian industry
- producing valuable intellectual property to expand Australian and regional capabilities and enhance business competitiveness
- providing industry with ready access to leading edge techniques for R&D, and new insights for advanced industrial processing
- building on and strengthening research and innovation links between Australia and countries in the region
- development of a multi-disciplinary user community leading to interchange of ideas and experimental techniques.

Table 1. Recommended initial suite of beamlines for the Australian Synchrotron

No	Beamline Description	Category	Energy Range
	Crystallography & Diffraction		
1	High-throughput Protein Crystallography	A	2–23 keV
2	Protein Microcrystal & Small Molecule X-ray Diffraction	A	5.5–20 keV
3	Powder X-ray Diffraction	A	4–60 keV
4	Small and Wide Angle X-ray Scattering	A	5.5–20 keV
	Spectroscopy		
5	X-ray Absorption Spectroscopy	A	4–65 keV
6	Soft X-ray Spectroscopy	A	0.1–2.5 keV
7	Vacuum Ultraviolet (VUV)	B	10–350 eV
8	Infrared Spectroscopy	A	0.001–1 eV
9	Microspectroscopy (submicron-XAS, XANES, & XRF)	A	5–20 keV
	Imaging		
10	Imaging & Medical Therapy	A, B	10–120 keV
11	Microdiffraction and Fluorescence Probe (XRD & XRF mapping)	C	4–37 keV
	Polarimetry		
12	Circular Dichroism	B	2–10 eV
	Advanced Manufacturing		
13	Lithography	C	2–25 keV

A Proposed Initial Suite of Beamlines

The National Scientific Advisory Committee to the Australian Synchrotron and the International Scientific Advisory Committee recommend consideration of the establishment of a suite of up to thirteen beamlines in the first few years of the facility's 30-year life.

The thirteen recommended beamlines have been grouped into three categories, as summarised in table 1. An outline of each of these experimental facilities is presented in chapter 10.

Category A

There are nine general purpose beamlines considered essential to be available or under construction at the commissioning of the synchrotron in 2007. This suite provides a comprehensive range of techniques that will meet most of the scientific, medical and industrial research needs. Preliminary cost estimates for these nine beamlines total to approximately $A49.5m.

Category B

Two beamlines (VUV and circular dichroism) are considered highly desirable for a balanced set of capabilities for the synchrotron; however the experienced user communities for these lines are small and will require time to develop. In addition, beamline 10 (imaging and medical therapy) can be extended for large-scale imaging and beamline 1 can be further developed. Preliminary cost estimates for these beamlines and modifications total $A14.9m, and consideration of funding for these will be sought separately after the Category A beamlines are established.

Category C

Two beamlines (microdiffraction and fluorescence probe and lithography) are principally for industrial and commercial use. Preliminary cost estimates for these are $A3.4m for the microdiffraction and fluorescence probe and $A4.2m for the lithography beamline. A separate funding plan is being developed for these beamlines based upon a combination of direct capital contributions and cost recovery fee-for-service policy.

Management Framework and Access Policy

It is the view of the National Scientific Advisory Committee that the synchrotron should be managed as a national facility consistent with the principles established for other major research facilities. There are several mechanisms by which this outcome may be achieved. While one approach is examined in chapter 9, a decision must await further discussions amongst the parties that invest in the facility. It will be essential for the achievement of breakthrough scientific outcomes that the facility is managed to the highest international standards. An outward view is vital to ensure that, in addition to local synchrotron users, some of the world's leading synchrotron scientists are attracted to the Australian facility.

It is proposed that access to Category A and B beamlines will be on a merit basis – consistent with the ASRP process developed by the Australian Government and with well-established access models used at other international facilities. Access guidelines would be established through peer review mechanisms to support the scientific management team at the synchrotron. It is anticipated that there would be the close involvement of the research funding agencies in this process.

Also consistent with international practice, overall access arrangements would facilitate priority to industry users, generally on a cost-recovery basis.

Under the proposed model, a proportion of the time available for scientific experimentation on these beamlines would be reserved for members of funding agencies and institutions that have invested in the capital funding of the Category A and B beamlines. Access would still be merit based and would be additional to any beam time sourced from the general pool.

It will be important to ensure that access arrangements enable researchers from across the country and New Zealand to have the same opportunity to participate in synchrotron research as their colleagues located in Melbourne. The ASRP and AINSE programs provide useful models for this.

Operating Costs

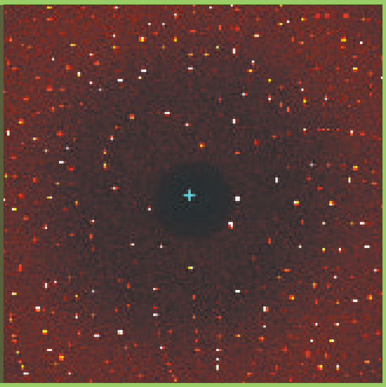
The annual operating costs of a synchrotron comprise the fixed costs to maintain and operate the machine and associated infrastructure as a leading edge facility and costs associated directly with the number of operating beamlines. The development and finalisation with key stakeholders of the coverage of operating costs and the methods by which these are met will be important elements of future stakeholder discussions. Further details are provided in chapter 4.

Beamline Funding Proposal

Following an extensive consultation process, the National Scientific Advisory Committee recommends on behalf of the Australian scientific and industrial user community:

- that the nine general access beamlines identified in this proposal be jointly funded in a partnership involving research institutions, State and other governments and industry, with the Australian Government. Details of the matching basis to be finalised in future discussions
- that two general access beamlines (beamlines 7 and 12) plus an extension of beamline 10 be funded when additional capital funds become available
- that usage guarantees and direct capital contributions be sought from industry to enable the construction of a microdiffraction and fluorescence probe and a lithography beamline, with these two beamlines being operated on a predominately fee-for-service, cost recovery (including capital) basis, once fully operational.

01



Overview

IMAGE: Laue diffraction pattern of a single crystal of the ribotoxin, restrictocin. Image taken at the Advanced Photon Source, Chicago, by Xiao-jing Yang and used with permission.

Chapter 01

Overview

The Australian Synchrotron, which will commence operations in mid 2007, is an essential piece of national science infrastructure needed to keep Australia and its region at the forefront of world class scientific and industrial research in the 21st century.

The machine provides an extremely intense light source covering a broad band of electromagnetic radiation – from deep infrared through to very hard x-rays. It enables a wide range of experiments and measurements to be performed simultaneously and these are done on separate specialised beamlines that run tangentially from the synchrotron ring.

The facility will be the latest 'third generation' design with world class capability, comparable to the new synchrotrons currently under construction in the UK, Canada and the USA.

Benefits to Australian Science and Industry

The Australian Synchrotron will be of immense value to a large section of the scientific community and it has been estimated that once the initial suite of beamlines is fully established it will be used by more than 1,200 members of the scientific research community in the country[1]. This has been the experience in other advanced countries where their scientists enjoy access to a local synchrotron[2,3].

For the life sciences it is an essential tool for the structural and conformational (i.e. shape) analysis of proteins, nucleic acids and viruses. It brings new techniques for the imaging of cells and biological structures, an area where Australia enjoys a first-rate reputation, and for studying cellular interactions in real time.

For the physical and chemical sciences the range of high resolution x-ray, VUV and infrared spectroscopic techniques, together with x-ray diffraction and imaging, plus the ability to follow reactions in real time, will bring new understanding to many areas from basic physics and chemistry through to the science of new advanced materials.

For the emerging area of nanoscience, where materials and chemical processes are controlled and manipulated at the atomic and molecular level, synchrotron techniques are vital not only for characterisation on this scale, but also for the production of the microtextured substrates on which nanoscience is carried out.

For agriculture it opens up new possibilities in understanding the proteomics of plant systems, in imaging cells and plant tissue, and following processes such as the uptake of metal-ion species or toxins into plant cells. It enables high throughput, rapid analysis of soils and can detect extremely low levels of trace elements.

For the minerals industry it is expected to revolutionise the way minerals exploration and processing are done. The extremely high beam intensity enables very high throughput of large quantities of exploration samples and the tunability of the source provides information on the speciation (i.e. the oxidation state) of the elements in minerals. This information is vital in evaluating the ease with which ore bodies can be treated.

For the oil and gas industry the ability to study reactions in real time under high temperature and pressure will assist in developing technologies for extracting additional oil and gas from depleted fields. Synchrotron science can also simulate and study reactions such as the corrosion by carbon dioxide of transmission pipelines.

For advanced materials development, the ability to characterise materials with unprecedented precision and with the unique technique of x-ray absorption spectroscopy that can only be performed with the synchrotron will bring new understanding of the nanostructure of advanced ceramics, the molecular structure and functioning of intelligent polymers and biomaterials, and the electronic and magnetic structures of new semiconductors and opto-electronic materials.

For the microtechnology industry the synchrotron will bring a unique capability for the manufacturing of micro-devices with very high depth to width ratios and ultra smooth surfaces.

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[1] J.W. Boldeman, 'The Boomerang Proposal, Part IV: Benefits and opportunities for Australian science and industry' ASRP, April 2000.

[2] See http://www.aps.anl.gov/aps/frame_science.html

[3] See http://www.srs.ac.uk/srs/annual_reports.htm

Conventional lithographic techniques used for the manufacture of microcircuits produce planar devices – components that are essentially a series of two-dimensional layers. Synchrotron based lithography (LIGA) provides access to the third dimension and this is required in many micro-mechanical and micro-fluidic devices.

The synchrotron also enables the measurement of very thin surface layers and extremely low trace elements – important in the latest generation of silicon micro-devices. These techniques enable the manufacture of intelligent integrated sensors and other novel micro-devices for commercialisation in the automotive, aerospace, defence, information and communication technology and biotechnology sectors. The availability of smart integrated micro-devices is expected to impact all aspects of manufacturing in the future.

For the scientific instruments sector, where Australia already has an excellent reputation for innovation, the ability to develop the underlying physics and detector technologies behind new measurement techniques by accessing the high brilliance and tunable synchrotron light will maintain this industry at the forefront of developments.

For the pharmaceutical industry, in addition to the techniques critical to advancing drug design and medical research mentioned previously, x-ray diffraction driven from a synchrotron source is becoming an essential tool for monitoring quality control systems and for trouble shooting in the manufacture of medicines.

Contributions to National Research Priorities

The Australian national synchrotron facility will make contributions to all four of Australia's National Research Priorities:

- an environmentally sustainable Australia
- promoting and maintaining good health
- frontier technologies for building and transforming Australian industries
- safeguarding Australia.

An environmentally sustainable Australia

The Australian Synchrotron will enable the measurement of very small concentrations of toxic materials in soils, streams, seawater or the atmosphere. Such measurements can be performed with sub-micron spatial resolution, so the levels of various elements can be mapped through a sample. For example, the uptake of heavy elements by plants and microorganisms has been investigated in order to develop mine and industrial site remediation strategies[4]. The role of microorganisms in zinc-related processes associated with acid mine drainage have been explored[5,6]. Investigations such as these using the synchrotron address the goals of transforming existing industries and overcoming soil loss, salinity and acidity.

It will be possible to characterise airborne pollutants with discrimination and accuracy hitherto unobtainable, and thus positively identify their sources. Pioneering work by scientists at ANSTO on pollutants in the Sydney Basin has already demonstrated this[7].

The synchrotron is an ideal tool for studying the operation in real time of catalytic systems for emission control and fuel processing, for the operation of fuel cells and developing new technologies for sustainable development. Such work addresses the goal of reducing and capturing emissions in transport, and waste and energy generation.

Fine particulate air pollution

Atmospheric fine particles (< 2.5 microns diameter) are produced by combustion processes, traffic, industrial plants and mining operations, as well as by such natural sources as windblown soils and seaspray.

These atmospheric aerosols can affect health and the environment; they may stay in the atmosphere for weeks and can travel many kilometres from their source.

To assess the potential effects and assist with anti-pollution programs, ANSTO researchers analyse the composition of air samples and try to identify the likely source. They use XRF at the APS to determine whether emissions from Hunter Valley coal combustion for power generation and industry are reaching the Sydney Basin and impacting air quality there. More at www.ansto.gov.au/ansto/environment1/iba/projects/aerosol_studies.htm

Image: Views of Sydney during clear and foggy days. Courtesy D Cohen, ANSTO

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[4] Studies at the Advanced Photon Source covered by Mark Rivers in his presentation at the workshop, titled 'The Australian Synchrotron: New opportunities for soil and environmental science', 3–4 October 2003.

[5] A. Gerson & R. Hill, ATSE Focus, No. 121, Mar/Apr 2002, 'Synchrotron Applications to the Earth Sciences', refer to website http://www.atse.org.au/publications/focus/focus-gerson.htm

[6] M. Labrenz, G.K. Druschel, T. Thomsen-Ebert, B. Gilbert, S.A. Welch, K.M. Kemner, G.A. Logan, R.E. Summons, G. De Stasio, P.L. Bond, B. Lai, S.D. Kelly & J.F. Banfield, 'Formation of sphalerite (ZnS) deposits in natural biofilms of sulfate-reducing bacteria', Science, 290 (2000) 1744–1747.

[7] D. Cohen, R. Siegele, E. Stelcer, D. Garton, A. Stampfl, Z. Cai, P. Ilinski, W. Rodrigues, D.G. Legnini, W. Yun & B. Lai, 'The complementarity of PIXE and synchrotron induced x-ray methods for the characterisation of combustion sources contributing to urban air pollution', Nucl. Instr and Methods, B189 (2002) 100–104.

Promoting and maintaining good health

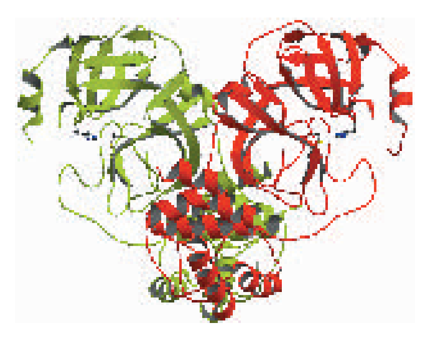
Australia has a fine reputation for leading-edge medical research in many areas.

Understanding the structure and shape of the genome and the proteins expressed by the genome is fundamental to understanding the basis of all life. This task is enormous – it is estimated that there are over one million proteins, all with different functions, expressed by the human genome, let alone the much greater number produced by the immune system. The synchrotron is an essential tool for this – not only for protein crystallography, which elucidates molecular structure, but also for envisioning the way protein chains are folded and change during cellular reactions.

Beyond this the synchrotron provides enhanced ability for the structural analysis of viruses, and the imaging of cells and biological structures. It is capable of studying cellular interactions in real time; this will bring new understanding of the processes of disease and be a major factor in rational drug design.

At a more fundamental level, it will be possible to measure the electronic properties and interactions at atomic level of the building blocks that make up biological molecules (for example, amino acids). Understanding these will provide new insights into many of the complex processes observed in biological systems.

The special characteristics of the synchrotron beam enable the imaging of biological tissues with much better contrast and more detail than is possible with conventional technologies[8]. Images of the fine detail of lungs and hearts, which were previously difficult to obtains will be possible with the synchrotron. The fine imaging of small animals, in particular, will have a major impact on Australian medical research – currently this is impossible to do on overseas facilities because of quarantine restrictions.



Structure determined for critical SARS enzyme

Scientists from California based company Structural GenomiX used x-ray diffraction techniques on their beamline at the Advanced Photon Source, Chicago, to determine the first structure of the main protease from the coronavirus that causes Severe Acute Respiratory Syndrome (SARS). The three-dimensional, high resolution (1.86Å) image will assist in development of a drug to inhibit SARS virus replication. A similar strategy succeeded with the HIV protease for treatment of AIDS. (More at http://www.anl.gov/OPA/whatsnew/030912sars.htm)

Highly intriguing research has shown that synchrotron radiation has great potential for development of new types of medical therapy – in particular the treatment of difficult cancers, such as brain tumours[9].

Food science, also, will benefit greatly from access to the Australian Synchrotron. The high beam intensities mean that it will be possible to follow food processing by infrared spectroscopy. It will also be possible to better characterise food pathogens.

Frontier technologies for building and transforming Australian industries

The special characteristics of the extremely intense, tunable, polarised, and pulsed synchrotron light will open up many new avenues for breakthrough science to be performed in Australia.

Breakthrough science

A small selection from examples of breakthrough science are:

- Australian researchers, particularly at La Trobe University and the University of Western Australia, have been at the forefront of the development of new synchrotron-based surface spectrographic techniques that can measure electron spin-dependent phenomena in atoms, clusters, ferromagnetic films and surfaces. This emerging area of 'spin-electronics' will impact technologies such as quantum computing, new artificially structured magnetic materials and transistors and the development of the next generation of hard disc storage systems.
- The operation of high temperature superconductors is not well understood and progress after the initial promising discoveries in the 1980s has been slow. Using synchrotron techniques it has recently been possible to probe the electronic structure of these unusual layered materials and reveal the 'stripe phase' that had been predicted by theorists in 1989. Study of the charge carrying mechanism of the stripe phase is expected to lead to new advances in the field.
- In the earth sciences synchrotron techniques will enable improved understanding of metal complexes and solubilities and the modes of transport of metal ions in molten magmas under high pressure and in hydrothermal systems, leading to better predictive models of ore formation.
- Over the past twenty years scientists at Melbourne and Monash Universities and the CSIRO have made major advances in the fundamental knowledge about x-ray imaging. This work has led to dramatic improvements in the contrast resolution that can be obtained. It has had important spin-offs in medical imaging, as described

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[8] S.W. Wilkins, T.E. Gureyev, D. Gao, A. Pogany, & A.W. Stevenson, 'Phase-contrast imaging using polychromatic hard x-rays', Nature, 384, (1996) 335–338.

[9] P. Suortti & W. Thomlinson, 'Medical applications of synchrotron radiation', Phys. Med. Biol., 48 (2003) R1–R35, online at stacks.iop.org/PMB/48/R1

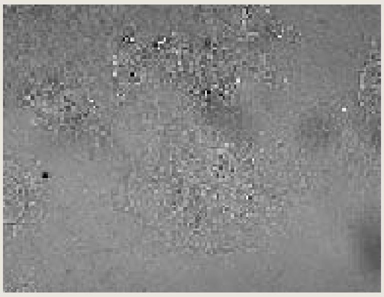
New microscope technology leads to global sales

Just as the study of lasers has opened up the new field of photonics, so ARC Federation Fellow Professor Keith Nugent and colleagues are using synchrotron science to open up the field of coherent x-ray optics.

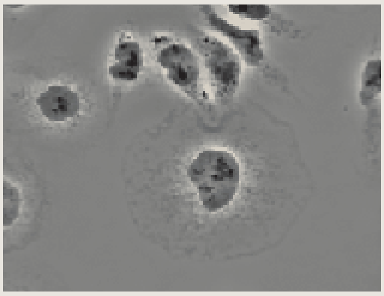
One of the first spin-offs of this work has been quantitative phase imaging which enables new and useful information to be gathered from light microscope images.

A Melbourne company IATIA has been established to develop and market this new technology and is already exporting to Europe, USA and Asia. The global market is estimated as hundreds of millions of dollars a year.

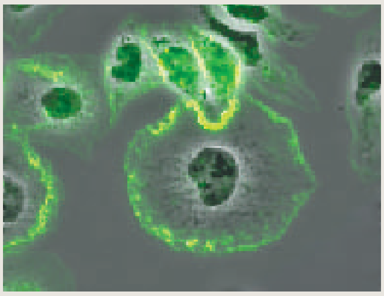
Images of rat mast cells taken three ways



A. Brightfield (conventional) shows no visible cellular contents



B. Quantitative phase image shows protein concentrations, increased density of cell surface and microfilaments, and locations of nucleus and cytoplasm areas.



C. Overlay of the fluorescence and phase image displays the localisation of proteins in the cells (Source: IATIA/Centre of Immunology, St Vincent's Hospital, University of NSW)

above, and the development of specialised new imaging instruments. To date much of the work been performed using overseas synchrotrons, and access to the Australian Synchrotron will enable this work to be continued more rapidly and at a higher level of intensity.

Frontier technologies

The Australian Synchrotron will have major impacts on the frontier technologies of nanotechnology, biotechnology, ultra broad-band communications (especially photonics) and genomics, proteomics and phenomics. An example where nanotechnology, biotechnology and proteomics have converged is research into ordered organic nanostructures or 'soft matter'. Soft matter covers many different types of systems, for example liquid crystals, functional polymers, di-block polymers, protein/lipid composites and organic/inorganic complexes. These have in common the self-assembly of component molecules into complex structures that have unique and different properties to their constituents. Synchrotron techniques enable detailed characterisation of these structures and can monitor in real time the dynamics of the self-assembly processes as well as their response to external environments.

Advanced materials

There are many examples of exciting new developments in advanced materials, and the synchrotron is expected to be an important tool in the development and refinement of most of them. An Australian example is the development of geo-polymers, a class of 'low temperature cements' with an outstanding combination of extremely high fire- and acid-resistance, high abrasion- and scratch-resistance, very low thermal conductivity and high compressive strength. These materials are based on alumino-silicates and can incorporate many other constituents, including waste products such as fly-ash[10]. Characterisation of these materials by conventional laboratory techniques is difficult because of their semi-amorphous nature, but synchrotron-based x-ray diffraction is providing new insights into the structure and method of synthesis.

Another Australian example is the development of materials for photonic devices. While silicon single- or poly-crystals are currently used in commercial devices, new work is seeking lower cost approaches. Highly oriented thin films of zinc oxide are an attractive alternative and these can be produced on novel organometallic precursors. Synchrotron techniques are important in measuring and optimising the properties of these films[11].

Smart information

The synchrotron beamlines will produce vast amounts of information-rich high quality data. Therefore a key supporting feature of the synchrotron is the smart and efficient handling and interpreting of data. Facing up to this challenge will lead to new developments, particularly in bio-informatics for interpreting the outputs of protein crystallography.

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[10] J.W. Phair & J.S.J. Van Deventer Int. Journal of Mineral Processing, 66 (2002), 121–143.

[11] E. Lee, N.H. Tran, J. Russell & R. Lamb, J. Appl. Phys 92 (2002), 2996–2999.

Large scientific infrastructures, such as the synchrotron, have a long history of groundbreaking developments in this area. The World Wide Web had its genesis in 1990 at the European Laboratory for Particle Physics, CERN, when researchers there were seeking a platform-independent method of communicating the large amounts of data generated every day by the facility.

Safeguarding Australia

Synchrotron methods are widely applied in forensic science. For example, the infrared beamlines at the Brookhaven synchrotron are used extensively by the Federal Bureau of Investigation. The intensity and focus of synchrotron light helps to characterise precisely micro-particles of paint, hair, skin or other substances at crime scenes or crash sites. In recent work, the structure of the anthrax lethal factor was solved using synchrotron protein crystallography, and now work is proceeding to develop anti-toxins[12]. Such work relates to the goal of protecting Australia from terrorism and crime.

Personnel at the Defence, Science and Technology Organisation (DSTO) are already synchrotron users. Their work has included the characterisation and development of improved ceramic coating materials for aircraft engine components[13] and the development of sensor technology, as part of automating military hardware.

DSTO users are strong advocates of the Australian Synchrotron and envisage that the new capabilities embodied in the initial suite of beamlines will be of great value in their ongoing programs for monitoring the health of aircraft, ships and land vehicles and their propulsion systems[14].

Synchrotron research helps the Australian Defence Force to extend the life of engine components in jet engines

Jet engines can reach 1,000°C. Engine designers want them to get hotter still – higher temperatures mean more thrust. However, the ceramic coatings in engines wear under stress. DSTO scientists used the Advanced Photon Source, Chicago, to develop improved ceramic coatings and make significant cost savings in maintenance bills. Source: DSTO

Education and Research Training

The Australian Synchrotron will have a major influence on the education and research training of the next generation of Australian and New Zealand graduate students, post-doctoral fellows and other emerging researchers in the physical, chemical, materials and biological sciences.

The wide range of advanced research techniques available in a single location at a synchrotron facility, together with the opportunity to work alongside leading national and international scientists, will broaden the scope and lift the sophistication and breadth of students' and young scientists' research. The variety of scientific disciplines that are simultaneously brought together is likely to open new opportunities for working across boundaries and in innovative clusters that are linked internationally to world-class science.

At most overseas synchrotron facilities research training and the development of the next generation of scientific and medical researchers is an important activity. For example, last year there were 320 PhD students who worked at the Advanced Light Source, Berkeley, USA[15]. The Australian Synchrotron Research Program, funded by the Australian Government, has already supported 68 Australian graduate students to access overseas synchrotron light sources for thesis research during 2002–03, and sixteen PhD theses that depended in part on synchrotron research were submitted in that period.

Managers of overseas synchrotrons have noted that the collegiate atmosphere which generally exists at these facilities provides the opportunity for students to mix and discuss their work with leading researchers from advanced research organisations located around the region, with industrial researchers and with fellow students. To encourage this, special provisions are made to train and induct research students and they are given additional assistance from scientific and technical staff.

A national synchrotron facility will also assist Australia's efforts to attract and retain the most talented people. Indeed this is already starting to happen, with lively interest in scientific opportunities offered by the Australian Synchrotron being expressed by world-ranking international scientists, including a number of expatriate Australians.

Promotion of regional collaboration

Australia has an important role to play in promoting regional collaboration in science and technology and the Australian Synchrotron will be a major new drawcard for this activity.

The Australian Synchrotron, as a medium energy 3 GeV facility, will complement the lower energy synchrotrons in Singapore (0.7 GeV), Thailand (1 GeV) and Taiwan (1.5 GeV), which are better suited to the ultraviolet and soft x-ray part of the spectrum. It is likely that reciprocal access arrangements will be made with these facilities.

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[12] T.Y. Wong, R. Scharzenbacher & R.C. Liddington, 'Towards understanding anthrax: structural basis of target recognition by anthrax lethal factor', refer to website http://www-ssrl.slac.stanford.edu/research/highlights_archive/anthrax.html.

[13] J. Thornton, D. Cookson & E. Pescott, 'The measurement of strains within the bulk of aged and as-sprayed thermal barrier coating using synchrotron radiation', Surface and Coatings Technology, 120–121 (1999) 96–102.

[14] C.R. Guy, DSTO, DPSL 643/03, pers.comm.

[15] E. Moxon, Technical Communications, ALS, pers. comm.

In addition, the Australian Synchrotron has performance characteristics that can support Japanese researchers while their machines are shut down during their routine maintenance periods or when there are power shortages.

A number of links have already been established. For example, the Photon Factory at Tsukuba in Japan has provided space and support for the Australian National Beamline Facility, and Taiwan's National Synchrotron will be hosting the new soft x-ray end station during its development phase prior to being transferred to the Australian Synchrotron. In addition senior scientists from SPring-8 (the world's largest third generation synchrotron in Japan) and the Singapore Synchrotron Light Source are represented on the Australian Synchrotron International Scientific and Machine Advisory Committees.

Effectively, a 'Pacific Rim' synchrotron community already exists, with close links established with synchrotrons similar to the Australian Synchrotron such as the Advanced Light Source at the Lawrence Livermore Laboratories, Berkeley, USA and the Stanford Synchrotron Radiation Laboratory, San Francisco, USA. A collaborative beamline design project is under way with the Canadian Light Source in Saskatoon, Canada (see chapter 10, beamline 11).

Further opportunities exist to link with the National Synchrotron Research Centre, Thailand, and to provide access to South East Asian scientists from organisations such as the Indonesian Institute of Sciences.

New Zealand has a strong contingent of highly skilled synchrotron scientists. However, like their Australian colleagues, they have to travel to the northern hemisphere for beamtime. The opportunity for the two groups to interact is thus very limited at present. This will change dramatically once the Australian Synchrotron is operational; indeed, New Zealand scientists have been involved in the selection process for the initial suite of beamlines and have already identified a number of opportunities for close collaboration.

Contents of the Proposal

This proposal summarises the current status of the project and the planned capability of the Australian Synchrotron in the context of other synchrotrons around the world, including several of the latest 'third generation' designs that are currently under construction. It outlines the returns to the nation that can confidently be expected from the investment in terms of the new science it enables, the health of the nation, and the new industries and new jobs created.

The proposal gives an introduction to Synchrotron technology and the techniques that it can perform in chapter 2. Then it describes some of the new science that will be enabled by the synchrotron in chapter 3 and the proposed initial suite of beamlines in chapter 4. The process for selection of the initial suite has been guided by both national and international scientific advisory committees, and has involved extensive information sessions, consultation and workshops with experienced and potential synchrotron users in Australia and New Zealand over the past two years (see appendix 3).

Guiding principles for the beamline selection process have been:

- The initial suite of beamlines should cover 95% of the techniques that it is anticipated the Australian and New Zealand scientific community will require
- All beamlines should be of world class standard, and where possible incorporate unique features that will attract a sizeable international group of users.
- The beamlines should be user-friendly, and accessible to scientists who may not be skilled synchrotron experimentalists.
- A number of the beamlines should be designed for flexibility and easy setting up of new instruments (e.g. the Infrared Spectroscopy and the Imaging and Medical Therapy beamlines), provided this does not compromise the overall performance and operational cost of the beamline.

The Australian and New Zealand research communities are geographically broadly spread. Special emphasis will be given to enable remote access to, and operation of, key beamlines. This feature is now possible because of developments in broadband communications, rapid data-processing and specialised robotics.

Chapter 4 also includes the cost estimates for construction of each beamline and for the overall annual operating cost of the facility.

Chapter 5 gives an analysis of the user base for each beamline, based on information from researchers who are either already using synchrotrons overseas or who have registered keen interest in using the techniques. Summary tables of key researchers at senior or 'principal investigator' level are provided and it is notable that many of these have registered interest in using a number of the beamlines. This is reinforced by an analysis of the disciplines that will be enhanced by each beamline, and it can be seen that in most cases access to several – not just one or two – of the beamlines will be required. (A detailed list of names of key research leaders and principal investigators is provided in volume 2, appendix 2.)

Chapter 6 places the Australian Synchrotron in the international and regional context. It can be seen that it will be a world-class facility, comparable with new facilities that are under construction in England, Canada, France, and the USA.

Chapter 7 summarises a number of studies on the national economic benefits of the synchrotron, indicating handsome returns in improved industry competitiveness, job growth and technical status of the country.

Chapter 8 gives the project timetable showing the parallel development of each beamline and the expected timetable for full commissioning of the initial suite.

Chapter 9 discusses possible approaches to the ownership and management of the facility, noting that final details will be decided in discussion with potential funding agencies and organisations. The terms for access to the beamlines are important and a possible model is described, based on best practice of successful synchrotrons overseas.

The function of each beamline is described in detail in Chapter 10.

Scientific Context for the Proposal

More than 350 scientists have been involved over the past two years in the development of this proposal.

Many have had experience of synchrotron research made possible through the federally funded Australian Synchrotron Research Program and the Access to Major Research Facilities Program, where access has been negotiated with synchrotrons in Japan, Taiwan, the USA and Europe. While this so-called ‘suitcase science’ is extremely valuable, and recently additional access has been arranged at synchrotrons in Chicago and Taiwan, the ASRP expects that opportunities will saturate within the next four years, as the local user communities increase. Currently access to beam time takes 3–6 months to arrange and, of course, involves the expense and inconvenience of international travel. This impacts on the nature and timeliness of the research.

Furthermore, it has sometimes been difficult or impossible to use this program due to the delicate nature of samples (protein crystals, for example, can be fragile and have limited shelf life) or due to quarantine restrictions, which limits the type of samples that can be transported (e.g. soil and tissue samples). The life sciences user community, in particular, has been disadvantaged in this way.

Finally, data gathered at overseas facilities can be subject to intellectual property ownership restrictions. For example, proprietary research at the Advanced Photon Source in the USA can only be carried out subject to restrictions regarding exploitation of the products of the research in the USA.

To date Australian users of synchrotron light have tended to confine their work to one particular technique, because of difficulties of access. Once the initial suite of beamlines is established, which will offer a comprehensive range of techniques, the user will be able to examine samples from a variety of viewpoints. The extra information that can be achieved by using several techniques will add immeasurably to the quality of the research output.

In addition, because there will be many researchers using the facility at the same time, the interaction that will be generated from the inevitable contact and discussion is sure to enhance and advance the research collaboration and output. This interaction is impeded when the Australian users are itinerant visitors to many different facilities.

The advanced experimental techniques which can be performed on the Australian Synchrotron will permeate through and raise the overall level of scientific performance of the Australian and New Zealand scientific community.

The Australian Synchrotron initiative builds on the successful outcomes of the ASRP and AMRFP facilitation. In many cases, the projects that have been carried out under these schemes are directly funded by ARC, NHMRC, CSIRO and to a lesser extent DSTO.

The Australian Synchrotron is a long-overdue piece of national scientific infrastructure and we confidently expect, based on overseas experience, that within five years after operations commence in 2007 it will transform many aspects of Australia’s scientific and industrial research capabilities.

02

Introduction to synchrotron science

IMAGE: Australian Synchrotron floorplan

Layout of the Australian Synchrotron showing the positions of the LINAC injector, booster synchrotron, storage ring, x-ray shielding and beamlines. It will be possible to accommodate more than 30 beamlines in the longer term.

Chapter 02

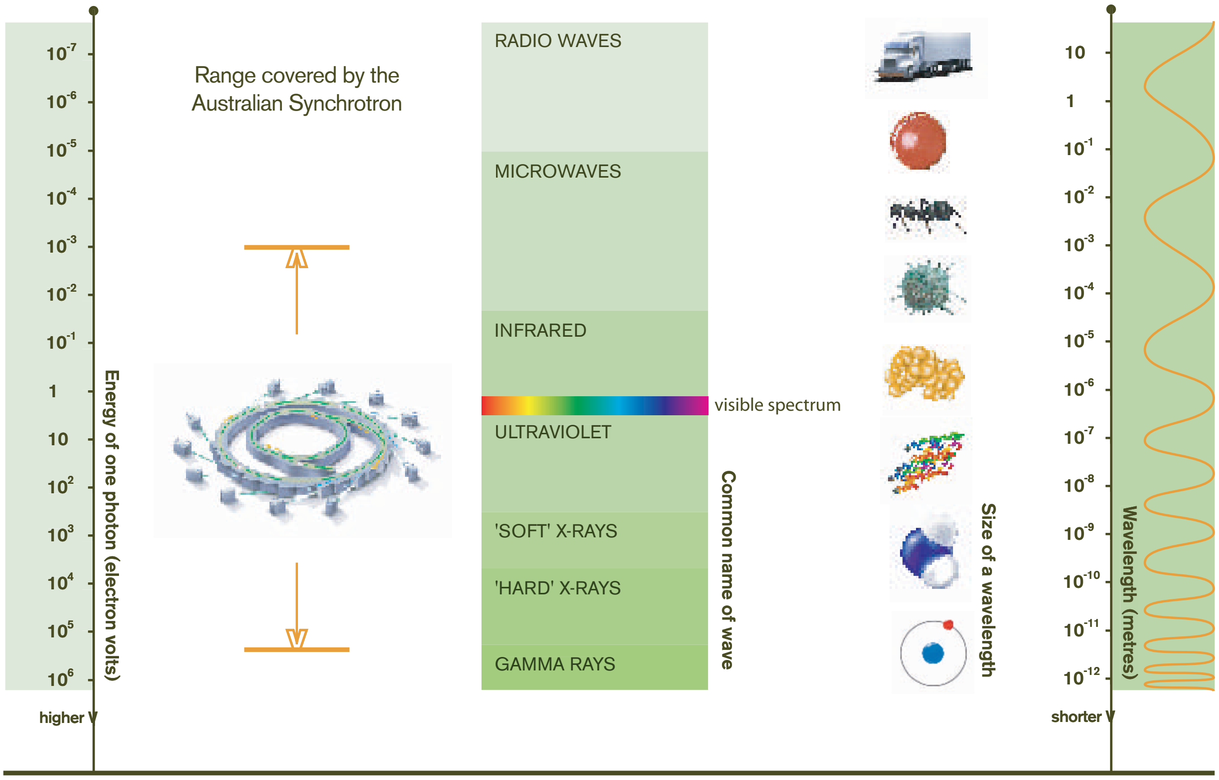
Introduction to synchrotron science

Synchrotron light (electromagnetic radiation) is emitted when charged particles, usually electrons or positrons, moving at velocities close to the speed of light, are forced to change direction under the action of a magnetic field. The electromagnetic radiation is emitted in a narrow cone in the forward direction, at a tangent to the orbit.

Characteristics of Synchrotron Light

Synchrotron light has a number of unique properties. These include:

- **High brightness:** synchrotron light is extremely intense (hundreds of thousands of times more intense than that from conventional x-ray tubes) and highly collimated.
- **Wide energy spectrum:** synchrotron light is emitted with energies ranging from infrared light to hard, energetic (short wavelength) x-rays.
- **Tunable:** through sophisticated monochromators and insertion devices (see below) it is possible to obtain an intense beam of any selected wavelength.
- **Highly polarised:** the synchrotron emits highly polarised radiation, which can be linear, circular or elliptical.
- **Emitted in very short pulses:** pulses emitted are typically less than a nano-second (a billionth of a second).



EMR The Electromagnetic Spectrum

Figure 2.1. *The electromagnetic spectrum, showing the energy range produced by the Australian Synchrotron*

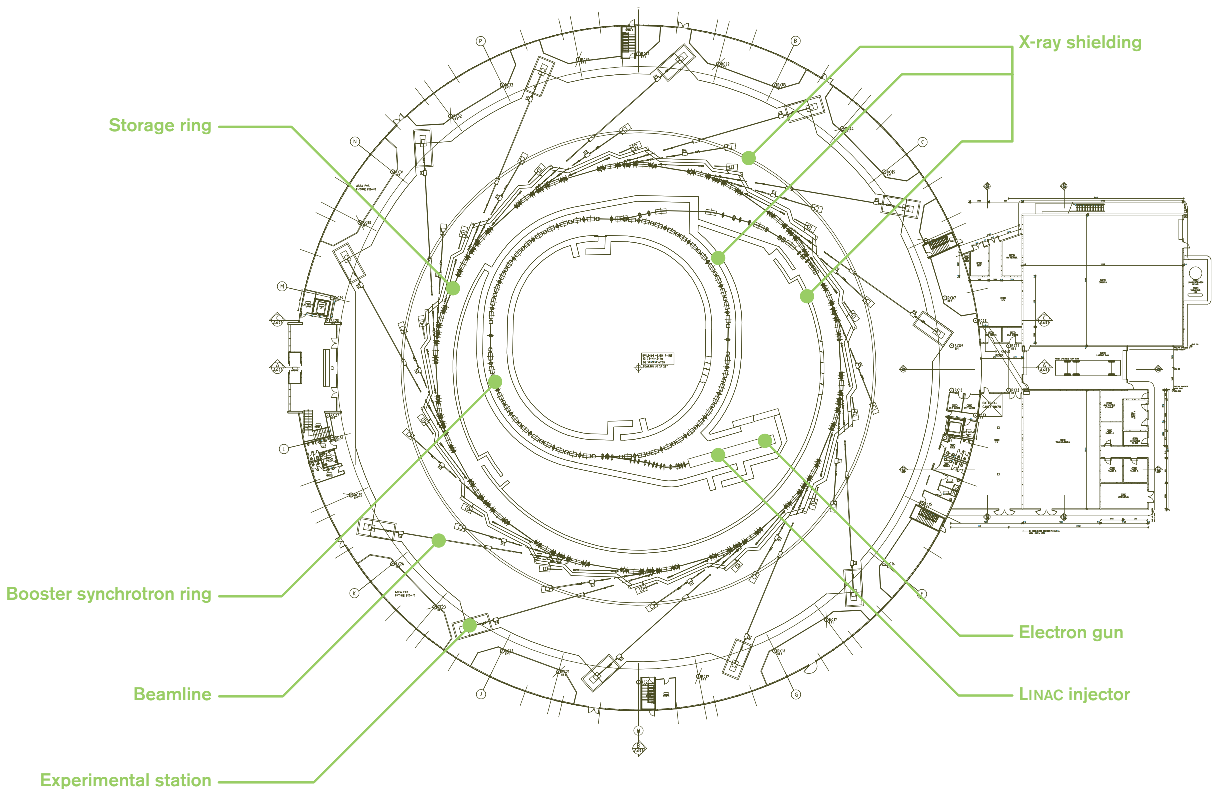
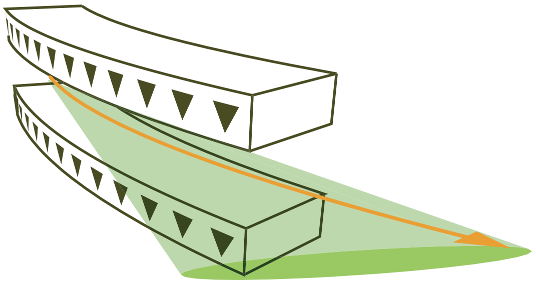


Figure 2.2. *Layout of the Australian Synchrotron showing the proposed positions of the LINAC injector, booster synchrotron, storage ring, x-ray shielding and beamlines. It will be possible to accommodate more than 30 beamlines in the longer term.*

Many techniques that provide information from materials on a microscopic and molecular scale require that the wavelength of the illuminating radiation must be of the same order as the structure. As shown in figure 2.1, synchrotron radiation is able to span the entire field of scientific interest – from lifesize imaging, down to nano-, molecular and atomic scale.



BENDING MAGNET Sweeping Searchlight

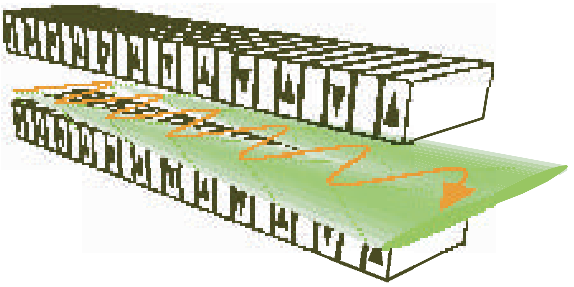
Figure 2.3. *A typical bending magnet – at each deflection of the electron path a beam of 'light' is produced. The effect is similar to the sweeping of a search light.*

Creation of Synchrotron Light

Figure 2.2 shows a plan view of the Australian Synchrotron. The electrons are generated in the centre (electron gun) and accelerated almost to the speed of light by the linear accelerator (abbreviated 'LINAC') and the booster ring, and then transferred to the outer storage ring. The electrons are confined to the circular orbit by a series of bending magnets separated by straight sections. When electrons moving at close to the speed of light are deflected they give off electromagnetic radiation, so that at each bending magnet a beam of synchrotron light is produced (see figure 2.3). These beams can be captured and used to perform a wide range of experiments – from x-ray diffraction to x-ray and light spectroscopy to x-ray imaging – by selecting parts of the beam's spectrum.

Synchrotron design has evolved rapidly over the past 20 years. In early designs the principal sources of synchrotron light were the bending magnets.

Although the intensity of synchrotron light from bending magnets is very high it was found that this can be increased by many orders of magnitude by the use of 'insertion devices' in the straight sections of the ring. These consist of two rows of small magnets with alternating polarity perpendicular to the electron beam, which move the beam from side to side. This sinusoidal trajectory causes more radiation to be emitted over and above that resulting from moving through the circular arc imposed by the storage ring's bending magnets.



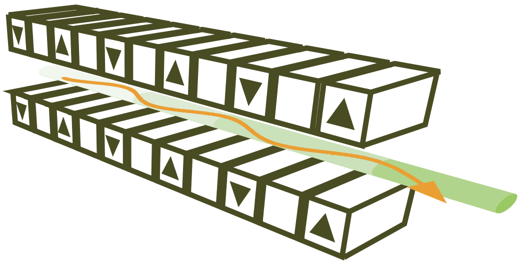
WIGGLER Incoherent Superposition

Figure 2.4. *A multipole wiggler – at the peak of each wave a beam of light is emitted. These beams reinforce each other and appear as a broad beam of incoherent radiation when viewed in the horizontal plane at a distance ahead of the wiggler.*

There are two classes of insertion devices. One is a multipole wiggler (MPW) in which a cone of light is emitted at each bend in the 'wiggle' so that the cones of light superimpose on each other, the intensity increasing with the number of bends (see figure 2.4).

The second type of device is an undulator that uses less powerful magnets to produce gentler undulations of the beam. In this case, the light cones just overlap and interfere with each other, so that certain wavelengths of light are enhanced perhaps by 10,000 times. These wavelengths can be changed by altering the gap between the component magnets so that the light is tunable to specific wavelengths (see figure 2.5).

Current ('third generation') designs of synchrotrons aim to optimise the intensity that can be obtained from insertion devices. In particular, attention is given to the size and positioning of the straight sections that accommodate the insertion devices.

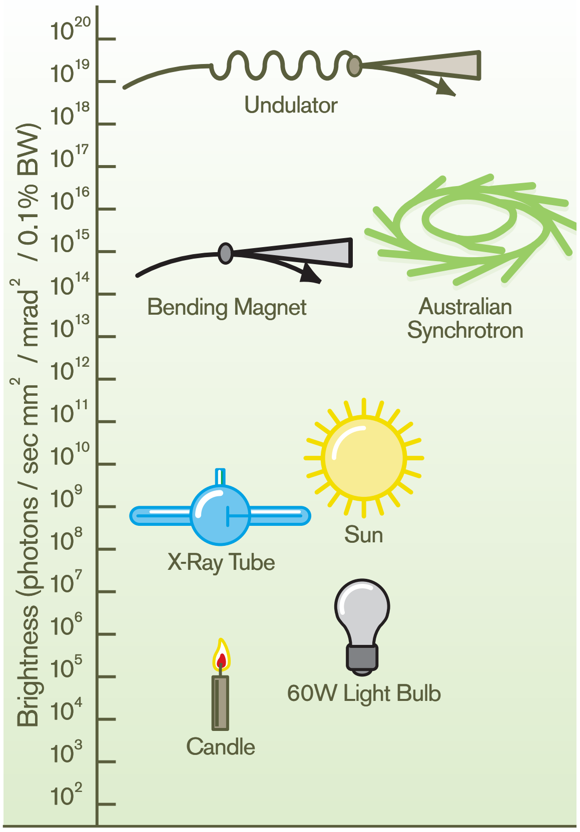


UNDULATOR Coherent Interference

Figure 2.5. *An undulator – the poles produce less deflection of the electron beam. This results in a narrow beam of coherent synchrotron light, with certain frequencies amplified by up to 10,000 times.*

In the Australian Synchrotron it is likely that the undulator magnets will be placed inside the vacuum of the storage ring; this will allow very close spacing of the magnets and extremely high light intensities. Conventional magnets can be used for the wigglers, but they may be wound with super-conducting wire, again enabling extremely high light intensities and the ability to easily tune the frequency of the light.

Thus the Australian Synchrotron, which is an advanced 'third generation' design, will be able to accommodate all the different types of light sources (bending magnets, multipole wigglers and undulators) to enable a wide range of advanced experiments or measurements to be carried out.



Comparative Brightness

Figure 2.6. *Intensity of light that can be obtained from the synchrotron compared to other sources.*

Experimental Techniques

To carry out experiments a beam originating from one of the sources travels out of the ring and down a tube that is under high vacuum, called a 'beamline'. The appropriate type of radiation is selected from the spectrum and then directed to the experimental 'end station'. The radiation can be light from deep infrared through to extreme ultraviolet light, or x-rays from soft to very hard (0.2 to 120 keV).

The experiments or measurements that can be carried out fall into four main categories:

- Diffraction/scattering for crystallography, including protein crystallography
- Spectroscopy for analysis of chemical composition and speciation in the bulk material and at surfaces, down to nanometre dimensions
- Polarimetry for measuring the shape of complex molecules, especially proteins, and the properties of magnetic materials
- Imaging from highly detailed imaging of small animals, and ultimately humans, down to the substructure of biological and physical material, using light from infrared through to hard x-rays.

It will be possible to combine imaging with analytical techniques to provide additional information in four of the beamlines – the Microspectroscopy, the Microdiffraction and Fluorescence Probe, the Infrared Spectroscopy, and the Imaging and Medical Therapy beamlines.

Apart from these measurement and imaging techniques it is possible to use the highly collimated hard x-rays for medical therapy and for micro-machining materials to micron sized dimensions, with exceptionally high depth to width aspect ratios.

Diffraction

X-ray diffraction is the most widely used approach for 'imaging' substances at atomic resolution and elucidating their structures. These substances include metals and alloys, chemical compounds, minerals, and molecular crystals ranging from several atoms to macromolecular assemblies of hundreds of thousands of atoms.

In a crystal the constituent atoms are arranged in regular arrays. When x-rays pass through the crystal they may be elastically scattered by the electron structure of the atoms. Because of the regular arrangement of the atoms the scattered waves periodically reinforce each other to form a diffracted beam (see figure 2.7). By rotating the crystal through all angles with respect to the x-ray beam, a complete diffraction pattern can be built up that is uniquely characteristic of the crystal. From this pattern it is possible to determine accurately the crystal structure by theoretical analysis and reference to molecular and crystallographic databases.

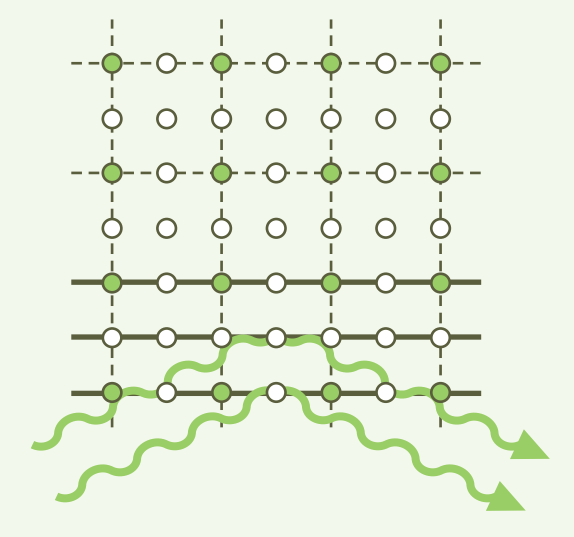


Figure 2.7. *The x-ray beam scattered by the electrons associated with the atoms in the crystal structure. Because of the regular array the scattered x-rays reinforce each other to form a diffracted ray, whose angle from the incident ray provides a measure of the distance between the planes of atoms.*

When a single crystal is examined, as will be the case for the protein crystallography and small molecule beamlines, a pattern of spots is produced on the detector – see figure 2.8.

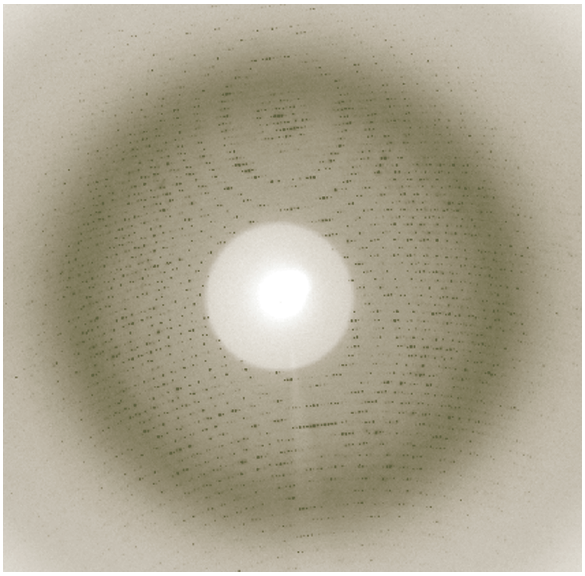


Figure 2.8. *A high resolution x-ray diffraction pattern obtained from crystals of a paramyxoviral haemagglutinin-neuraminidase. Courtesy of M.C. Lawrence, CSIRO Health Sciences and Nutrition, Parkville, Victoria*

Because the x-rays are scattered by the electrons in the crystal structure it is possible to compute not only the atomic structure of crystal but also its electron density map.

Single-crystal diffraction is the preferred method for determining the structure and electron density map. However, the preparation of diffraction-quality crystals often lags months or even years behind pioneering scientific breakthroughs, such as high temperature superconductivity. This is particularly true of many materials of major industrial or commercial importance, including zeolites, catalysts, pigments and pharmaceuticals, as well as many minerals. The ability of the synchrotron to produce intense, highly collimated x-rays and to focus them with x-ray optics to a very small spot size enables diffraction to be performed on small single crystals of many of these materials where previously this has been impossible.

Powder diffraction

When single crystals cannot be obtained, the material can be ground into a powder of tiny micro-crystals and analysed by powder diffraction. Powder diffraction is frequently chosen when the behaviour of the crystal structure under external conditions such as high pressure or high or low temperature is to be observed. In this technique a three-dimensional diffraction pattern is collapsed onto two dimensions by spherical averaging, and as a result, reflections, which would otherwise be separately measured, overlap. The resulting pattern is a collection of concentric rings, often with fine structure from the individual crystallites in each ring (see figure 2.9).

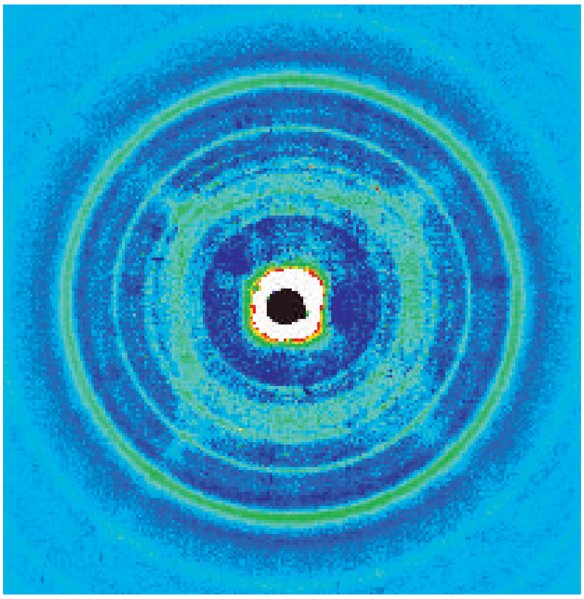


Figure 2.9. *Powder diffraction pattern of a human heart valve, showing some collagen structure and also the calcification that led to the failure of valve. (courtesy of Prof. R. Lewis (Monash University) and Dr K Rogers (Cranfield University), taken at the Synchrotron Radiation Source, Daresbury (UK).).*

The resolution that can be obtained from powder diffraction is limited by the degree of monochromaticity, the signal to background noise level ('noise' can result from scattering by the cell or air) and by the range of observations (d-range). Synchrotron radiation with its high intensity and highly collimated incident beam can be of great assistance in resolving overlaps of the diffraction rings experimentally; it also improves the signal to noise level and can increase the range of observations. Thus diffraction data obtained from synchrotron-based instruments provide much greater accuracy and resolution compared with conventional instruments.

Anomalous dispersion

Another important aspect of synchrotron light is its tunability, enabling anomalous dispersion effects to be exploited. This means that by the use of a monochromator the wavelength of the beam can be selected to maximise the visibility of certain elements in the sample. Many advanced materials contain elements that may be disordered over a number of sites within the crystalline phases, either as a result of the processing conditions or due to deliberate doping. Such disorder is often inherent in mineral samples. Anomalous dispersion effects produce element-specific information, enabling such disorder to be identified and quantified.

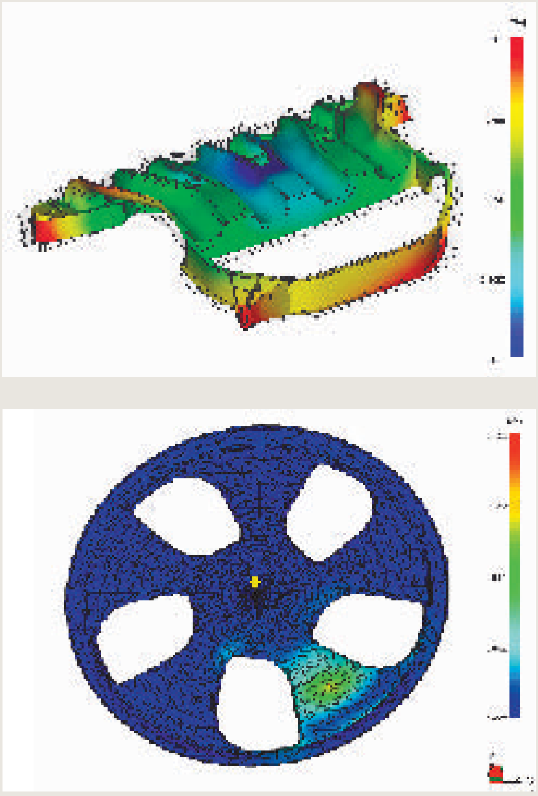
Anomalous dispersion is particularly useful for protein crystallography, especially of proteins containing seleno-methionine, where selenium replaces sulfur in the amino-acid methionine. In this technique, called 'multiple wavelength anomalous dispersion' (MAD), the diffraction patterns are measured at a number of wavelengths close to the x-ray absorption edge. The technique has formed the basis of many structural genomics initiatives, where the gene products of entire genomes are produced with seleno-methionine.

Small and wide angle scattering

Small angle scattering (SAXS) is the process of elastic scattering of x-rays from a sample, where those scattered at a small angle with respect to the original direction of the beam are detected. The information gained is primarily structural, especially for materials whose features are in the range 500 nm to 0.1 nm. Because of the inverse relationship between scattering and size, x-rays scattered at small angles give information about the size and shape of relatively large structures such as polymers and proteins.

For many experiments (such as nucleation and crystallisation) it is necessary to observe both the SAXS and the wide angle scattering (WAXS) from growing crystallite phases, e.g. from hydrothermal processes such as zeolite formation or Bayer liquor crystallisation. The wide angle diffraction gives information about structure at far smaller scales, similar to that obtained from the more standard x-ray diffraction technique. At a synchrotron beamline it is possible to collect SAXS and WAXS data simultaneously with specially designed detectors.

One of the first instruments to be built at the Replacement Research Reactor at Lucas Heights, NSW, will be a small angle neutron scattering instrument. The x-ray and neutron scattering methods complement one another, and the simultaneous refinement of data produced using a combination of both methods on the one system is very powerful. The major benefit of such analysis is the removal of potential ambiguity in the interpretation of data.



Structural analysis of a plastic part showing warp, and a plastic hubcap showing maximum stresses.

Improving plastic products

Australian researchers are using synchrotron SAXS and WAXS techniques on the Australian beamline in Japan to improve injection-moulded polymers.

- In Australia, injection-moulded plastics are an $8b industry. They are used in cars, medical devices, mobile phones, computers, TVs, toys and many other consumer goods.
- The industry needs accurate information about how polymers set after injection into the moulds.
- Monash University researcher Dr Graham Edward works with the CRC for Polymers. He says “using a synchrotron means we take days to complete work that would need months in the lab and the synchrotron results are more accurate”.

Sources: G Edward, Monash University; CRC for Polymers; Moldflow Corporation

Spectroscopy

When photons pass through any material a proportion of their energy will be absorbed by the atoms. Depending on the amount of energy absorbed an electron in an inner orbital may be ejected completely from the atom, figure 2.10a, or may be raised to a higher energy, unoccupied orbital state, figure 2.10b.

This gives rise to a number of spectrographic techniques, including:

- X-ray photoelectron spectroscopy (XPS) where the emission of photoelectrons is measured.
- X-ray absorption spectroscopy (XAS), where the degree of x-ray absorption is measured as the energy level of the radiation is increased. A typical plot that is obtained is shown in figure 2.12; it can be seen that the absorption suddenly changes at a specific energy level, which is related to the threshold energy at which an electron is ejected from its base orbital state. The position of the absorption edge is characteristic of a particular element and can be used to discriminate between elements with a high degree of precision.

When an electron is ejected from its base orbital state, a ‘hole’ or vacancy is created which is subsequently filled by an electron moving from a higher energy state to the lower state. During that process energy is given off by the electron, which can be in the form of a photon, see figure 2.10c, and the energy of the photon is characteristic of the particular atomic element. This gives rise to a third spectrographic technique termed x-ray emission spectroscopy (XES). (Sometimes XES is known as x-ray fluorescence (XRF)).

Alternatively the excess energy may be transferred to another electron in an outer orbital so that this electron now has sufficient energy to escape from the atom, see figure 2.10d. These escaped electrons are known as Auger electrons, and measurement of the emission of Auger electrons is known as Auger electron spectroscopy (AES).

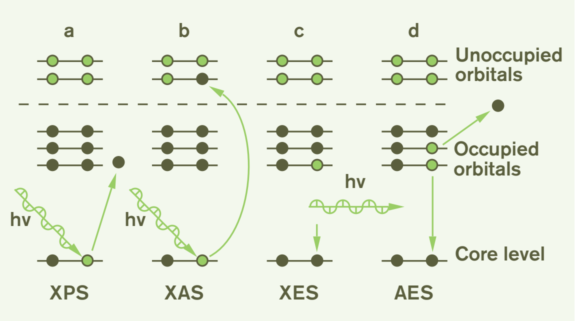


Figure 2.10. *Illustration of the changes in electron state when a photon is absorbed by an atom. These mechanisms enable (a) x-ray photon spectroscopy, (b) x-ray absorption spectroscopy, (c) x-ray emission spectroscopy and (d) Auger electron spectroscopy.*

X-ray absorption spectroscopy (XAS)

X-ray absorption spectroscopy (XAS) is a well-established, quantitative analytical technique used by both academia and industry to garner atomic-scale structural information for a wide range of systems in both liquid and solid form. XAS probes both the short and medium range order of a sample and measures disordered samples, and as such is complementary to x-ray diffraction.

As a crystal is not needed for XAS, it is not only possible to study liquids but also to analyse the elemental structure of most biological (cells, plant roots, etc.) and environmental (soils etc.) samples.

XAS measurements are made over the energy range covered by soft, intermediate and hard x-rays. Intermediate and hard x-radiation is used for studying elements from atomic number Z=20 (calcium) upwards. Soft x-radiation is used for studying the lighter elements, and also to obtain additional chemical information about elements above Z=20. For example, in the case of chromium, K-edge (~6 keV) XAS is carried out on a hard x-ray beamline, but L-edge (~0.6 keV) XAS, which provides valuable additional information, is carried out on a soft x-ray beamline.

The physical processes governing x-ray absorption are shown schematically in figure 2.11 – a photon of energy *hv* is absorbed by an atom and a photo-electron is ejected. The latter is considered quantum mechanically as an out-going spherical wave that may be scattered by neighbouring atoms. At the absorbing atom, out-going and scattered waves interfere, modulating the absorption coefficient. Accordingly, an absorption spectrum such as that shown in figure 2.12 exhibits oscillations or fine structure extending beyond the absorption edge. These gradually die away as the x-ray energy increases. The oscillations, which occur relatively close to the edge (within about 40 eV), are known as NEXAFS (near edge x-ray absorption fine structure) or XANES (x-ray absorption near edge structure), and those further out are termed EXAFS (extended x-ray absorption fine structure).

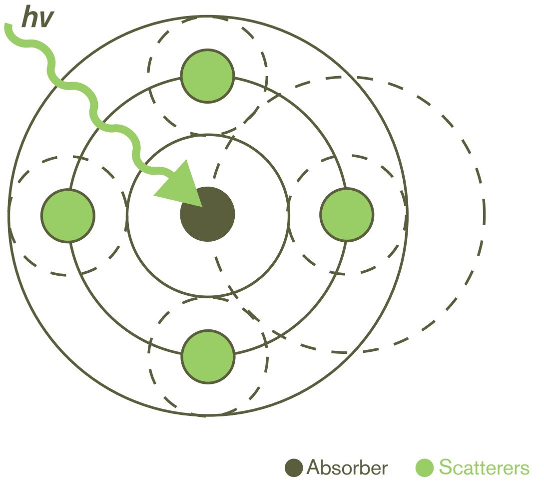


Figure 2.11. *Schematic representation of the x-ray absorption process. A quantum of light is absorbed by the central atom and scattered by adjacent atoms.*

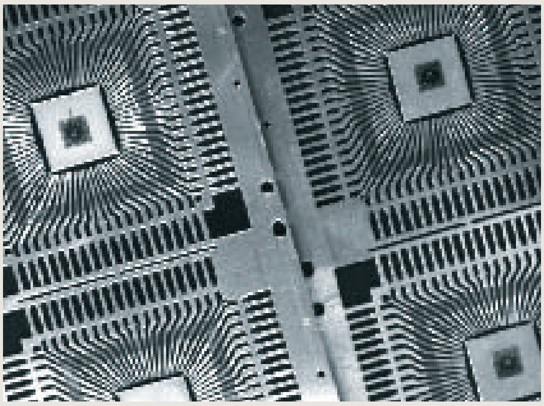
Analysis of the extended x-ray absorption fine structure (EXAFS) yields structural information such as bond lengths and coordination numbers. In closer proximity to the absorption edge, analysis of the electronic transitions and multiple-scattering processes that dominate XANES yields chemical information such as the local coordination geometry and oxidation state of the absorbing atom.

Though the fine structure of an absorption spectrum was first observed experimentally approximately 100 years ago, it was not until the 1970s and the availability of the intense, tunable source of photons from synchrotron light that the underlying physics was correctly established and XAS forever changed from a qualitative observation to a quantitative analytical technique. Despite a 30-year history and current widespread usage, the XAS technique continues to evolve both experimentally (for example, time-resolved measurements) and theoretically (for example, improved ab-initio calculations).

X-ray emission spectroscopy (XES)

XES provides similar and complementary information to XAS and XPS. A wide variety of materials including solids, liquids and gases can be analysed.

The characteristic photons measured in XES are those that arise when an electron vacancy in an inner shell is filled by an electron from one of the outer shells. The energy, E, of the characteristic photon is equal to the difference in the binding energies between the two electron levels involved in the transition. Lines are called K series lines if the initial ionisation is in the K shell, L series lines if it is in the L shell and so on.



Semi-conductor image captured with a Redlake MegaPlus Camera. Used with permission from Redlake http://www.redlake.com

Semiconductor Science

Australian materials scientists are using XAS to determine the nature of ion-implantation-induced disorder in semiconductor substrates.

- This research impacts the fabrication of both electronic and photonic devices.
- The ion implantation process is one of several basic processes used in the production of all such modern devices. The form and extent of ion-implantation-induced disorder ultimately governs device performance.
- Synchrotron XAS is the only analytical technique capable of unambiguously identifying and quantifying the homopolar bonding observed before the crystalline-to-amorphous phase transformation. (See chapter 3 for further details.)

Source: Dr Mark Ridgway, Australian National University

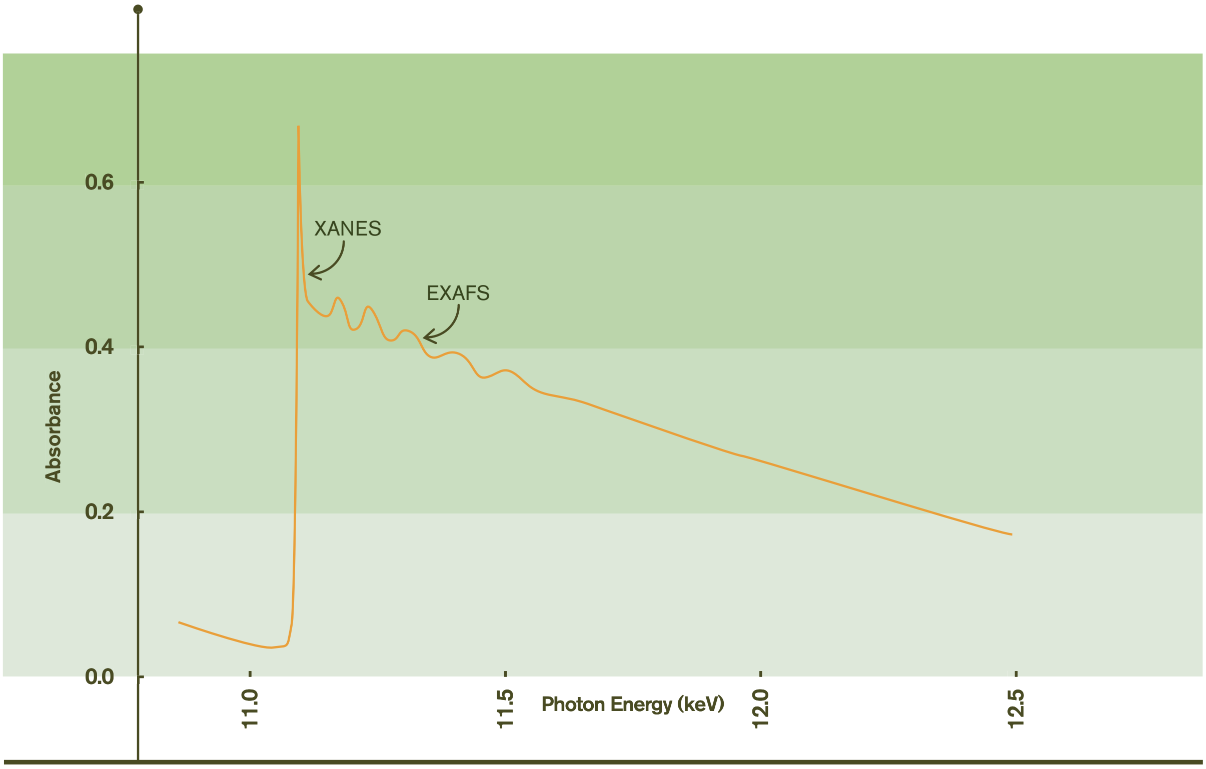


Figure 2.12. *A typical x-ray absorption spectrum*

Because XES measures photons that arise from transitions between inner electron energy levels in atoms, the technique can provide very detailed, element-specific information about the valence electron states in a compound or alloy.

The interpretation of XES spectra obtained from conventional laboratory x-ray sources, is sometimes made difficult by overlaying lines due to satellite transitions or close-lying core holes. Also, irrelevant inner core transitions may accidentally fall in the wavelength region under study. These problems can be removed by using monochromatised synchrotron radiation.

Thus the use of XES has developed rapidly in the past decade as access to tunable soft x-ray synchrotron radiation has become more readily available. Most work has been on solids, particularly electronic materials, but recently the technique has been applied to investigating metalloproteins where light elements contained in peptide chains or water molecules can be detected.

X-ray photoelectron spectroscopy (XPS)

X-ray photoelectron spectroscopy (XPS) is the most important and versatile technique for the chemical characterisation of the surface of a material. In conventional XPS, soft x-rays of fixed energy are obtained from an aluminium anode, and because this photon energy is near 1.5 keV, depending on the binding energies of the core electrons of interest, the photoelectron kinetic energies are such that the typical analysis depth is 2–5 nm. Clearly only a small proportion of this analysis depth can be considered to be the true surface layer.

In synchrotron XPS, the photon energy can be tuned to vary the kinetic energy of the ejected photoelectrons, thereby varying the analysis depth. In particular, a photon energy can be selected to result in the photoelectrons of interest having a kinetic energy near 45 eV, the energy for which the inelastic mean free path is a minimum. In this way, the surface sensitivity of XPS can be maximised and an analysis depth of two atomic layers can be achieved. By increasing the photon energy, the analysis depth is increased and information for a non-destructive chemical depth profile can be obtained.

In synchrotron XPS, the photon energy can also be tuned to alter the photo-ionisation cross-section for the electrons of particular interest. In practice, it is often highly desirable to optimise the cross-section to enhance the sensitivity for a particular element, or to change the relative cross-section for a sub-shell in two elements, but of course in both cases, a concomitant change in the depth analysed would occur. Thus, in synchrotron XPS, it is the tunability of the photon energy that is of greatest importance, but of almost equal importance is the high photon flux, because this allows high energy resolution to be selected in the trade-off between monochromator resolution and transmission. The high flux also allows photoelectron diffraction measurements to be made.

Angular Resolved Ultraviolet Photoelectron Spectroscopy (ARUPS)

Angular resolved ultraviolet photoelectron spectroscopy (ARUPS) is the pre-eminent technique for the elucidation of the electronic structure of atoms, molecules and solids. The method enables the determination of absolute binding energies of electrons in solids.

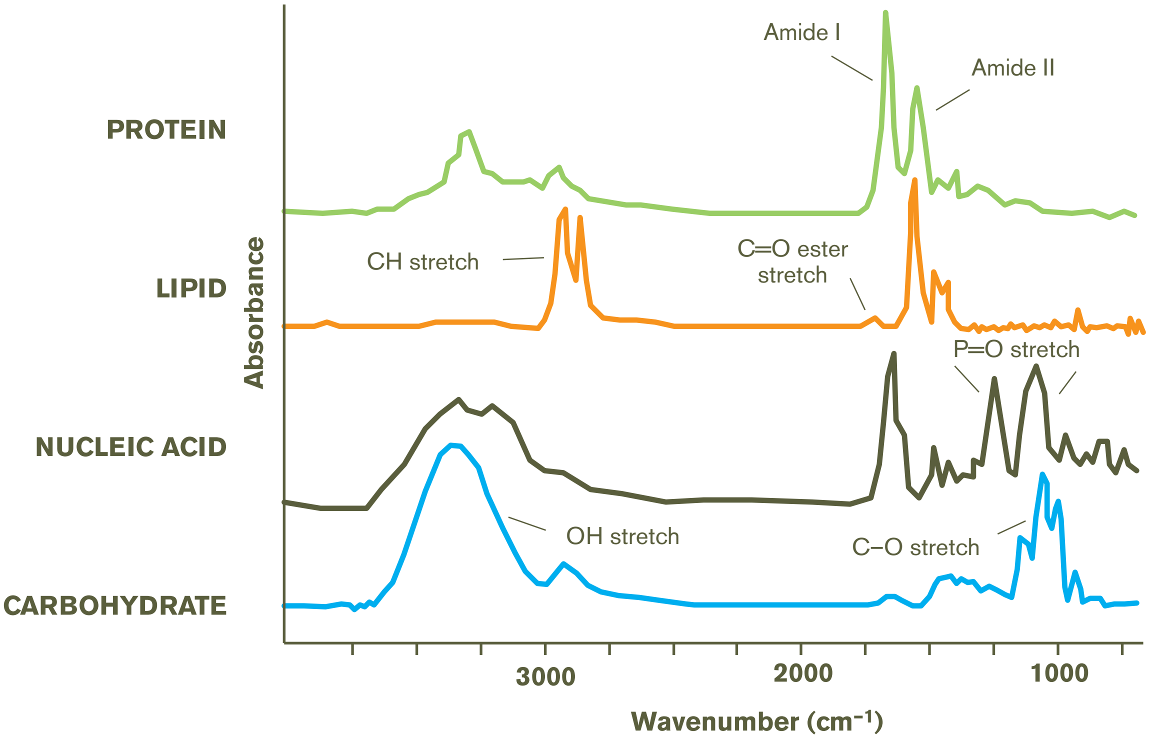


Figure 2.13. *Typical infrared spectra of a protein, lipid, nucleic acid and carbohydrate. Each has a separate, characteristic profile because of the different types of chemical bonding in the structure.*

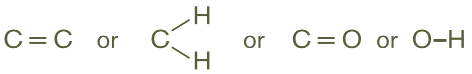
For ARUPS the sample is irradiated with VUV light (energy range from 5 to 100 eV) to excite photoelectrons into the vacuum above the surface of the sample.

In general, the emission pattern of photoelectrons is not isotropic in space, but produces a characteristic angular distribution of energies. From measurement and analysis of the kinetic energy and angular distribution of the photoelectrons, information on the electronic structure of the material in the sample, particularly Fermi surfaces, can be determined.

Due to the limited mean free path of the photoelectrons, ARUPS is a surface sensitive technique, and is especially suited to the analysis of thin films.

Infrared Spectroscopy

Infrared illumination causes atoms in a molecule to vibrate. The frequency of vibration is specific to the type of interatomic bond. For example, in a biological or polymer molecule the bonds are mostly between carbon, hydrogen and oxygen.



Each of these bonds vibrates at a different, characteristic frequency. Typical infrared absorption spectra for a protein, lipid, nucleic acid, and carbohydrate obtained by Fourier Transform infrared spectroscopy (FTIR) are shown in figure 2.13. The types of bonds present and their intensity provides a unique 'signature' for each molecule.

By analysing the spectra it is possible to identify the structures and types of molecule with a high degree of discrimination. If a characteristic peak is selected and then imaged it is possible to build a picture of the distribution of specific molecules in the sample.

Infrared spectroscopy is very widely used in Australia. Every reputable research or analytical laboratory (chemistry, physics, materials, biochemistry and microbiology) would possess an infrared system and many production facilities use the technique for quality control.

Laboratory-based microspectroscopy instruments are usually driven by globar light sources, which limit the achievable spatial resolution to 20–30 microns. Synchrotron light, which is highly collimated, polarised and much more intense (at least 100 times more intense) and stable (see figure 2.14), vastly increases the potential of the techniques:

- Using a synchrotron, spatial resolution down to the diffraction limit of 5–10 microns can be obtained. As a result it is possible to locate and analyse individual components in a sample with dimensions typical of biological cells.
- Recent advances in focal plane array detectors, when coupled with high intensity illumination from a synchrotron and scanning confocal microscopy, will enable high resolution infrared imaging in three dimensions in a realistic time frame, leading to wide application in anatomy and forensic science.
- The high brightness enables high resolution infrared spectroscopy, which is important in atmospheric monitoring, gas analysis and molecular structure determination.

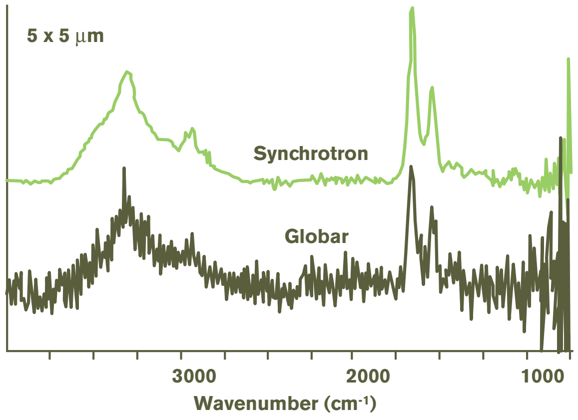


Figure 2.14. *Comparison of infrared spectra obtained from the same sample using a conventional globar-based laboratory instrument and a synchrotron IR beamline. The signal to noise ratio is substantially improved due to the greater stability of the synchrotron source.*

In isolation or when combined with other techniques, particularly diffraction and fluorescence, infrared spectroscopy is highly effective for characterising the structure, composition and state of samples – from minerals through to biological tissue.

Polarimetry

X-ray circular dichroism (MXCD)

It is possible to obtain circularly polarised x-radiation from a synchrotron which, with the appropriate design of insertion device, can be rapidly switched between both helicities.

This can be used to obtain information on a wide range of magnetic properties of materials. Examples include measurement of the spin and orbital components of element-specific and site-specific magnetic moments, measurement of element specific hysteresis loops, determination of Lz/Sz ratios, and determination of absolute local moments.

Magnetic X-ray Circular Dichroism (MXCD) arises because a magnetic material may have a different photon absorption cross-section at a particular photon energy for left- and right-circularly polarised light, see figure 2.15. This is known as the Faraday effect. By comparing the absorption spectra measured with the two opposite signs of polarisation, the MXCD spectra is obtained, which can then be interpreted to determine the various magnetic properties. Thin films, bulk materials and the interfaces between thin films can all be analysed.

The technique is essential for development of the next generation of hard disk storage devices.

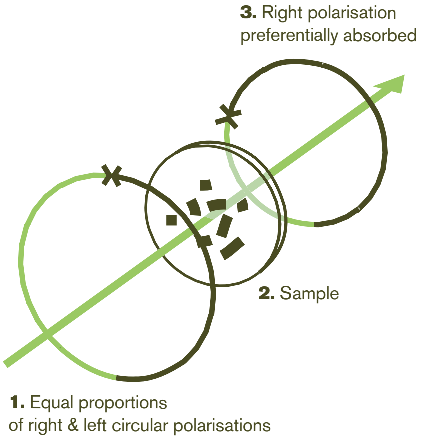


Figure 2.15. *Illustration of the principle of 'circular dichroism'. The sample may absorb circularly polarised light asymmetrically because of its electronic spin-orbit structure (in the case of magnetic materials), or its molecular bond structure (in the case of complex molecules such as proteins).*

VUV circular dichroism (VUV CD)

In the ultraviolet region of the spectrum circular dichroism can be used to analyse the conformational structure (i.e. shape) of complex molecules – for example the folding of proteins. It can also be used for examining the binding of ligands and drugs to proteins, as well as for deciphering the nature of interactions between proteins and other macromolecules. It is particularly valuable for examining both soluble and membrane proteins, which are difficult to analyse by other means because of the difficulty in crystallising them. Membrane proteins are important for drug development, because most drug delivery systems involve transfer across membranes using them.

Circular dichroism (CD) spectroscopy is possible in these materials because their polypeptide backbones are optically active and differ in their absorption of left- and right- circularly polarised UV light.

Conventional laboratory based CD instruments have been available since the 1960s and typically cover from about 190 to 250nm wavelengths. While these provide very valuable information, further information exists in the vacuum ultraviolet (VUV) wavelength region (below 190 nm), but its measurement is generally limited in a conventional instrument by the high absorption of the sample, buffer and solvent, and the low intensity of the light source.

Over the past few years synchrotron radiation has been used to extend CD measurement into the VUV region. Apart from the additional information provided it has been found that synchrotron radiation is a much more stable source so that the spectra are much clearer and provide more detail (see figure 2.16).

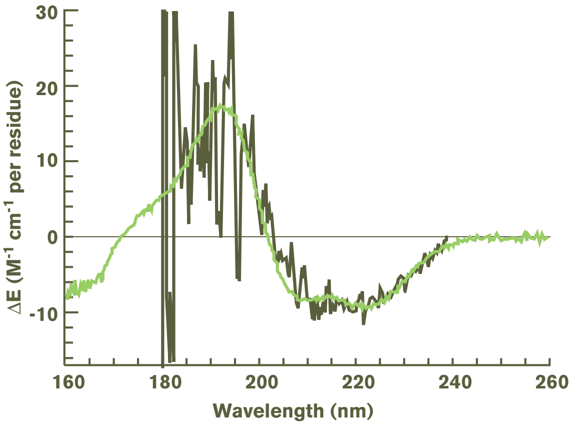


Figure 2.16. *Comparison of CD spectra for the same sample from a conventional laboratory instrument (black line) and from a synchrotron VUV CD beamline (green line). Note the improved signal to noise ratio, and the additional information at wavelengths shorter than 180 nm provided by the synchrotron. Courtesy G.R. Jones and D.T. Clarke, SRS, Daresbury, UK.*

In addition, it has recently been demonstrated that VUV irradiation in an SRCD instrument is non-damaging to protein integrity.

Parallel developments in bioinformatics are providing better definition and classification of a wide range of protein structural types, and the rapid growth in crystal structure analyses has provided a large number of protein structures from which more comprehensive reference databases can be constructed.

Taken together, these developments mean that SRCD is becoming a vital part of the suite of techniques required for modern structural biology.

Imaging

X-ray imaging

Conventional imaging with x-rays based on the absorption of the radiation has been in use for over 100 years. The contrast produced in a conventional x-ray image results from differing absorption by components in the object caused by varying composition, thickness or density. Effectively, a shadowgraph is obtained, which works well when there are very large differences in absorption between constituents – such as bone and soft tissue. However, conventional x-ray imaging of soft tissues, such as skin, cartilage, ligaments, tendons, lungs, breast tissue and tumours, produces information of poor quality.

Phase contrast

Pioneering work at The University of Melbourne, CSIRO,[1] Monash University and several synchrotron laboratories has shown that a suite of techniques, collectively known as phase contrast x-ray imaging, can exploit the valuable information that arises from the refraction of the x-ray beam by the soft tissue[2]. The different refractive indices of the various types of soft tissue cause changes in the direction and phase of the illumination and this can be detected when the highly collimated, tuned radiation of a synchrotron is used. The magnitude of the phase shift effect is approximately 1,000 times larger than the absorption, allowing much greater contrast from weakly absorbing objects such as soft tissue.

Diffraction enhanced x-ray imaging

Diffraction enhanced imaging[3] is one type of phase contrast imaging and relies upon the very small range of angles over which a perfect crystal reflects x-rays. If the crystal is placed just after the sample as an analyser and rocked through this small angular range (approximately 3 microradians) it can separate out the refraction or phase information from the absorption information in the image. The resulting images have greatly improved contrast.

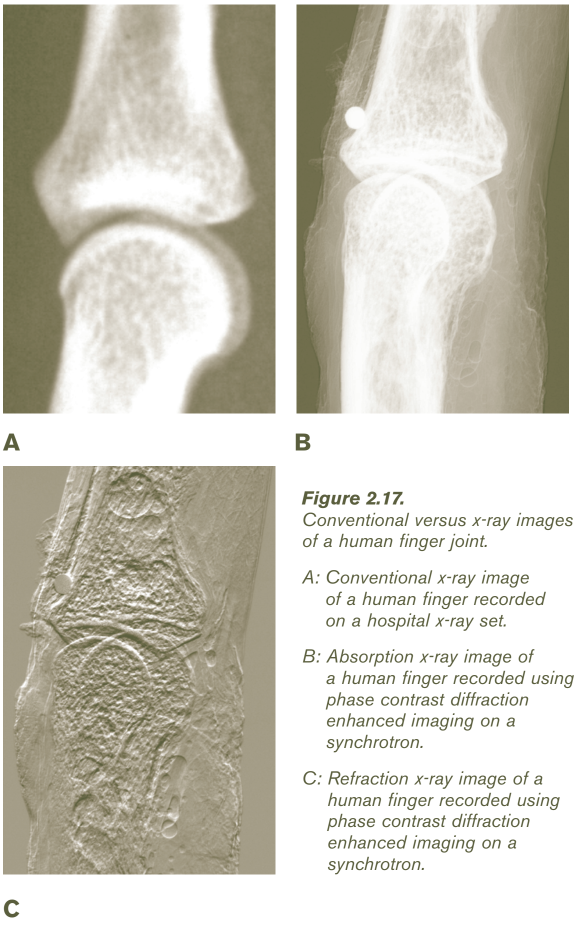


Figure 2.17.
Conventional versus x-ray images of a human finger joint.

A: Conventional x-ray image of a human finger recorded on a hospital x-ray set.

B: Absorption x-ray image of a human finger recorded using phase contrast diffraction enhanced imaging on a synchrotron.

C: Refraction x-ray image of a human finger recorded using phase contrast diffraction enhanced imaging on a synchrotron.

Images: R. Lewis, Monash University, obtained using Elettra synchrotron, Italy

Time Dependent Studies

A major advantage of a synchrotron source is that, because of the extremely high beam intensities, it is possible to study processes that are changing with time. These dynamic processes are of enormous interest in both the life sciences and physical sciences, and they represent an area where synchrotron sources are contributing valuable knowledge, unobtainable by other experimental techniques.

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[1] S.W. Wilkins, T.E. Gureyev, D. Gao, A. Pogany & A.W. Stevenson, 'Phase-contrast imaging using polychromatic hard X-rays', Nature, 384, 1996 335–338.

[2] R.A. Lewis, C.J. Hall, A.P. Hufton, S. Evans, R.H. Menk, F. Arfelli, L. Rigon, G. Tomba, D.R. Dance, O. Ellis, A. Evans, E. Jacobs, S.E. Pinder & K.D. Rodgers, 'X-ray refraction effects: application to the imaging of biological tissues', British Journal of Radiology, 76 (2003), 301–308.

[3] D. Chapman, W. Thomlinson, R.E. Johnston, D. Washburn, E. Pisano, N. Gmür, Z. Zhong, R. Menk, F. Arfelli & D. Sayers, 'Diffraction enhanced x-ray imaging', Phys. Med. Biol., 42 (1997) 2015–2025.

Time dependent studies can be done using all of the techniques that have been described. They usually require sample containment chambers that will change an external factor to the sample, for example increase or decrease temperature or pressure, vary the atmosphere surrounding the sample, introduce a chemical or biological reactant or irradiate the sample with a laser.

Some of the beamlines (for example the powder diffraction beamline) will have an environmental chamber as a standard part of their set-up, and others (for example the infrared and the imaging beamlines) will be sufficiently flexible to accommodate special purpose experimental chambers.

Micro-machining by X-ray Lithography

Lithography is the process of making mechanical parts and structures by photographically exposing a light-sensitive material (usually a photo-resist) to create patterns that may be either directly used, or act as shields to allow selective etching of lower layers. Alternatively it can produce moulds to fill with metals, ceramics, polymers, glasses or even bio- and nano-engineered materials. Lithography is the cornerstone of the semiconductor industry where the world's top ten manufacturers have combined sales in excess of US$4b annually.

The semiconductor microchip is a planar device, and the lithography techniques used are essentially two-dimensional. The emerging field of microtechnology, or MEMS, where additional functions such as actuation, sensing or microfluidics are integrated with intelligent microchips, has brought the need to manufacture devices with three-dimensional structure. Techniques used for this to date include excimer laser micromachining, UV lithography, electrodischarge machining and electrochemical machining. However none of these are capable of manufacturing structures with high depth to width aspect ratios.

In 1986 researchers at the German atomic research centre (Forschungzentrum Karlsruhre) announced the development of a deep x-ray lithography technique using synchrotron light. They called the technique LIGA, a German acronym that stands for lithography, electroplating and replicating by injection moulding or embossing.

LIGA is a major advance; it produces structures with:

- micron sized features
- aspect ratios (depth : width) of more than 100 – this is essential for power transfer in micro-devices
- optically smooth side walls – vital for telecommunication applications
- almost perpendicular walls – made possible by the highly collimated synchrotron x-ray beam.

By way of comparison excimer laser lithography achieves aspect ratios in the region of 4–16, has side wall roughness of around 75 nm R.A. or more, and produces a 7°–12° wall angle.

LIGA was developed using polymethylmethacrylate (PMMA) as the x-ray sensitive material. Pre-cast sheets of PMMA are glued to a previously plated holder and exposed to x-rays. PMMA requires exposure times of about 2–3 hours on the synchrotron. More recently an epoxy-based resist has been used that requires exposure times of the order of 60 seconds. This completely transforms the cost analysis of LIGA and has brought the process into prominence as a competitive mass production process.

Capabilities of the Proposed Beamlines

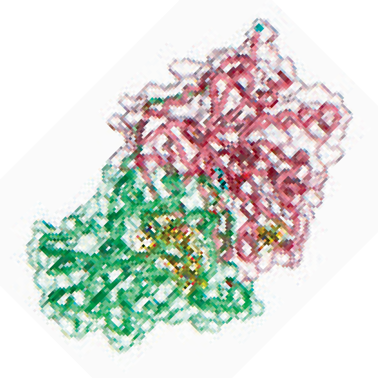
The proposed initial suite of beamlines has been selected to perform all of the techniques described in this chapter. The capabilities of each beamline are described in table 2.1.

Further information on the beamlines is given in chapters 4 and 10.

Table 2.1. Techniques available using the proposed initial suite of beamlines

Beamline Name	Techniques	Capabilities
Beamline 1 High Throughput Protein Crystallography	Medium energy, multiple wavelength anomalous dispersion XRD	Dedicated facility for crystallography of large protein crystals, set up with robotic loading and centring, and for remote operation
Beamline 2 Protein microcrystal and small molecule diffraction	Medium energy, multiple wavelength anomalous dispersion XRD	Facility with finely focussed x-ray beam for determining the crystal structure and electron density maps of weakly diffracting, hard–to-crystallise proteins, nucleic acids, and for small molecules
Beamline 3 Powder diffraction	Medium to high energy powder XRD	Versatile high resolution powder diffraction facility equipped with sample chambers for a wide range of in-situ experiments
Beamline 4 Small and wide angle x-ray scattering	Medium energy SAXS/WAXS	Measurement of long range order in complex molecules and materials
Beamline 5 X-ray absorption spectroscopy	Medium and high energy XAS, XANES, XAFS and XES	Measurement of short and medium range order, bond lengths, coordination numbers and local coordination geometry, and the oxidation state of atoms from atomic number $Z=20$ upwards
Beamline 6 Soft x-ray spectroscopy	Low energy XAS, XES, XPS and AES	As above, for the light elements , $Z < 20$. Also for the analysis of surfaces and thin films
Beamline 7 VUV spectroscopy	ARUPS, MXCD	Determination of the electronic structure and surface characteristics of solid, soft matter and gas phase substances
Beamline 8 Infrared spectroscopy	FTIR spectroscopy and IR microspectroscopy	Analysis of bond structures in complex molecules, biological materials, minerals and band structures in certain semiconductors
Beamline 9 Microspectroscopy	XAS, XANES, XAFS and XES at a submicron scale	For producing high resolution maps of elemental distribution in a sample. Also for determination of the oxidation state and coordination geometry of atoms in particles down to sub-micron size.
Beamline 10 Imaging and medical therapy	Phase contrast enhanced high energy x-ray imaging	Very flexible beamline for research into high contrast imaging of objects from small animals through to engineering components. For research into the physics and biophysics of cancer therapy techniques
Beamline 11 Microdiffraction and fluorescence probe	Simultaneous medium energy micro-XRD and fluorescence	Fast mapping of micro-XRD and fluorescence information. Especially intended for the minerals industry, environmental sciences, and manufacturing investigations
Beamline 12 Circular dichroism	VUV CD	Determination of the 'secondary' structure of biological molecules, e.g. protein folding
Beamline 13 Lithography	LIGA	Production of micro-components with very high depth to width ratio and excellent surface finish

03



New science enabled by the synchrotron

IMAGE: Two domain exoglucanase enzyme that removes glucose from plant cell walls and is used by plants for softening the plant skin so that new shoots can grow.

Image by Jose Varghese, CSIRO Structural Biology Program

Chapter 03

New science enabled by the synchrotron

Australian Nobel Prize winners William Lawrence Bragg and William Henry Bragg. Courtesy Edgar Fahs Smith. Memorial Collection, Special Collections, University Pennsylvania Library

There are many fields of new science where access to a synchrotron is essential. It is noteworthy, for example, that the Nobel Prize for Chemistry this year for 'discoveries concerning channels in cell membranes' was supported with research done at synchrotrons in the USA and France for solving the structure of the potassium ion channel.

This chapter provides an insight into the opportunities in just a few of the fields that will be possible for researchers who have access to the proposed beamlines on the Australian Synchrotron. The examples are illustrative, not comprehensive, and have been sourced from Australian research where possible.

Structural Biology

Tremendous strides have been taken over the past twenty years in the understanding of biology and the processes that make life possible. Central to this has been the understanding of the role of genes, and the sequencing of the DNA code. Recent unravelling of the human genome had led to the perception that this knowledge will help cure many intractable diseases, and that the control and manipulation of biota is possible.

Understanding the genome is important, but of greater interest in the post-genomic era is understanding the structure and function of the many proteins that are expressed by the gene. This is a very large undertaking – it is estimated that there are over one million different protein products expressed by the human genome alone.

Nobel Prizes for research with x-rays

The Australian Synchrotron will provide x-rays over a wide energy range. Since their discovery in 1895, x-rays have had an extraordinary effect on society. There have been no fewer than fifteen Nobel prizes awarded for x-ray research, listed below.

X-rays are already vital to research ranging from molecular biology through to high-energy astrophysics and there is continuing potential for exciting new science.

1901	W. C. Roentgen in Physics for the discovery of x-rays.
1914	M. von Laue in Physics for x-ray diffraction from crystals.
1915	W. H. Bragg and W. L. Bragg in Physics for crystal structure derived from x-ray diffraction.
1917	C. G. Barkla in Physics for characteristic radiation of elements.
1924	K. M. G. Siegbahn in Physics for x-ray spectroscopy.
1927	A. H. Compton in Physics for scattering of x-rays by electrons.
1936	P. Debye in Chemistry for diffraction of x-rays and electrons in gases.
1962	M. Perutz and J. Kendrew in Chemistry for the structure of haemoglobin.
1962	J. Watson, M. Wilkins, and F. Crick in Medicine for the structure of DNA.
1964	D.C. Hodgkin in Chemistry for the structure of vitamin B_{12} and penicillin
1979	A. McLeod Cormack and G. Newbold Hounsfield in Medicine for computed axial tomography.
1981	K. M. Siegbahn in Physics for high resolution electron spectroscopy.
1985	H. Hauptman and J. Karle in Chemistry for direct methods to determine x-ray structures.
1988	J. Deisenhofer, R. Huber, and H. Michel in Chemistry for the structures of proteins that are crucial to photosynthesis.
2003	R. MacKinnon in Chemistry for structural and mechanistic studies of ion channels.

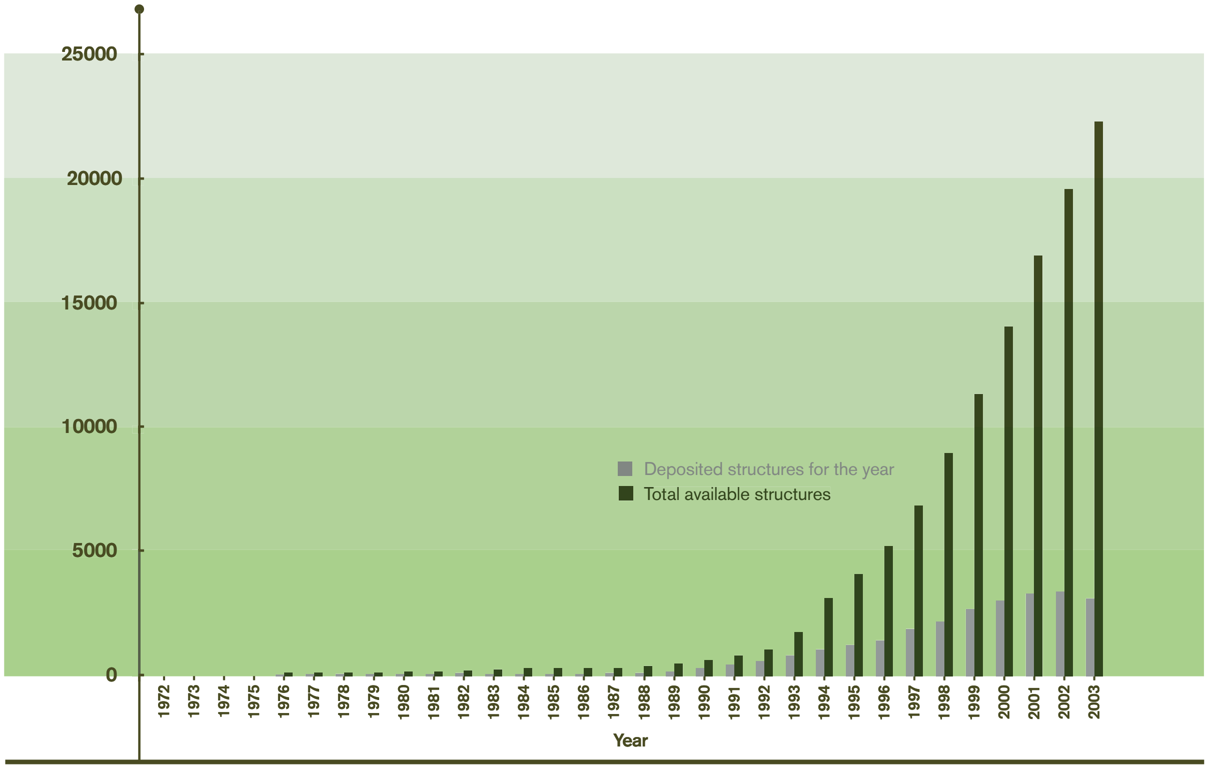


Figure 3.1. *Number of protein structures lodged with the Protein Data Bank over the period 1972 to December 2003*[1]

Thus a new field of 'proteomics' has emerged that is the systematic characterisation of the gene products of entire organisms.

Beyond proteomics, there are many more proteins produced by the immune system, and in addition to proteins, there are other complex macromolecules of key importance in biological processes, such as viruses and nucleic acids.

The determination of the three-dimensional structures of these complex macromolecules is known as 'structural biology'. Perhaps the best-known technique employed by structural biologists is protein crystallography using single-crystal x-ray diffraction, which provides the 'primary' structural information – that is, the structure of the molecule. While knowledge of the molecular structure of the crystal alone is useful, of additional and sometimes greater importance is to elucidate the shape of the molecule and how the molecule is folded – the so-called secondary or 'conformation' structure.

Although nuclear magnetic resonance (NMR), mass spectrometry and cryo-electron microscopy do provide valuable information on the primary and secondary structure of complex macromolecules, x-ray diffraction, small angle scattering, circular dichroism and microspectroscopy are the key techniques for structural biology.

Early attempts to analyse macromolecular structures used conventional x-ray and laboratory light sources; the most famous of these is probably the determination by Watson and Crick of the structure of DNA. However it was not until developments over the past decade in cloning and over-expression of proteins, more effective methods of protein crystallisation, better data collection and manipulation, cryogenic cooling of the crystals (to minimise degradation by the radiating beam), advances in computer and detector technology and, in particular, access to synchrotron light that structural biology on a large scale has been possible.

The latest developments in synchrotron techniques, using the finely focussed, high intensity beam coupled with multiple wavelength anomalous dispersion (MAD) techniques, are enabling the analysis of smaller and weakly diffracting crystals, which has previously been impossible to do.

The growth in activity has been spectacular. Figure 3.1 shows the number of protein structures registered in the international Protein Data Bank over the period 1972 to June 2002. At 7 December 2003 the number of proteins in the data bank was 23,552 of which 20,018 were determined by x-ray diffraction. The remarkable rise after 1992 has coincided with the commissioning of a number of synchrotron-based protein crystallography beamlines (see figure 3.2, which shows the proportion of protein structures determined by synchrotron techniques to 1999. It is now believed to be close to 100%.)

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[1] Annual Report of the Protein Data Bank, 2002, http://www.rcsb.org/pdb/annual_report02.pdf

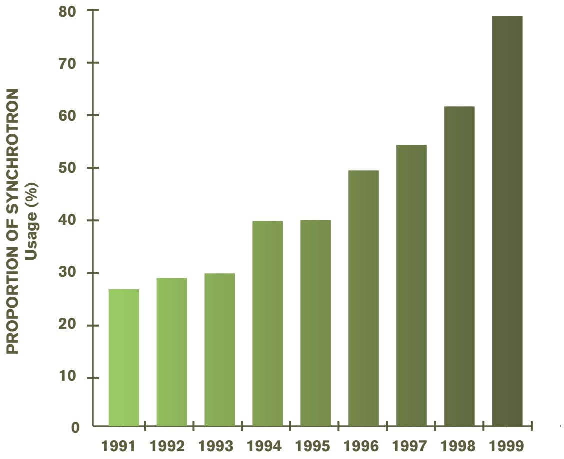

Figure 3.2. *Proportion of protein structures determined via synchrotron-based techniques*

Australia has been a significant player in proteomics – indeed the term 'proteomics' was first coined by researchers at Macquarie University – and access to the protein crystallography, SAXS/WAXS and circular dichroism beamlines on the Australian Synchrotron will be vital to remaining at the forefront of the field.

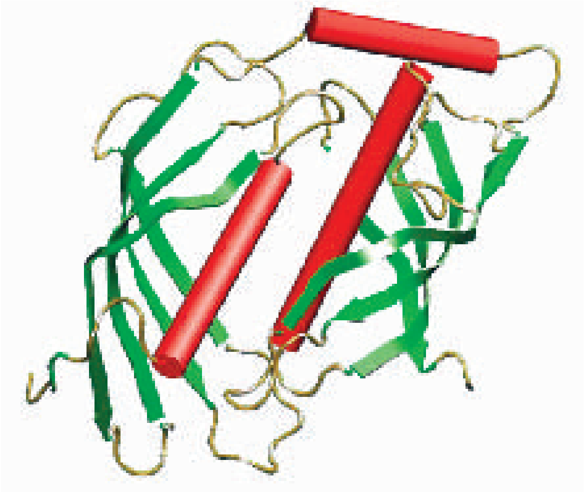

Figure 3.3. *Structure of mouse latexin, solved as a part of the structural genomics of macrophage proteins initiative at The University of Queensland. Latexin's known function is as carboxypeptidase inhibitor, and the protein is expressed at high levels in mouse macrophages and the expression increased in response to lipopolysaccharide*[2]*.*

Cellular Biology

In concert with the advances in structural biology there has been spectacular progress in understanding the molecular basis of a number of processes in the fields of cellular and developmental biology. The structure of the major histocompatibility antigen (MHC) and its complexes with other immuno-modulating factors has revolutionised molecular immunology, and similar new insights are being made into other biological processes. The structures of many hormone–receptor, protein–protein and protein–DNA complexes have now been determined, and these have laid down the foundations of the mechanisms of cellular processes.

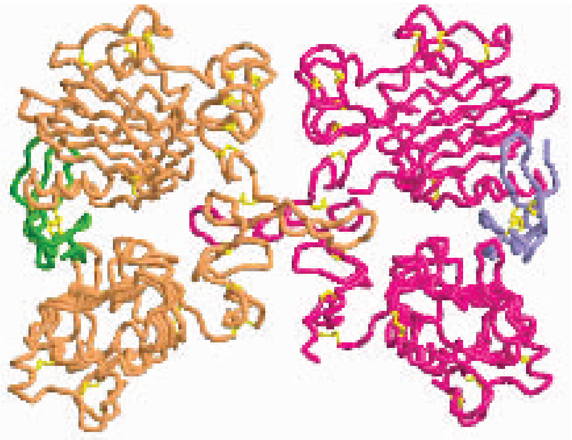

Figure 3.4. *Crystal structure of a dimer of a truncated epidermal growth factor receptor extracellular domain bound to transforming growth factor alpha*[3]*. This receptor–ligand complex is involved in the growth of many cancers. It was determined by a collaboration between the Walter and Eliza Hall Institute, Ludwig Institute for Cancer Research and CSIRO.*

An important new area, which until the advent of the synchrotron has been impossible to research, is the study of how biological signals are transmitted across cellular membranes. Areas of study include pore-forming toxins, receptors and channels.

Fundamental to further progress in this area will be the ability, using the synchrotron, to image cellular and molecular events in both normal and pathological processes. Significant advances in this field will be made by coupling knowledge of the physical sources of contrast, technological capabilities of the instrumentation and cellular and/or molecular processes.

Two major approaches are possible using synchrotron techniques – infrared microspectroscopy and x-ray microspectroscopy – and Australian researchers are at the forefront of both.

Projects at the Royal Women's Hospital in Melbourne and Monash University School of Chemistry have demonstrated that synchrotron-based infrared microspectroscopy can add a new capability to the diagnosis of cervical cancer.

Researchers, primarily at The University of Sydney, are making major advances using x-ray absorption microspectroscopy at overseas synchrotrons to image the uptake and metabolism of metal-containing pharmaceuticals in cells and tissue.

In the next few years, progress in x-ray microspectroscopy will be limited by the sensitivity of the detectors, as radiation damage issues become more important; by the precision with which the scanning can be performed; and by the ability to produce a very small x-ray focus in the scanning system.

Beamline 9 on the Australian Synchrotron will be designed with the latest technology for x-ray focussing to obtain a spot size of 0.2 microns on the sample, and with new detector systems to enable this important program to advance rapidly.

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[2] A. Aagard, P. Listwan, N. Cowieson, T. Huber, C. Wells, T. Ravasi, D. Hume, B. Kobe & J. Martin. University of Queensland.

[3] T.P. Garrett, N.M. McKern, M. Lou, T.C. Elleman, T.E. Adams, G.O. Lovrecz, H.J. Zhu, F. Walker, M.J. Frenkel, P.A. Hoyne, R.N. Jorissen, E.C. Nice, A.W. Burgess, C.W. Ward. Cell, 110(6) (2002) 763-73.

Rational Drug Design

Many medicines have been developed by traditional ‘drug discovery’ methods in which the myriad of naturally occurring compounds have been surveyed for their ability to control disease. However the explosion in the fundamental knowledge of biological protein interactions has enabled a rational approach to drug design based on theory and structural biology. The impact of structural biology on the design of medically important drugs has been exemplified by the development of the anti-influenza drug Relenza. This work was carried out within CSIRO and was the first structure-based anti-viral drug to be developed, and also a very early example of the rationally based drug design methodologies. Subsequently the new generation of drugs active against HIV such as the HIV-protease inhibitors were developed by similar methodology. Other examples have been the development of the anti-inflammatory inhibitors that were selective inhibitors of the COX-2 enzyme. There are many drugs undergoing late stage clinical trials at present for a number of human diseases ranging from cardiovascular disease to cancers that are based on the information discovered by structural biology. It is expected that this approach to finding solutions to human health problems will accelerate in the future, as it is becoming increasingly important in the fight against newly emerging and re-emerging viral and microbial diseases.

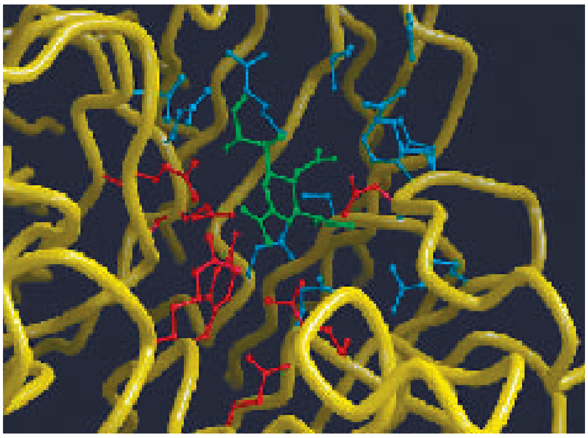

Figure 3.5. *The anti-influenza drug Relenza™ in the conserved active site of influenza neuraminidase*[4].

Rational drug design is currently being applied to many areas of drug development. Anti-viral drug developments include efforts to abate the HIV pandemic; the serious human health threat posed by hepatitis C virus, which is mutating at a rate that makes vaccine treatment ineffective; and measles, which continues to kill over a million children per year in Africa alone. Currently no drugs are available for many Third World protozoan pathogens such as sleeping sickness, and malaria is becoming increasingly resistant to current drug therapy, as are several microbial diseases such as tuberculosis and *staphylococcus aureus* infections.

Almost all drugs used in the treatment of cancer cause serious side effects because they lack selectivity for tumours over normal tissues. Selective activation relies on successful exploitation of the differences between the environment in tumours and that in healthy tissues. Tumour hypoxia, the lower than normal oxygen levels present in solid tumours, is the result of the rapid growth and poor vascularisation of tumours. For a drug to be activated in a hypoxic environment it must have an inactivated higher oxidation state and an activated lower oxidation state. To date, the development of hypoxia-selective agents has been carried out in the absence of information on the oxidation status of the agents in tumours and, in particular, how this status is affected by the degree of hypoxia. Extensive investigations of Co and Pt anti-cancer drugs using x-ray absorption spectroscopy are in progress to determine the oxidation state in-situ in different regions of tumours and in models of hypoxic tumours. This will enable the rational tuning of the reduction potentials to achieve activation in the desired regions of the tumours. Simultaneously, the project will provide information on the relationship between reduction potential and the extent of activation in hypoxic environments.

Infrared spectroscopy and circular dichroism are complementary techniques that are able to monitor the up-take of anti-cancer drugs and their effect on the conformational changes that these cause in critical proteins. Synchrotron light will add a new dimension to these studies because it will be possible to follow these processes in real time.

Co, Cu, Ni and Zn anti-inflammatory drugs are potent veterinary drugs and are likely to enter human clinical trials in the near future. X-ray absorption spectroscopy and powder diffraction have been used extensively in the characterisation of new drugs in the solid state, solution, pharmaceutical formulations and biological fluids. This research has been essential in determining the stability of the drugs in pharmaceutical preparations[5], and is providing a better understanding of the pharmacology of these drugs for the development of better and safer systems.

Toxicology

The synchrotron is a unique and powerful tool for determining the speciation of chemicals, with applications in the fields of environmental science, forensics and medicine.

Of all carcinogens, Cr has the widest occupational exposure to workers and is of growing environmental concern. Although Cr(VI) is the carcinogenic form of Cr, it does not interact with DNA in the absence of cellular reductants. X-ray absorption spectroscopy is being used to characterise for the first time the structures of a range of reactive Cr(VI), Cr(V) and Cr(IV) complexes with biological reductants. Many Cr(III) complexes, which are the ultimate products of the reductions, have also been characterised[6].

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[4] J. Varghese, V. Epa & P. Colman, Protein Science, 4 (1995) 1081–1087.

[5] J.E. Weder, T.W. Hambley, B.J. Kennedy; P.A. Lay, G.J. Foran & A.M. Rich, ‘Determination of the structures of anti-inflammatory copper(II) dimers of indomethacin by multiple-scattering analyses of XAFS’, Inorg. Chem., 40 (2001), 1295–1302.

C.T. Dillon, T.W. Hambley, B.J. Kennedy, P.A. Lay; J.E. Weder, Q. Zhou, ‘Copper and zinc complexes as anti-inflammatory drugs’ in A. Sigel & H. Sigel, (Eds) Metal Ions and Their Complexes in Medication, Vol. 41 of Metal Ions in Biological Systems, Marcel Dekker, Inc., New York, in press.

Using microfocus synchrotron radiation induced x-ray emission (Micro-SRIXE), researchers at Sydney University and ANSTO have been able to follow the uptake of Cr(III) and Cr(VI) chemical species into individual cells with sub-micron resolution[6].

In a collaboration between the Schools of Biological Sciences and Chemistry at Monash University, synchrotron based infrared spectroscopy techniques are being developed to monitor the chemistry and toxicity of microalgae and to use infrared signatures for classification of species. Apart from toxological effects, the study of microalgae is relevant to environmental research; microalgae, as marine phytoplankton, perform more photosynthesis in the world's oceans each year than do the tropical rainforests on land, and thus their life cycle has a primary effect on greenhouse gas control.

Biosystems

The electronic properties and interactions of matter at an atomic level in biological environments is very much unknown. Yet the detailed understanding of these systems is crucial to the successful development of many new technologies that have direct impact on biosystems. These include medical implants, delivery systems (for example of radiopharmaceuticals), bio-sensors and chips for diagnostics, biomimetic materials (such as the construction of artificial skin or organs) and novel artificial photosynthetic devices. Vacuum ultraviolet (VUV) light is able to probe the valence and low-lying core states of many elements in the periodic table. The interaction of such states ultimately controls the complex interactions and properties observed in biological systems.

The high flux and small spot size produced by the VUV beamline will allow for many ground-breaking experiments and studies to be performed on biosystems. Studies will initially focus on more traditional (but still not understood) systems such as the electronic properties and structure of amino acids (an essential building block) on various surfaces. One significant new direction would be the in-situ study of liquid–solid interfaces and multi-layered systems. As most biosystems are made of several functioning parts, small spot microscopy of objects as tiny as only a few nanometres to as large as a few microns in size would be of tremendous importance in order to determine the electronic state of each part accurately.

Surface science, which is supported by soft x-ray, VUV and infrared spectroscopy techniques, has recently been increasing in prominence in the biomedical area, based on the fact that many biological reactions occur at surfaces. Thus any fundamental understanding of the biocompatibility of a medical device must take into account the properties of proteins and cells at interfaces, and the characteristics of local biological reactions. Principles worked out in surface science laboratories are likely to become the basis for ways of improving the function and durability of materials featured in a wide range of medical products.

As an example, the hemocompatibility of synthetic surfaces can be improved by various biologically active substances, of which heparin is perhaps the most promising. To immobilise heparin onto biomaterial surfaces, its physiochemical properties are modified by incorporation of a specific binding agent onto the heparin molecules. The resulting modified-heparin coating material has a high affinity for a variety of synthetic surfaces, and retains all biological properties of the unmodified heparin. This offers the prospect of heparin-coated bypass circuits for use in open heart surgery, for example.

Biotechnology

Access to synchrotron light is becoming increasingly important for researchers developing industrial applications of biotechnology, in such areas as bio-remediation and biological sensors. Enzymes to degrade industrial and environmental pollutants are being designed to alter their substrate specificity by modification of the active sites of natural enzymes that degrade similar chemical moieties, by protein engineering based on the three-dimensional structure of the native enzyme. These modified enzymes themselves, or the genes that code for them, can be inserted into biological organisms that can then be used in the remediation of contaminated environments. These techniques can also be applied to the removal of toxic metals and the concentration of metals from low-grade ores. The engineering of the thermostability of enzymes used for industrial purposes at various temperature regimes can be carried out based on structural information.

The design of insecticides with increased efficacy and species specificity is also being investigated through structural biology. The new classes of insecticides target insect hormone receptors, enabling the disruption of normal insect growth, by the design of agonists or antagonists to modulate the function of these receptors. Such biotechnological applications can have an enormous impact on the environment and the rural sector, for example by the control of specific insect pests in the agriculture and livestock industries.

Nanotechnology

Nanotechnology, the science and engineering of the small or, equivalently, the study and manufacture of structures and devices of nanometre-scale dimensions, has the potential to impact our way of life profoundly. Nanoparticles (with distinctly different properties from bulk material) can be exploited in a multitude of potential technological applications (for example, non-linear optical switches). Accordingly, funding agencies worldwide are allocating considerable resources towards nanoscience and, in Australia, the Australian Research Council has designated nanoscience as a research priority area.

Synchrotron-based powder diffraction combined with x-ray absorption spectroscopy (XAS) is the ideal technique, for determination of the local arrangement of atoms within the nanoparticles.

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[6] A. Levina, R. Codd, C.T. Dillon & P.A. Lay, 'Chromium in Biology: Nutritional Aspects and Toxicology', Prog. Inorg. Chem., (2003), 51145–250.

Many nanomaterials have a disordered structure and conventional powder diffraction (e.g. Rietveld refinement) is unsatisfactory, so it is necessary to use pair distribution function (PDF) analysis. Such analysis requires the data to be collected to a much higher q-range than is possible with a conventional powder diffractometer and high energy synchrotrons are emerging as the only x-ray source capable of this.

XAS also provides information on short- and medium-range order and disorder, and studies using this technique have been initiated by Australian scientists to study both semiconducting and metallic nanoparticles in a variety of matrices for application to photonic devices and chemical catalysis, respectively. An example of semiconducting nanoparticles is shown in figure 3.6. Given that both the optical and catalytic properties are governed by the structural properties, XAS structural determinations have the potential to yield fundamental insights into the unique nature of science at the nanoscale[7].

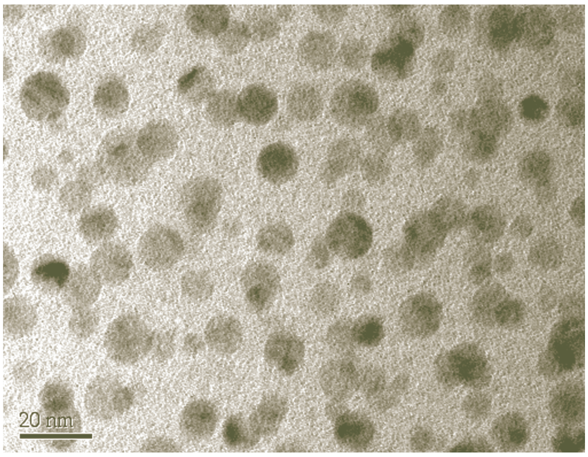

Figure 3.6. *Semiconducting Ge nanoparticles in a SiO_2 matrix for application in advanced photonic devices in telecommunications and the electronics industry[7].*

In addition the ability to focus the x-ray spot size down to the order of 0.2 microns in the microspectroscopy beamline means that for the first time it will be possible to analyse the chemical composition of individual nanoparticles.

There is clear overlap in biotechnology and nanotechnology when biological molecules are used for non-biological purposes. Knowledge of the three-dimensional structure of antibody molecules obtained through the use of synchrotron-based techniques is leading to the development of biosensors that are able to detect both biological and other chemical moieties. Rapid developments in the field of diagnostics are enabling the design and construction of biosensor chips using these antibody molecules as the detection front-end to facilitate the diagnosis of cancer and other disease states. This is proving useful in particular for future medical diagnostics 'point of care' technology. There is also an increasing interest in using biological molecules as sensors for the detection of chemicals and pathogens. This has particular relevance in the area of detection of chemical and biological weapons. Currently there are programs within CSIRO and several CRCs that are directed towards finding solutions to these goals.

Devices exploiting nanotechnology developments, such as biosensors, usually require micro-machined substrates to support the nano layers, and provide intelligence or other functions such as microfluidics. Synchrotron-based lithography provides unequalled capability to produce such substrates with truly deep three-dimensional structures and optically flat surfaces, and will become an essential tool as nanotechnology develops.

The chemical compatibility and reactivity of surfaces is also an important factor in producing nanolayers, and the synchrotron-based soft x-ray techniques will be important for characterising these surfaces as well as the layers.

Advanced Materials

Solid metal oxides – magnetic, superconducting and battery materials

The majority of advanced inorganic materials used in magnetic, conductivity, superconductivity, ferroelectric, catalytic and battery applications are solid metal oxides. Numerous groups across Australia are actively studying the properties and structures of metal oxides. In general such inorganic materials are prepared and used as polycrystalline ceramics or powders. Powder x-ray diffraction is a key characterisation method and synchrotron radiation is often required.

Metal oxide chemistry is dominated by classes of materials having crystal structures derived from a simpler parent structure, such as perovskite or rutile. Small lattice distortions, which are critical to the key electronic and physical properties of these oxides, usually lead to lower symmetries and superstructures. These distortions are characterised by subtle peak splittings and the appearance of weak superlattice reflections in the diffraction data. The detection and understanding of such distortions using powder diffraction methods usually requires high resolution that is only afforded by synchrotron radiation. Typical examples include the polar distortions in bismuth oxide ferroelectrics, Jahn-Teller distortions in manganese oxide battery materials and valence ordering in CMR (colossal magnetoresistance) materials. Phase transitions between the distorted structural variants influence the stability and processing of the materials. Such distortions often lead to twinning making it impossible to synthesise diffraction-quality single crystals easily. This is critical in emerging areas. Powder diffraction does not suffer from this problem and historically has been the tool of choice to study novel oxides.

An underlying feature of many of the most interesting materials is the strongly correlated behaviour of the electrons and coupling of the electronic charge and spin degrees of freedom with those of the electron orbitals and the lattice. The greatest potential for functionality is

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[7] M.C. Ridgway, G. de M. Azevedo, C.J. Glover, D.J. Llewellyn, R.G. Elliman, B. Johannessen, D.A. Brett & G.J. Foran, 'EXAFS characterisation of Ge nanocrystals in silica', Nucl. Instrum. Meth., submitted (2003) (invited contribution).

in materials at the edge of a structural and/or electronic instability, where small changes in chemical or physical conditions lead to a major change in properties. Establishing the role of these perturbations requires careful variation. The success of such parametric studies is reliant on rapid data collection (about 5 minutes per data set) without compromise of data quality. The importance of such studies is illustrated in the identification of an intermediate thermal phase in the unusual 4d ferromagnet $SrRuO_3$. This phase was only correctly identified after collecting high resolution data in 5°C temperature intervals over a wide temperature range[8].

Australian researchers have an enviable reputation in the study of incommensurate structures. Previously such studies have been limited to samples where high quality single crystals are available. However, the presence of structural modulations can by themselves preclude the formation of suitable single crystals. The superb signal-to-noise at synchrotron powder diffractometers can reveal the extremely weak superlattice reflections associated with such modulations, and considerable effort is being directed towards the analysis of such structures from powder diffraction data. A number of key materials exhibit modulated structures, including Cu superconductors and layered Bi oxide ferroelectrics[9].

Electronic and opto-electronic materials

A niche area in which Australian research has made a significant contribution is the development of thin film materials for electronic and optoelectronic devices. Thin films of materials with particular chemical and/or physical properties such as piezoelectricity are typically deposited onto an appropriate substrate by one form of chemical vapour deposition, and during the development phase for both precursor and deposition conditions the physical and chemical properties of the film must be determined. As in most surface characterisation, conventional x-ray photoelectron spectroscopy (XPS) is used for initial chemical analysis, but XPS is rarely able to reveal the orientation of film crystallites. Synchrotron-based variable-angle XAS is the most effective technique for determining this important characteristic.

A major thrust for new knowledge and understanding of spin-dependent phenomena in atoms, clusters, ferromagnetic films and surfaces is developing from the ‘two-particle coincidence reflection spectroscopy’ technique which leads to surface information unobtainable by any other method. The technique allows a description of spin-dependent interaction potentials and electron correlations which determine the enhanced magnetic moments of atoms, surfaces and magnetic coupling between, for example, a magnetic and a non-magnetic material or magnetic layers separated by a spacer layer. This information is the basis of spin-electronics (or magneto-electronics) in which the spin as well as the charge of the electron is a determining factor. For example, a system of alternating ferromagnetic and non-magnetic metal layers can change its electrical resistance from small (with parallel magnetisation) to large (with anti-parallel magnetisation) to form a ‘spin-valve’ in the 'read head' of hard disks. It allows the 'write/read head' to be made smaller and the storage density on hard disks to increase to above 10^{10} bits/cm^2. Research using a synchrotron is expected to provide a basis for further reduction in size and greater density.

Trace metallic impurities at ultra-dilute levels have become a significant concern for silicon microchip manufacturers seeking ever improving performance. Recent research has shown that it is possible to trap these impurities on the inner surface of nanocavities in the silicon substrate. Figure 3.7 shows an example of nanocavities that effectively getter or trap the metal impurity atoms at depths beyond the device’s active region. The very high intensity of a beam derived from a wiggler, planned for the XAS beamline (beamline 5), enables measurement of concentrations of these impurities at parts per billion level using XAS and can be used to study the trapping mechanism.

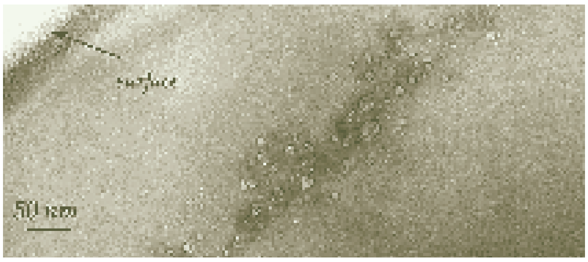

Fig 3.7 Nanocavities for entrapping and immobilising impurities at the parts per billion level in silicon substrates for ultra-high performance micro-circuits (Source: M. Ridgway, ANU)

Catalysts

Catalysts are vital for many industrial, biotechnological and food manufacturing processes, but how they work is often not well understood. Understanding their reaction mechanisms on an atomic scale is a key part of developing new and better catalysts. Combining microspectroscopy and imaging will provide new information on the chemistry and physical structure of a material’s surface, which will give important clues to how catalysts function.

The redox state dependence of the reactions and reactivity of transition-metal complexes is a key distinguishing characteristic of the d-block elements. This characteristic is pivotal to their remarkable ability to act as catalysts for an extraordinary range of reactions and explains the vital role of transition metals in a broad range of enzymes. Both in biological and abiological contexts transition-metal catalysis is essential for life as we know it. Metalloenzymes are examples of exquisitely designed low-temperature, low-pressure, low-volume catalysts. In contrast, the catalysts typical of the chemical industry are capable of high-volume chemical transformation but at the cost of high-temperature and/or pressure. Elucidation of the molecular details of the chemistry associated with enzyme catalysis is thus important because of the potential this offers for the

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[8] B.J. Kennedy, B.A. Hunter & J.R. Hester, ‘Synchrotron X-ray diffraction reexamination of the sequence of high temperature phases in $SrRuO_3$’, Phys. Rev. B., (65), 224103 (2003).

[9] C.D. Ling, J.G. Thompson, R.L. Withers & S. Schmid, Acta Crystallographica., B55 (1999) 306–312.

discovery of energy-efficient large-volume catalysts and the light that these investigations cast on our general understanding of chemistry. Accordingly, XAS studies are in progress to improve understanding of the influence of redox or charge state on the electronic and molecular structure of metal complexes or clusters so as to better anticipate (and ultimately control) the reactions and reactivity of transition-metal catalysts. The metal clusters that lie at the active site of the nitrogenase and hydrogenase enzymes provide challenging, but important, target molecules for this work. Techniques, including the use of infrared, ultraviolet and electron paramagnetic resonance spectroscopies, have been developed to permit in situ spectroscopic examination of reactive electro-generated species to complement direct structural characterisation with XAS.

XAS studies will be used to identify efficient abiological catalysts to provide a low-cost, energy-efficient production of ammonia and catalysts for H_2 fuel cells based on cheap and abundant chemicals. Progress depends upon the determination of the molecular structure of reactive intermediates that, with the aid of the increasingly powerful suite of theoretical techniques, can then be used to drive catalyst design. XAS studies enable time-resolved XAS measurements of dynamic systems. These advances will be essential toward the implementation of the catalyst into a process control environment.

Microporous materials such as zeolites have great potential as catalysts, sorbants and micro-reactors. These materials typically have large unit cells and often contain large voids that are invariably responsible for their key properties. Analysis of their structures is vital to understand the way they function, but is very difficult. It is not uncommon to observe weak and complex x-ray diffraction patterns due to low symmetry or subtle distortions. The small molecule diffraction end station on beamline 2 will be an important new tool for this task.

Metals and Alloys

The development and production of metals and alloys are of fundamental importance for any advanced society that is dependent on sophisticated elaborately transformed manufactures.

Many different types of metals and alloys are now available, each tuned with the required combination of physical, mechanical and chemical properties to suit a specific application. These combinations of properties are achieved by the development of highly complex microstructures through the addition of alloying elements, together with thermal and mechanical treatments.

The understanding of the role of microstructures and their influence on the alloy properties has been made possible by access to a wide range of measurement and imaging techniques, especially optical and electron microscopes and microprobes, x-ray imaging and x-ray diffraction. As a result, remarkable progress has been made, but there are still many aspects of alloy design not fully understood and plenty of opportunity for further improvement. The advanced techniques possible with the synchrotron are bringing new tools to this task.

Particular techniques that will make valuable new contributions are:

- x-ray absorption spectroscopy to obtain knowledge on the short and medium range order, coordination numbers and local coordination geometry of the elements at an atomic level in complex alloys
- higher resolution x-ray diffraction on a micro scale to be able to understand subtle changes to crystal structure that occur with the addition of alloying elements and to be able to measure internal thermal and residual strain distributions in microstructures
- phase contrast enhanced hard x-ray imaging to be able to see microstructures and defects in structures inside the material on a three-dimensional basis
- in-situ imaging of the liquid to solid transformation that occurs during the casting of an alloy, to observe the nucleation and growth of grains and dendrites and the segregation of alloying elements
- in-situ imaging of the microstructural transformations that occur on thermal treatment or mechanical deformation of alloy systems
- in-situ observation of the corrosion mechanisms that occur at the surfaces of alloys under a wide range of environmental conditions.

Australia is a major producer and exporter of metals and alloys, particularly for manufactured goods such as motor vehicles. While the major material used in a modern automobile is steel, the move to improve fuel economy in order to reduce greenhouse gas emissions has led to a search for high strength, low density alloys. Australia is responding to this with the Light Metal Action Agenda and initiatives such as CSIRO's Light Metals Flagship. Major programs are under way to develop new low-cost magnesium, aluminium and titanium alloy systems. Synchrotron techniques will be extensively used by the researchers in these programs because of the ability of high energy, high brightness x-rays to penetrate deeply into these metals.

In some of the most advanced light metals the incorporation of ultra-fine refractory fibres has been considered to strengthen the material. The performance of this type of strengthening mechanism depends critically on the residual strains and the efficiency of stress transfer at the fibre/matrix interface. Synchrotron x-ray diffraction techniques are an excellent method for measuring internal stresses, particularly for monitoring in real time the changes that can occur when straining or thermally treating the material.

Engineered Components

The measurement of residual strain fields in the surface and subsurface (0.01 to 1 mm) region is important in understanding the long-term performance of mechanical engineering components. This depth range is where most of the degradation of mechanical components during service originates. It also covers the thickness range of many protective coatings (for example, thermal barrier coatings) and surface engineering treatments (for example, laser shot peening).

The large flux of high energy x-rays coupled with the ability to scan components in beamline 10 will enable the two-dimensional mapping of strain and grain texture in practical times. It will be a major advance over the alternative techniques that are currently used – neutron methods which have insufficient spatial resolution (1 mm) and laboratory sourced moderate energy x-rays which are limited to investigating the top 0.01 to 0.05 mm.

Earth and Environmental Sciences

It is clear that earth and environmental sciences are of crucial importance to Australia. Environmentally sustainable ore extraction, mineral processing, coal combustion and soil use are merely a few of the areas that will continue to require significant research support. Synchrotron techniques are already opening up new ways to address the complex problems arising from earth resource utilisation, and this contribution is expected to increase.

Evaluation of an ore body

The economic viability of a potential new ore body depends on many factors. One of the most important factors is the ease of mineral processing. Mineral bodies contain a number of crystalline and amorphous phases that contain complex distributions of metal cations. The optimising of mineral processing conditions is often dependent on the precise composition of the ore and this generally requires very high resolution data. Although the presence of major phases is often easily established using conventional x-ray methods, the quantification of all the species present, including establishing the distribution of the metal cations, requires extremely high resolution coupled with high signal-to-noise data. The use of lower grade ores with increasing complexity in mineralogy is accelerating this requirement.

Often, an understanding of mineralogical changes that occur during processing is derived from equilibrium studies that only provide information about the final product in an idealised 'steady state' operation. However, few mineral processing operations operate in this mode. In order to understand chemical and physical properties of minerals, it is important to obtain information under conditions that emulate the 'real' processing conditions. This information can be derived from so called in-situ experiments where the sample is subjected to elevated temperature, pressure (typically hydrothermal pressure), sample pH and so on during powder x-ray diffraction data collection.

Two recent Australian examples of the use of in situ XRD (x-ray diffraction) experimentation in the mineral processing area are:

- the pressure acid leaching of Ni-laterites at real processing conditions of 250°C and 600 psi in H_2SO_4. The experiments showed the formation of an intermediate phase kieserite $MgSO_4.H_2O$ that cannot be observed in ex situ experiments due to its negative temperature coefficient of solubility[10].
- the formation of silico-ferrite of calcium and aluminium (SFCA). SFCA is the major bonding phase for the iron-ore sinters used in the production of iron and steel. The experiments have allowed study of the mechanism of SFCA formation, observation of intermediate phases directly with respect to time and temperature, and derivation of the order and comparative rates of phase formation throughout the experiments.[11]

Mineral beneficiation – flotation

The surface chemistry of metal sulfides is of major importance in the separation of the valuable and unwanted components in base metal ores, in the hydrometallurgical processing of a concentrate to produce the corresponding metal from the sulfide, and in the leaching of rejected material in waste heaps. Over the past thirty years, conventional x-ray photoelectron spectroscopy (XPS) has provided a wealth of information in these areas, however, because of the several nanometre analysis depth, establishing the chemical nature of the true surface layer has been difficult. Since the application of synchrotron XPS to mineral fracture surfaces, the importance of surface chemical states arising from relaxation of the outermost layer following fracture has become evident. Enhanced surface sensitivity is achieved by determining the S 2p spectrum from a sulfide mineral fracture surface with ~200 eV synchrotron x-rays compared with 1,487 eV x-rays in conventional XPS. For example[12], in the case of pyrite, the additional states present at the surfaces are believed to be S^{2-}, arising from broken S–S bonds, and S_2^{2-}. The relevance of surface states to industrial-scale processes lies in their influence on surface reactivity, and this reactivity can be monitored by synchrotron XPS when mineral fresh fracture surfaces are subsequently exposed to different environments.

The enhanced surface sensitivity provided by synchrotron XPS, as well as the ability of angle-dependent NEXAFS (near edge x-ray absorption fine structure) to reveal orientation, have also assisted elucidation of the mechanism by which flotation reagents interact with the surface of minerals. By contrast, investigation of passivation layers that slow the dissolution kinetics in the hydrometallurgical processing of mineral concentrates is usually hindered not by a lack of surface sensitivity but because a near-surface, yet buried, interfacial layer must be characterised. In that situation, it is the non-destructive chemical depth profiling ability of NEXAFS spectroscopy that is exploited, and attempts are currently being made to augment the XAS data with threshold XAES (x-ray Auger-electron spectroscopy) measurements. The principle underpinning the threshold XAES approach is that, by incrementing the photon energy through the

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[10] Unpublished data from CSIRO Division of Minerals, supplied by I. Madsen et al.

[11] I. Madsen, et al., paper submitted to J. Applied Cryst.

[12] A.G. Schaufuss, H.W. Nesbitt, I. Kartio, K. Laajalehto, G.M. Bancroft, & R. Szargan, 'Reactivity of surface states on pyrite', Surf. Sci., 411, (1998) 321-328; A.G. Schaufuss, H.W. Nesbitt, I. Kartio, K. Laajalehto, G.M. Bancroft, & R. Szargan, 'Incipient oxidation of fractured pyrite surfaces in air', J. Electron Spectrosc. Relat. Phenom., 96 (1998) 69–82.

absorption edges for the different species present, it should be possible to identify an interfacial species under resonance conditions, even if that species might be present in only a thin interfacial layer.

Environmental issues

Mineral weathering resulting in the release of acid mine drainage (AMD) is now of considerable environmental concern. It is estimated that in Australia remediation costs will be in the order of $900m over the next 15 years[13]. The dual XRF–XRD (x-ray fluorescence–x-ray diffraction) mapping facility of the Microdiffraction and Fluorescence Probe will enable the identification of reaction and re-precipitation layering on mineral surfaces as a functioning of weathering. Understanding the evolution of these layers in terms of both their elemental composition and crystalline phase is important to the prediction and control of AMD[14]. This combination of analyses will enable significant contributions to be made to the understanding of the release of toxic elements, which often accompanies AMD, and their bioavailability[15].

Another example is mine tailings containing arsenic. Arsenic (As) can exist structurally bound in compounds such as $FeAsO_4$ or adsorbed onto the surface of minerals such as goethite (FeOOH). The manner in which the As is incorporated has a strong impact on its 'availability' to the environment and hence on the steps that must be taken in the remediation of contaminated sites. The synergistic use of the XRF-XRD mapping facility together with x-ray absorption spectroscopy (EXAFS) is important in understanding the nature of contaminant metals at the molecular level so that appropriate action can be taken at the macro level.

Imaging

Perhaps better than any other method, images provide us with an intuitive understanding of the subject. It is therefore perhaps surprising that the exploitation of synchrotrons for imaging arrived rather later than their use for diffraction and spectroscopy. Nevertheless, the three largest synchrotrons now have substantial numbers of people and several beamlines dedicated to advanced x-ray imaging techniques, and imaging is one of the most rapidly expanding areas of synchrotron science. The use of synchrotrons for imaging has led to the development of new approaches that provide unprecedented resolution and contrast of nature's smallest details. Australian scientists, based largely in Melbourne, have helped pioneer the development of many of these techniques and are regarded as among the world leaders in the field. One aspect of this work relates to the development of phase-contrast based imaging techniques that transcend the conventional reliance on absorption to produce contrast. A second relates to the development of theory to make these imaging techniques quantitative. These developments provide the basis for major advances in x-ray imaging science that are not only relevant for synchrotron-based imaging but also to radiography with conventional sources.

Biomedical imaging

Despite being by far the most popular medical imaging modality, lack of soft tissue contrast is a significant problem in both medical and biomedical x-ray imaging. The relatively small variations in density and composition of soft tissues mean that their x-ray attenuation characteristics are very similar. Conventional radiography produces images through the differential absorption of x-rays, and so provides very little soft tissue contrast unless high doses are employed as in computed tomography. Synchrotron-based imaging techniques produce high resolution images using differences in the refraction and scatter of x-rays as they pass through tissue. Genuine soft tissue contrast with micrometre-scale resolution is possible.

Furthermore the collimation and monochromaticity of an imaging beamline allows high resolution images to be recorded at far lower doses than required by conventional equipment. This capability permits longitudinal studies (serial imaging) to be performed for investigations where the dose required by conventional imaging would confound the experiment.

The power of these imaging techniques is particularly suited to the study of living processes. It will be possible to exploit the proximity between the Australian Synchrotron, Monash University, CSIRO, Melbourne University and the Monash Medical Centre to bring together the expertise and facilities that will make the imaging beamline (beamline 10) one of only two beamlines in the world capable of work on live animals. The studies of live animals for medical research is an area that is impractical under overseas access programs, and so relates to an essentially new and numerous Australian synchrotron user class that has not been served in the past.

One of the problems at present is that animals are often sacrificed in order to obtain anatomical information at high resolution. The proposed imaging beamline will allow in vivo imaging of small animals and so provide the major advantage of allowing longitudinal studies to be carried out. This has the significant advantage of following the same animal through the process and also dramatically reducing the number of animals sacrificed in a study.

Mammography

Two major areas where soft tissue contrast is vital are breast and lung imaging. Both breast and lung cancer are major killers and better methods of imaging these diseases would have a major impact on health care.

Screening for breast cancer, which is the biggest killer of women in the 35 to 55 age group, is based entirely upon soft-tissue x-ray absorption contrast. As a result,

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[13] G. Parker, 'A critical review of acid generation resulting from sulfide oxidation: Processes, treatment and control', in Acid Drainage. Australian Minerals and Energy Environment Foundation, Melbourne, 1–182 (1999).

[14] J.L. Jambor, J.E. Dutrizac & T.T. Chen, 'Contribution of specific minerals to the neutralisation potential in static testes', Proc. Fifth Int. Conf. Abatement of Acid Mine Drainage (Denver, May 2000) Soc. Min. Metall. Explor. Inc. (SME), U.S.A. 1, (2000) 551–565.

[15] S. Kurunczi, S. Torok & P. Chavallier, 'A micro-XRF study of the elemental distribution on the growth front of mussel shells', Mikrochimica Acta 137, (2001) 41–48; M. Labrenz et al., 'Formation of sphalerite (ZnS) deposits in natural biofilms of sulfate-reducing bacteria', Science, 290, (2000) 1744-1747 'Reactivity of surface states on pyrite', Surf. Sci., 411, (1998) 321-328; A.G. Schaufuss, H.W. Nesbitt, I. Kartio, K. Laajalehto, G.M. Bancroft, & R. Szargan, 'Incipient oxidation of fractured pyrite surfaces in air', J. Electron Spectrosc. Relat. Phenom., 96, (1998) 69–82.

mammography, while having been proven to reduce mortality, suffers from some major deficiencies.
In particular it is non-specific, resulting in a very large number of unnecessary biopsies, and it does not work well in women below the age of 50. The potential benefits of phase contrast imaging to improving the success of mammography in detecting cancer are enormous. Work by others has shown that the contrast increases by as much as 25 times by employing phase contrast.[16] The beamline to be constructed would be used as a 'gold standard' facility to develop improved techniques for breast imaging.

Lung Imaging

Anyone who has seen a chest x-ray knows that the lungs are largely invisible to all but the highly trained eye of a radiologist. However, the air–tissue interfaces in the lung appear with startling clarity using phase contrast imaging (illustrated in figure 3.8 showing the differences between conventional and two synchrotron phase contrast images of mouse lungs). The resolution of the synchrotron images is around 10 microns, which enables individual alveoli to be visualised. This is particularly applicable to human babies, and an Australian project at a SPring-8 beamline is planned to investigate the potential for developing technology to image lung clearance at birth.

Phase contrast techniques offer enormous opportunities for the study of lung function and disease in both humans and animals. Examples include:

- The detailed study of the development of respiratory function in marsupials that are born in an embryonic state and yet can still breathe
- Longitudinal studies of the effect of anti-cancer therapies on mice and other animal models.

In addition to the dramatic improvements offered by phase contrast, workers at the ESRF have demonstrated xenon contrast respiration-gated synchrotron radiation computed tomography (SRCT) with a spatial resolution at the level of the respiratory lobule (terminal bronchiole and alveoli). This technique allows direct quantification of xenon as an inhaled contrast agent based on K-edge subtraction imaging and hence the dynamics of xenon wash-in can be used to calculate regionally specific quantitative maps of lung ventilation. Examples of the use of this technique are:

- Identifying local variations in lung function caused by diseases such as asthma and chronic obstructive pulmonary disease
- Testing the efficacy of pharmaceuticals on respiratory dysfunction.

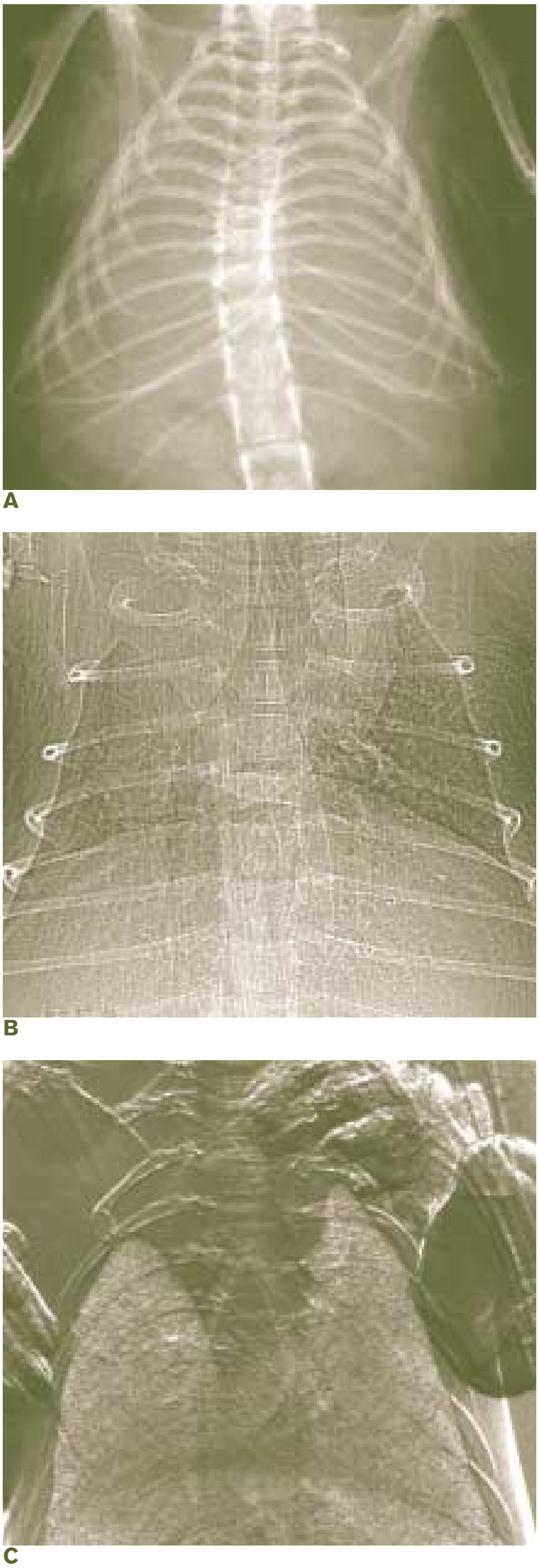

Figure 3.8. *X-ray images of mouse lungs, showing the differences between the conventional x-ray absorption image (A) and two synchrotron phase contrast images (B, C). Source: Image A was obtained by R. Lewis with a Facitron. Images B and C taken by R. Lewis et al, Monash University, at SPring-8, Japan.*

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[16] M.Z. Kiss, D.E. Sayers, Z. Zhong 'Measurement of image contrast using diffraction enhanced imaging', Physics in Medicine & Biology, 48 (3), 325-40, 2003. F. Arfelli et al "Phase detection techniques for possible developments in mammography with synchrotron radiation", Radiology, 215, (2000), 286–293.

Imaging of advanced materials and manufactured products

The high contrast and microtomography capabilities can be exploited to great effect in the areas of materials science, non-destructive testing and mineralogy.

Examples include:

- studies of precipitation and voids in industrially important light metal alloys
- the study of membranes for use in advanced fuels cells
- studies of fracture in ceramics
- investigation of micro/nano structured devices by micro-CT, e.g. for use in automotive applications
- the use of high resolution computed tomography for the study of porosity in oil-bearing rocks. By tuning to different energies it will also be possible to image the amount of residual oil left in the rock following extraction
- the study of advanced materials following and during various stresses, both mechanical and environmental. Many advanced materials, for example those in aerospace applications, are composed of materials that cannot be imaged with conventional x-ray techniques due to lack of contrast (figure 3.9 image of graphite fibres in aluminium). These features would be essentially invisible in conventional absorption contrast radiography.

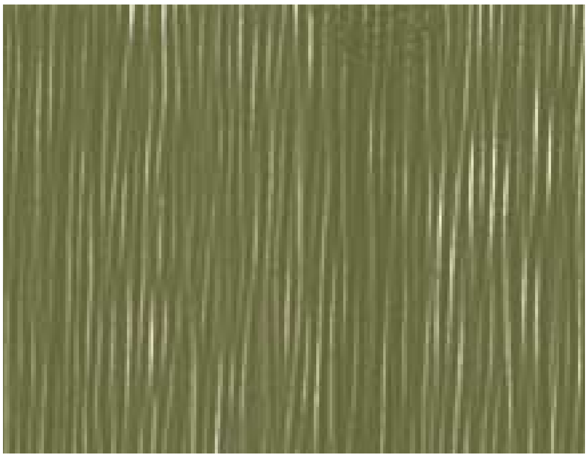

Figure 3.9. *Synchrotron phase contrast image of graphite fibres in aluminium*[17]

Imaging of plants

The contrast mechanisms employed to visualise soft tissues in animals can also render visible many of the structures inside plants. An enormous range of studies is envisaged, but of particular interest is the study of drought- and salt-tolerant species, with a view to developing more efficient crops for Australia. Phase contrast computed tomography techniques will be employed to study the development of root structures without removing the plant from the soil, while K-edge imaging will be used to study protein hormone flow dynamics.

Further developments of imaging

Imaging may be regarded as any process by which spatial structural information about an object is acquired. A paradigm shift occurred with the Nobel Prize winning work of Gabor where he demonstrated that the information in a coherent wave could be captured on film and then decoded afterwards.

Australian researchers have already made major contributions to the fundamental understanding of this, leading to the algorithms for decoding the information and thus the ability to extract readily interpretable information about a sample from the images that have been described above. However there is still much to be done, and access to the Australian Synchrotron will be important for advancing the field.

Some fundamental topics that will be pursued are the non-crystallographic phase problem and complete wavefield recovery, leading to the detailed structural analysis of a sample.

This work will be of great value in obtaining structural information from proteins that are impossible to crystallise, such as membrane proteins. It will also enhance the ability to obtain very high resolution three-dimensional images of objects with poor contrast such as biological cells and tissue.

Progress in this field is currently limited by lack of detailed theoretical understanding of the problems of coherence and phase recovery; by the need for custom optics, such as cylindrical lenses; by the sophisticated software required to recover the multi-dimensional image information; and by access to a suitable imaging detector. Beamline 10 will be designed for flexibility to support the development of the optics systems and detectors that are needed.

Radiotherapy

In cancer biology, imaging and therapy are inextricably linked. In the case of beamline 10 (the imaging and medical therapy beamline) also, the capabilities designed for excellent imaging are ideally suited for the study and development of novel radiotherapy techniques.

The major problems with radiotherapy lie in determining the extent of the spread of the disease and delivering sufficient radiation to the tumour without damaging surrounding healthy tissues. These problems are particularly acute in tumours where the surrounding tissue is extremely sensitive. Synchrotron radiation is able to deliver high dose only to the targeted area significantly better than current clinical techniques. Three methods are currently under investigation at overseas synchrotrons: photon activation therapy (PAT), computed tomography (CT) therapy, and microbeam radiation therapy (MRT).

Photon activation and CT therapy both use specific x-ray energies that are preferentially absorbed by an element that has been delivered into the tumour. In PAT a chemical agent (e.g. cis-platinum, which is also used for chemotherapy) is introduced and concentrates in the

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[17] A.W. Stevenson et al. "Phase-contrast x-ray imaging with synchrotron radiation for materials science applications", Nucl. Instr. and Methods in Phys. Res. B 199 (2003), 427–435.

tumour. By choosing the correct energy the x-ray beam interacts preferentially in the tumour and delivers a high localised dose. CT therapy also uses a contrast agent (e.g. iodine) that concentrates in the tumour but takes advantage of beam spreading effects and stereotactic methods to spare normal tissues.

Perhaps the most exciting possibility is MRT. Here extremely large radiation doses are applied to tissues in an array of micrometres-thick highly collimated x-ray beams (figure 3.10).

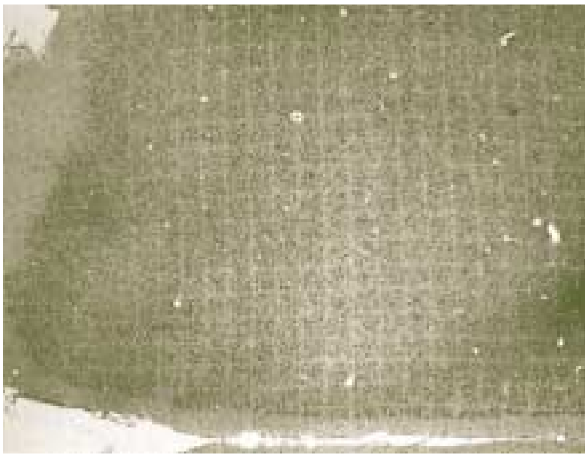

Figure 3.10. *The right cerebral hemisphere of a young adult rat after cross irradiation with x-ray beams from a multi-slit collimator. Two arrays of vertical, 0.5 cm-high and approx. 25 mm-wide microbeams with centre-to-centre distances of 210 mm were used. Subsequent examination showed that normal tissue was able to regenerate the blood vessels after one month, even in the irradiated slices. Tumours, however, do not recover from this treatment*[18].

The extraordinary aspect of microbeam radiation is that it spares healthy tissue far better than large-area beams of the same dose and yet the tumour is still damaged. The method has been used with great effectiveness to deliver doses in excess of 1000 Gy to live animals. (Note that 10 Gy delivered in a conventional method is lethal.) The reason for this effect is unknown, and is a fertile area for study.

It is possible that therapies utilising this effect may revolutionise the treatment of some kinds of cancers, which are currently untreatable. A strong programme of research into the nature of this effect, together with determining the most effective way of delivering the dose, is planned to be a significant activity on the Australian Synchrotron. However it should be noted that much research will be required before MRT could be considered for clinical application.

Future Beamline Possibilities

The flexibility of the Australian Synchrotron as a light source means that beyond the initial suite of beamlines there are other possibilities for new techniques that could be added to the facility in the future.

One of the new techniques is imaging in the terahertz (THz) region of the spectrum. So-called 'T-ray imaging' uses pulsed, far-infrared light. It has great potential as a medical imaging tool because there is no ionisation hazard for biological tissue and Rayleigh scattering is many orders of magnitude less for THz wavelengths than for the neighbouring infrared and optical regions of the spectrum[19].

The THz frequencies correspond to energy levels of molecular rotations and vibrations of DNA[20] and proteins[21], and these may provide characteristic fingerprints to differentiate biological tissues in a region of the spectrum not previously explored for medical use. In addition THz wavelengths are particularly sensitive to water[22], which can indicate tissue condition.

Another possibility is to build a micro-focussed soft x-ray beamline, which utilises the unique capabilities of the toroidal geometry electron spectrometer that has been developed by researchers at La Trobe University[23]. This would bring a new approach to the imaging of self-assembling structures on the nanometre scale and enable researchers to follow the self-assembly process in real time. Not only could imaging be achieved but it should also be possible to investigate the electronic and magnetic properties of self-assembling systems using the techniques that have been developed in recent years for 'bulk angle resolved spectroscopy'.

A second approach to imaging self-assembling systems that could be incorporated on this beamline involves illuminating a macroscopic area of sample and relying on the spatial resolution obtainable using a low energy electron microscope column. This is the PEEM or XPEEM (x-ray/photoelectron emission microscopy) system pioneered by Ernst Bauer and others[24].

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[18] J.A. Laissue, N. Lyubimova, H-P. Wagner, D.W. Archer, D.N. Slatkin, M. Di Michiel, C. Nemoz, M. Renier, E. Brauer, P.O. Spanne, J-O. Gebbers, K. Dixon, H. Blattmann, 'Microbeam radiation therapy', In H. Bradford Barber, H. Roehrig (Eds), Medical Applications of Penetrating Radiation, Proceedings of SPIE, 3770 (1999) 38–45. See also http://www.pathology.unibe.ch/Forschung/microbeam/microbeam.htm

[19] D.D. Arnone, C.M. Ciesla, & M. Pepper. Terahertz imaging comes into view. Physics World, April 2000 pp 35–40.

[20] A.G. Markelz, A. Roitberg & E.J. Heilwiel. Chemical Physics Letters, 320 (2000) 42–48.

[21] M. Walther, B. Fischer, M. Schall, H. Helm & P. Uhd Jepsen. Chemical Physics Letters, 332 (2000) 389–395.

[22] D.M. Mittleman, R.H. Jacobsen & M.C. Nuss. IEEE Journal of Selected Topics in Quantum Electronics, 2(3) (2000) 679–691.

[23] R.C.G. Leckey, J.D. Riley. Appl. Surf. Sci. 22/23 (1985) 196 – 205. Aust Patent No. 539 588 U.K. Patent No. 2 098 797. U.S.A Patent No. 4 758 722

[24] E. Bauer. J. Phys. C. Condens. Matter 13 (2001) 11391–11404

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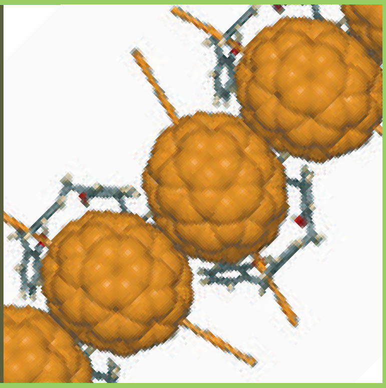


Proposed initial suite of beamlines and cost estimates

IMAGE: Fullerenes

Structure of a complex between fullerene C70 and a cavitand molecule, calix[5]arene.

A recent example of the capability of a synchrotron source is the determination of the structure of a complex between fullerene C70 and a cavitand molecule, calix[5]arene, which is important in understanding molecular recognition/purification of the fullerene, and also in building up new material with novel function. Data was collected at the SRS facility, UK, with the small crystals (10 microns) too weakly diffracting for data collection from conventional x-ray sources.

Chapter 04

Proposed initial suite of beamlines and cost estimates

The versatility of synchrotron light enables many different experimental techniques to be used, each technique requiring a separate dedicated beamline.

It is proposed that the Australian Synchrotron should commence with a core suite of between nine and thirteen world class beamlines. As the user community grows and as new techniques are developed (synchrotron science is moving rapidly) further lines will be established. In the long term the lattice has the potential to accommodate in excess of 30 different beamlines.

In some American synchrotrons (notably the Advanced Photon Source in Chicago and the Advanced Light Source in San Francisco) the beamlines have been funded and constructed by groups separate from the core synchrotron operators. Experience has shown however that this results in unnecessary duplication, and also that many of the beamlines have been designed to perform too many functions, which adds extra complication and expense. To avoid this, it is proposed to construct a comprehensive and complementary range of specialist beamlines for the Australian Synchrotron and to provide scientific and technical support for the broad community of users. Wherever possible common equipment should be used – particularly vacuum equipment, electronic controls and data handling software and hardware – to simplify and reduce maintenance costs. In deciding the beamlines to establish initially the objective is to create a suite of techniques that would cover 95% of the Australian scientific community's anticipated needs.

A National Scientific Advisory Committee (NSAC) and an International Scientific Advisory Committee (ISAC) – comprising senior scientists experienced in synchrotron research – have guided the selection, and the research groups currently working through the Australian Synchrotron Research Program (ASRP) have been extensively consulted. NSAC has met on six occasions, ISAC has had two major meetings, and members of both committees participated in a large workshop attended by 350 delegates in January 2003. Resulting from all of these discussions, the thirteen beamlines listed in table 4.1 have been recommended as the optimum configuration for Australia's scientific and industrial needs. Page vi lists the members of the advisory committees. Beamlines 3, 5, and 10 will require wigglers and 2, 4, 6, 7, and 9 will require undulators for their radiation source. These insertion devices add significant expense and need to be individually commissioned, so their beamlines are likely to be introduced progressively in the construction schedule. At 'first light' it would be expected to have beamlines 1, 3, 5, 8, 9, 11 and 13 operating (High-throughput Protein Crystallography, Powder X-Ray Diffraction, X-ray Absorption Spectroscopy, Infrared Spectroscopy, Microspectroscopy, Microdiffraction and Fluorescence Probe and Lithography), with beamlines 2, 4, 6 and 10 (Protein Microcrystal and Small Molecule X-ray Diffraction, Small and Wide Angle X-Ray Scattering, Soft X-ray Spectroscopy, and Imaging and Medical Therapy) under construction and progressively introduced during 2007 and 2008.

Once these core beamlines are commissioned, it is planned that beamlines 1 and 3 will be upgraded to operate from an in-vacuum undulator and wiggler respectively, beamline 10 will be extended and beamlines 7 (Vacuum Ultraviolet) and 12 (Circular Dichroism) will be established.

Table 4.1. Proposed initial suite of beamlines for the Australian Synchrotron

No	Category	Beamline Description	Source	Energy Range
		Crystallography & Diffraction		
1	A	High-throughput Protein Crystallography	Bending magnet	2–23 keV
2	A	Protein Microcrystal & Small Molecule X-ray Diffraction	In-vacuum undulator (22 mm period)	5.5–20 keV
3	A	Powder X-ray Diffraction	Stage 1: Bending magnet Stage 2: Wiggler	4–60 keV
4	A	Small and Wide Angle X-ray Scattering	In-vacuum undulator (22 mm period)	5.5–20 keV
		Spectroscopy		
5	A	X-ray Absorption Spectroscopy	Wiggler (2T)	4–65 keV
6	A	Soft X-ray Spectroscopy	Undulator (75 mm period)	0.1–2.5 keV
7	B	Vacuum Ultraviolet (VUV)	Undulator (185 mm period)	10–350 eV
8	A	Infrared Spectroscopy	Bending magnet	0.001–1 eV (2–10,000 cm^{-1})
9	A	Microspectroscopy (submicron-XAS, XANES, & XRF)	In-vacuum undulator (22 mm period)	5–20 keV
		Imaging		
10	A, B	Imaging & Medical Therapy	Wiggler (4T)	10–120 keV
11	C	Microdiffraction and Fluorescence Probe (XRD & XRF mapping)	Bending magnet	4–37 keV
		Polarimetry		
12	B	Circular Dichroism	Bending magnet	2–10 eV
		Advanced Manufacturing		
13	C	Lithography	Bending magnet	2–25 keV

Category A: Nine general purpose beamlines are considered to be essential to be available or under construction at the commissioning of the synchrotron in 2007. This suite is selected to ensure access by the widest possible discipline groupings to photons from low energies (infrared) to high energies (x-rays) to achieve balance between physical and biological scientific investigations.

Category B: Beamlines 7 and 12 are considered to be highly desirable in order to have a balanced set of capabilities for the synchrotron. In addition it is planned that, after beamline 10 is fully established and proven, it should be extended out to a separate building equipped for full-body medical imaging research and that beamline 1 should be up-graded to be sourced from an in-vacuum undulator. Mechanisms to fund these lines will be sought once funding for the first nine beamlines is achieved.

Category C: These two beamlines are viewed as high throughput facilities, principally to service the diagnostic and production needs of industry. A funding plan is being developed for these beamlines based upon a combination of capital contributions and cost recovery fees.

Capital cost estimates for the beamlines

Preliminary cost estimates for the design, construction and commissioning of the beamlines are given in Table 4.2.

Work is continuing on the specifications for each beamline, and as details are finalised these cost estimates will be refined. Appendix 1 contains costing breakdowns for each beamline.

Cost estimate assumptions

Items that are included in the budget for the machine and as such are not included in Table 4.2:

- the ‘front end’ equipment (i.e. vacuum equipment, interlocks, controls and electronic equipment on the inner side of the shielding wall)
- a distributed liquid nitrogen system
- the labour costs of the beamlines manager and corporate technical staff. (However, an allowance has been included for labour for design, construction and commissioning of each beamline.)
- costs for survey and alignments, vacuum and control interfacing with the machine and radiation monitoring.

Prices quoted are in current Australian dollars. Conversion rates used:

$A1 = $US0.65
$A1 = $CAN0.90
$A1 = GBP 0.385
$A1 = Euro 0.58
$A1 = Yen 75

Table 4.2 Preliminary cost estimate for the initial suite of beamlines

BL	Title	Category A	Category B	Category C
		$(A)	$(A)	$(A)
1	High throughput Protein Crystallography	5,823,000	1,655,000	
2	Protein Microcrystal & Small Molecule Diffraction	7,983,000		
3	Powder Diffraction	5,300,000		
4	Small & Wide Angle Scattering	4,785,000		
5	X-ray Absorption Spectroscopy	5,110,000		
6	Soft X-ray	4,939,000		
7	Vacuum UV		4,990,000	
8	Infrared Spectroscopy	2,600,000		
9	Microspectroscopy	5,339,000		
10	Imaging & Medical Therapy	7,610,000	5,120,000	
11	Microdiffraction and Fluorescence Probe			3,442,000
12	Circular Dichroism		3,100,000	
13	Lithography			4,240,000
Total		**49,489,000**	**14,865,000**	**7,682,000**

Contingency

No contingency has been made for currency fluctuation or uncertainties of the cost of components. Synchrotron technology is evolving rapidly and it is possible that by 2006 some devices may be of lower cost; however this is impossible to predict at present.

Operating Costs

The annual operating costs of a synchrotron comprise the fixed costs to maintain and operate the machine and associated infrastructure as a leading-edge facility and costs associated directly with the functioning beamlines. The cost of operating the total facility has been estimated as being around $15 million per year (real 2003) on commencement of operations in 2007 rising to around $17 million per year (real 2003) in the more mature operating phase.

Operating costs associated with the mature synchrotron can be considered in two broad categories:

- scientific, technical and management staff; and
- general operating costs.

The approximate full-time employee requirement for the Australian Synchrotron with 12 to 13 beamlines is around 80 staff. The majority will be employed directly on the storage ring or the beamlines.

General operating cost categories include:

- administration and consumables
- computing and office equipment
- workforce support (non-salary items: recruitment, training, security, safety etc)
- communication and conferences
- engineering and maintenance
- utilities.

Within the general operating costs a major variable is the level of electricity consumed during operation. This will be determined by the operating approach and the equipment selection, which will in turn affect the conditions for the purchase of electricity.

The development and finalisation with key stakeholders of the coverage of operating costs, and the methods by which these are met will be an important element of future stakeholder discussions. It is expected that the bulk of operating funds, at least in the initial years after commissioning, will be provided predominantly from national science funding sources, with possible contributions from other governments (State and overseas), some research institutions, and the private sector.

Further discussion of possible approaches to financing and management of the facility are contained in chapter 9.

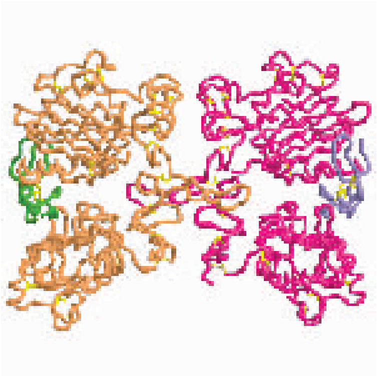
Access to Ancillary Services

The synchrotron will be sited next to Monash University and the Monash cluster, which includes the CSIRO Clayton facilities and the Monash Health Sciences precinct, and not far from the Baker Institute, Melbourne University and the 'Parkville Strip' of research institutes. It is anticipated that ready access can be provided to ancillary services by these institutions and this will enable capital and operating costs to be kept to a minimum.

For example, access will be available to:

- the sample preparation facilities (including growing of protein crystals) at Monash and CSIRO
- the confocal microscopy, electron microscopy and NMR suites at Monash and CSIRO
- the Scanning Nuclear Microprobe facility of the CSIRO, which will be relocated to Melbourne in 2004
- the animal breeding and housing facilities of Monash and Melbourne Universities, and
- several specialised instrument-making workshops.

05



User communities and the beamlines of interest to them

IMAGE: Crystal structure of a epidermal receptor bound to a transforming growth factor.

This receptor/ligand complex is involved in the growth of many cancers and was determined by collaboration between the WEHI, LICR and CSIRO. From T. Garrett et al. Cell. 2002 Sep 20; 110(6):763-73.

Chapter 05

User communities and the beamlines of interest to them

Over the past 10 years a rapidly growing group of Australian researchers has been carrying out experiments on overseas synchrotrons, initially through a national consortium managed by ANSTO, with the assistance of the federally funded Access to Major Research Facilities Program, and from 1996 by the Australian Synchrotron Research Program (ASRP), which incorporated the original consortium. Figure 5.1 shows the growth in the number of spokespersons for ASRP experiments from 1996 to 2002. In 2002 there were 140 research groups participating in this scheme.

Many disciplines have been involved (see figure 5.2). If anything, the biotechnology and medical research community is under-represented at present because of the great difficulty in taking biological samples overseas. However this gives an indication of the broad scientific and industry user group that will develop for the Australian Synchrotron.

It is important to note that an experienced synchrotron user will usually need access to several techniques, in some cases with the techniques being performed simultaneously, to obtain the greatest benefit. Thus it is imperative that the full complement of beamlines envisaged in this proposal is constructed to service user needs properly. As an indication of this, the beamlines that will be of primary interest to researchers in the various fields are listed in table 5.1.

Several beamlines will be developed to be easy to use by occasional or inexperienced users, and others are likely to offer high throughput and remote access, primarily to service industry needs.

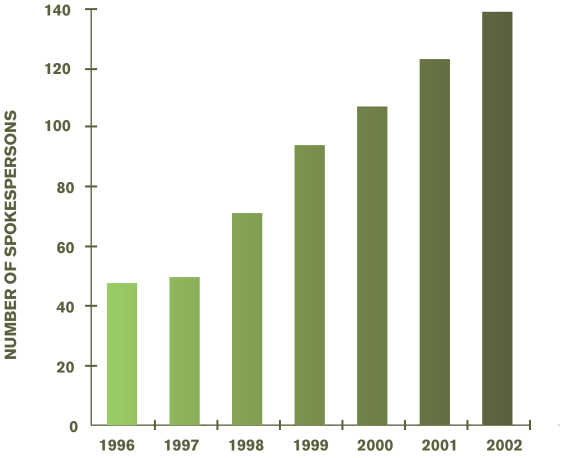


Figure 5.1. *Number of spokespersons for experiments funded by the Australian Synchrotron Research Program. Each of these typically speak on behalf of three or four researchers.*

While the beamline descriptions in chapter 10 provide details about the user communities currently associated with each beamline technique, the key features of each group are summarised here. A list of known key principal investigators is provided in Volume 2, appendix 2, although a summary of their organisations is given in table 5.2. A sample of the most recent work conducted by Australian researchers at overseas synchrotron facilities is provided in table 5.3.

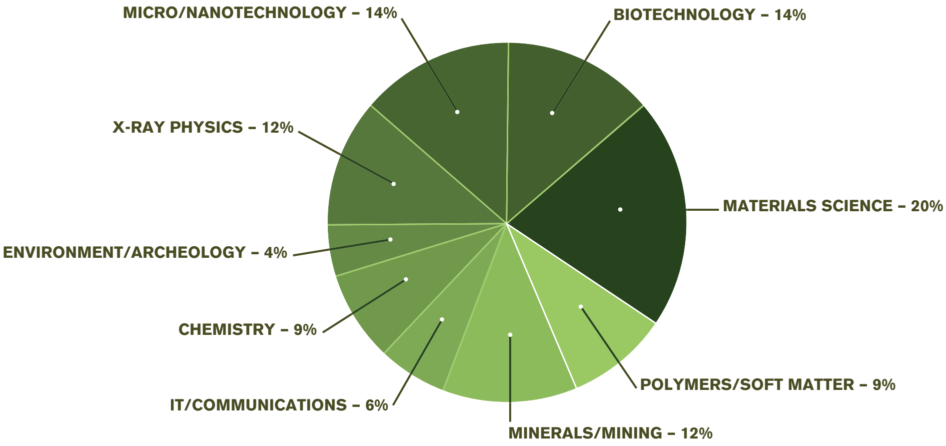


Figure 5.2. *Research disciplines for experiments funded by the Australian Synchrotron Research Program.*

Table 5.1 The research fields that will be enhanced by the synchrotron, with the beamlines primarily needed for each field indicated by shading.

RESEARCH FIELDS	BL 1 Protein crystallography	BL 2 Protein microcrystals and small molecules	BL 3 Powder diffraction	BL 4 Small & wide angle scattering	BL 5 X-ray absorption spectroscopy	BL 6 Soft X-ray spectroscopy	BL 7 Vacuum UV	BL 8 Infrared spectroscopy	BL 9 Microfocus spectroscopies	BL 10 Imaging & medical therapy	BL 11 Microdiffraction and fluorescence probe	BL 12 Circular dichroism	BL 13 Lithography
Life Sciences													
Biological research & drug design	🟩	🟩	🟩	🟩	🟩		🟩	🟩	🟩	🟦		🟩	
Biotechnology & bio-sensors	🟩	🟩			🟩	🟩		🟩	🟩				🟩
Biomedical & medical imaging								🟩	🟩	🟩			
Medical therapy										🟩			
Plants & crops	🟩		🟩		🟩		🟩			🟩		🟩	
Physical Sciences													
Sustainable environment		🟩	🟩		🟩			🟩	🟩				
Forensics			🟩	🟩	🟩	🟩		🟩	🟩	🟩			
Advanced materials:													
– functional polymers		🟩		🟩		🟩		🟩		🟩		🟩	
– ceramics			🟩	🟩	🟩	🟩		🟩	🟩	🟩	🟩		
– nanomaterials & composites		🟩	🟩	🟩		🟩	🟩	🟩	🟩	🟩	🟩		🟩
– metals & alloys			🟩			🟩	🟩		🟩	🟩	🟩		
– micro-electronic & magnetic materials					🟩	🟩	🟩	🟩		🟩			🟩
– biomaterials		🟩	🟩		🟩	🟩	🟩	🟩		🟩	🟩	🟩	
Engineering			🟩							🟩			🟩
Mineral exploration & beneficiation			🟩		🟩	🟩			🟩	🟩	🟩		
Earth sciences		🟩	🟩	🟩	🟩	🟩		🟩	🟩		🟩		
Oil & gas production and distribution		🟩		🟩	🟩			🟩	🟩	🟩	🟩		
Agricultural technology	🟩		🟩	🟩	🟩	🟩				🟩		🟩	🟩
Food technology	🟩	🟩	🟩	🟩				🟩				🟩	🟩
Chemical reactions & catalysts		🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩		🟩		🟩
Advanced manufacturing													
Production and testing of micro-devices					🟩	🟩				🟩	🟩		🟩

🟦 Small animal imaging

Beamline User Communities

Beamlines 1 and 2

A survey in early 2003 of the Australian protein crystallography community indicated that there are about 42 protein crystallography users or user groups interested in national synchrotron facilities. On current usage, total synchrotron beam time requirements have been estimated at 216 days per year. If the number of protein crystallographers continues to grow at the current rate to 2007, demand will saturate available beam time, particularly if the likely interest of New Zealand and other regional scientists is included. The small molecule community in Australia currently using single-crystal x-ray diffraction (XRD) for molecular structure determinations is estimated to be at least 100 members. Awareness of synchrotron capabilities in this area is low at present, but is expected to rise dramatically when the local facility is commissioned. The dedicated single crystal facility at SRS in the United Kingdom is over-subscribed by more than a factor of two.

Beamline 3

The synchrotron powder diffraction community exceeds 23 independent research groups from thirteen Australian institutions at present, due to rapid growth in the use of synchrotron powder diffraction in the past decade. Demand of existing users is estimated to utilise all beamtime on beamline 3 already.

Beamline 4

There is currently an active SAXS (small angle x-ray scattering) community in Australia, using several laboratory-based SAXS instruments and the recently commissioned ChemMatCARS instrument at the Advanced Photon Source in Chicago, through the ASRP. Demand for this instrument already exceeds supply.

Beamline 5

The Australian x-ray absorption spectroscopy (XAS) user community exceeds 70 practitioners at present, estimated to increase to 150 with a local synchrotron. In spite of flux limitations with the ANBF beamline at the Photon Factory, Japan, XAS measurements comprised 42% of all experiments performed (2001, ASRP). It is estimated that total current Australian XAS demand will utilise all available beamtime on a wiggler-based XAS beamline.

Beamline 6

The current Australian synchrotron soft x-ray user community comprises approximately fifteen research groups. Worldwide, all overseas synchrotron soft x-ray beamlines are oversubscribed, which limits the access of Australian researchers. With access to a dedicated soft x-ray beamline, purpose-built for the Australian community at a local facility, it is estimated that 30 groups from eighteen research institutions have the potential to use all available beamtime.

Beamline 7

There are at least eight Australian synchrotron vacuum ultraviolet (VUV) research groups at present with extensive experience and advanced capabilities. Access to VUV beamlines has not been available through the ASRP. Because of the nature of the experimental techniques, VUV experiments take 2–3 weeks at a time, so using overseas facilities is costly and difficult to obtain. Taking usage rates at the German VUV beamline as a guide, the existing Australian VUV community will fully utilise a VUV beamline from the outset.

Beamline 8

Worldwide, the demand for infrared spectroscopy (IR) beamline time has been heavy, which has limited the access of Australian researchers to overseas synchrotron IR facilities. The ASRP has recently provided access to an IR beamline on the Taiwan synchrotron, in response to rapidly increasing requirements from the local user community. Combined with strong interest from New Zealand researchers, it is expected that the user community will grow to 200 members in 2007.

Beamline 9

Australian researchers have been international leaders in the development of microprobe techniques for two decades. There are currently 64 known potential Australian users or teams, from nineteen universities and research organisations including government institutions and industry.

Beamline 10

Most of the potential medical and biomedical users of the imaging and medical therapy beamline will be new, because the types of live animal and patient studies envisaged cannot currently be addressed at overseas synchrotron facilities. There are at least fifteen biomedical research institutions, five CRCs and several private enterprises that have indicated interest as potential users. Materials imaging is expected to attract direct or collaborative research interest from manufacturing (including automotive), aerospace and defence industries.

Beamline 11

The combination of simultaneous micro-XRD and x-ray fluorescence is particularly attractive to industry, through either direct or collaborative research projects. It will also provide a high level resource for fundamental research. A significant number of industry sectors have expressed interest and support, in particular the minerals industry and manufacturing research sectors. In addition, a strong collaborative venture is under way with a similar beamline on the Canadian synchrotron.

Beamline 12

Synchrotron circular dichroism (CD) is a recent development and Australian CD users have had no access to a CD beamline to date. However, 32 users or user groups have expressed interest in synchrotron CD techniques. Extrapolating from the rate of expansion of biomedical and structural biology research in Australia, it is estimated that the number of users would exceed 100 within two years of local access to a CD beamline, which would fully utilise available beamtime.

Beamline 13

An industrially focussed, high volume production Australian LIGA beamline has already attracted substantial local industry interest. It is planned to operate the beamline in tandem with the nearby MiniFAB facility, making it an attractive option for international users. The beamline is also strongly supported by the CRC for Microtechnology and there are possibilities for international partnerships.

Table 5.2 Number of key principal investigators and research team leaders from major institutions, with their beamlines of interest

ORGANISATION	BL 1 Protein Crystallography	BL 2 Protein Microcrystal & Small Molecules	BL 3 Powder Diffraction	BL 4 Small and Wide Angle Scattering	BL 5 X-ray Absorption Spectroscopy	BL 6 Soft X-ray Spectroscopy	BL 7 Vacuum Ultraviolet	BL 8 Infrared Spectroscopy	BL 9 Microspectroscopy	BL 10 Imaging and Medical Therapy	BL 11 Microdiffraction/Fluorescence Probe	BL 12 Circular Dichroism	BL 13 Lithography
ANSTO ASRP			1								1		
ANSTO Bragg Institute		2	6	5	3	2	1		4			1	
ANSTO Environment				1	1				6				
ANSTO Materials and Engineering Science			3	2	4	1			3				
ANSTO Radiopharmaceuticals Division					1								
Applied Sorting Technologies P/L										1			
Austin Health Centre for Positron Emission Tomography												1	
Austin Health Radiation Oncology										1			
Austin Research Institute Inflammatory Diseases												1	
Austin Research Institute Structural Immunology		1	1										1
Australian Minerals Industry Research Association												1	
Berthold Aust. P/L										1			
BHP Billiton Minerals Technology											1		
Boeing/ASTA Components Advanced Manufacturing Research and Development										1			
Canesis Network Ltd, New Zealand Corporate Research							1						
Central Queensland University Department of Biology									2				
Ceramic Fuel Cells Limited Manufacturing										1			
Cetec Pty Ltd										1			
CRC for Microtechnology													3
CSIRO Energy Technology			1	1	1	1		1	1	1	1		
CSIRO Exploration and Mining					2	1			1				
CSIRO Forestry and Forest Products			1	1	1				1	1	1		
CSIRO Health Sciences and Nutrition	3	3		2	2						1	1	
CSIRO Land and Water			1		1	2		1	2		1		
CSIRO Livestock Industries		1											
CSIRO Manufacturing and Infrastructure Technology			4	1					9	9	4		2
CSIRO Minerals			2	2	4	2			2	1	3		
CSIRO Molecular Science				4		5		3	1				
CSIRO Petroleum Resources										1			
CSIRO Telecommunications and Industrial Physics									1				
CSIRO Textile and Fibre Technology					1			1	1	1			1
Curtin University of Technology Department of Applied Physics			4	2									
Curtin University of Technology Dept of Applied Science			1		1								
Curtin University of Technology School of Applied Chemistry		2	2	1	2	3		1					
Cyclotek (Aust) Pty Ltd										1			
DSTO Air Vehicles Division			1						1	1	1		
DSTO Maritime Platforms													1
Edith Cowan University School of Engineering and Mathematics									1				

Elbicon/Barco										1			
Environmental Geochemistry International Pty Ltd											1		
Flinders University School of Biological Sciences	1	1											
Flinders University School of Chemistry, Physics and Earth Sciences						3	1				1		
Food Science Australia Ultrasonics				1									
Geoscience Australia Petroleum & Marine Division				1						1			
Griffith University Institute for Glycomics	1	1											
Griffith University Natural Product Drug Discovery, The Erskitis Institute	1	1											
Griffith University School of Science		2	1			1	1	1	1				
Ian Potter Conservation Centre										1			
Industrial Research Limited, New Zealand Materials Performance Technologies		1			1								
Industrial Research Limited, New Zealand Materials Technologies Group		1			2			1					
Industrial Research Limited, New Zealand Measurement Standards Laboratory					1			1					
Institute of Geological and Nuclear Sciences					1								
James Cook University Biochemistry & Molecular Biology	1	1											
James Cook University School of Pharmacy and Molecular Sciences		1											
La Trobe University Department of Chemistry						1	1						
La Trobe University Department of Physics						6	4						
Macquarie University Department of Chemistry								1					
Magotteaux Australia Pty Ltd											11		
Massey University Centre for Structural Biology, New Zealand	1	1											
Massey University Institute of Natural Resources, New Zealand								1					
Massey University Institute of Technology and Engineering, New Zealand					1								
Massey University Institute of Molecular Biosciences, New Zealand	4	4											
Medical Imaging Australia Group				1									
Monash Medical Centre Urology				1									
Monash University Department of Anatomy and Cell Biology, School of Biomedical Sciences										1			
Monash University Department of Biochemistry and Molecular Biology	2	2										4	
Monash University Department of Medicinal Chemistry, Victorian College of Pharmacy	1	2											
Monash University Department of Pharmaceutics, Victorian College of Pharmacy												2	
Monash University Department of Physiology										1			
Monash University Institute of Reproduction and Development										1			
Monash University School of Applied Science				1						1			
Monash University School of Chemistry		6				1		2	1			2	
Monash University School of Physics and Materials Engineering			4	3		1	1			1			
Murdoch University CRC for Hydrometallurgy					1								
Murdoch University Science and Engineering Division						1	1						
National Gallery of Victoria Conservation Department										1			
New Zealand Institute for Crop and Food Research		1											
Pacific Lithium NZ Limited ILiON Technology Corporation					1								
Peter MacCallum Cancer Centre Diagnostic Imaging										1			
Peter MacCallum Cancer Centre Radiation Oncology										5			
Queensland University of Technology School of Physical and Chemical Sciences								2					
Radiation Oncology Victoria Physics										1			
Research Laboratories of Australia, South Australia											1		
Rio Tinto Technology Support											1		
RMIT Faculty of Applied Science				2	2				1				
Robert Bosch (Aust) P/L										1			
Shimadzu (Aust) P/L										2			

SOLA International Holdings Ltd Research and Technology, South Australia											1		
South Australian Museum Minerals											1		
St Vincent's Hospital Melbourne Medical Engineering and Physics										1			
St Vincents Institute of Medical Research Biota Structural Biology Laboratory	2	2										1	
St Vincents Institute of Medical Research Pharmacogenomics										1			
Swinburne University Industrial Research Institute/MiniFAB				1		1			1				3
Swinburne University School of Engineering and Science				2									
TGR Biosciences											1		
The Alfred Radiation Oncology										2			
The Alfred William Buckland Radiotherapy Centre										2			
The Australian National University Geology, Faculty of Science									1				
The Australian National University Chemistry, Faculty of Science		1											
The Australian National University Research School of Chemistry	2	3	1	2	2			1	1			1	
The Australian National University Research School of Earth Sciences					1	1			1		1		
The Australian National University Research School of Physical Sciences and Engineering			1	1	5	4	8	1	2	1			1
The Royal Melbourne Hospital Department of Radiology										1			
The University of Adelaide Department of Chemistry								2					
The University of Adelaide Earth and Environmental Sciences											1		
The University of Adelaide Geology and Geophysics					1				1				
The University of Adelaide School of Electrical & Electronic Engineering								1					
The University of Adelaide School of Molecular and Biological Science												1	
The University of Auckland Department of Chemical and Materials Engineering					1								
The University of Auckland Department of Chemistry	1	2			2	2		2					
The University of Auckland School of Biological Sciences	4	4											
The University of Melbourne Bionic Ear Institute										1			
The University of Melbourne Department of Biochemistry and Molecular Biology										1		4	
The University of Melbourne Department of Genetics									1				
The University of Melbourne Department of Microbiology & Immunology												1	
The University of Melbourne Department of Pathology										1			
The University of Melbourne Department of Physiology										1			
The University of Melbourne Howard Florey Institute												1	
The University of Melbourne School of Chemistry		1		1	2	1		2				1	
The University of Melbourne School of Dental Science										1			
The University of Melbourne School of Physics			2	1	1				4	2			1
The University of New England Chemistry										1			
The University of New England Physics & Electronics								1		1			
The University of New England School of Biological, Biomedical and Molecular Sciences		1											
The University of New South Wales Centre for Membrane Science and Technology				1									
The University of New South Wales Centre for Photovoltaic Engineering						1							
The University of New South Wales Department of Applied Physics				1									
The University of New South Wales School of Biological, Earth and Environmental Sciences									1				
The University of New South Wales School of Chemical Engineering and Industrial Chemistry				1									
The University of New South Wales School of Chemical Sciences				1	3	6							
The University of New South Wales School of Civil and Environmental Engineering									1				
The University of New South Wales School of Physics	1	1										1	

The University of Newcastle Faculty of Engineering and Built Environment			1										
The University of Newcastle School of Mathematical and Physical Sciences					1	1	1						
The University of Queensland Centre for Magnetic Resonance					1								
The University of Queensland Department of Biochemistry and Molecular Biology	2	2										2	
The University of Queensland Department of Chemistry					1								
The University of Queensland Division of Chemical Engineering			1										
The University of Queensland Faculty of Biological and Chemical Sciences				1		2							
The University of Queensland Institute for Molecular Bioscience	1	1										3	
The University of Queensland School of Molecular and Microbial Sciences					1			1					
The University of Sydney Department of Chemical Engineering			1		1								
The University of Sydney Electron Microscope Unit									1				
The University of Sydney School of Chemistry	1	7	4		8	4		2	4				
The University of Sydney School of Land, Water and Crop Sciences			1		1								
The University of Sydney School of Molecular & Microbial Biosciences	3	2										3	
The University of Western Australia School of Medicine and Pharmacology												1	
The University of Western Australia School of Physics				1		1	2						
University of Canberra Corrosion and Spectrochemistry Lab								1					
University of Canberra Heath Design and Science								1					
University of Canterbury Department of Physics and Astronomy								1					
University of Canterbury Electrical and Computer Engineering					1								
University of Canterbury Department of Chemistry		3											
University of Cape Town, South Africa, Mineral Processing Research Unit											1		
University of Notre Dame MG Kailis Group										1			
University of Otago Department of Biochemistry	4	4											
University of Otago Department of Chemistry		3						1					
University of Otago School of Chemistry		1											
University of South Australia Ian Wark Research Institute			1	3	2	2			2		2	1	
University of South Australia IT, Engineering and the Environment											1		
University of South Australia Research Services						1							
University of Tasmania School of Chemistry		3											
University of Technology Sydney Department of Applied Physics		1				1							
University of Technology Sydney Department of Chemistry, Materials and Forensic Science					1						1		
University of Waikato Department of Materials and Process Engineering					1								
University of Waikato School of Chemistry		1											
University of Western Australia School of Biomedical and Chemical Sciences	1	5	1									1	
University of Western Sydney School of Science Food and Horticulture				1									
University of Wollongong Centre for Medical Radiation Physics									2	1			
University of Wollongong Department of Chemistry		1											
Victoria University of Wellington School of Chemical and Physical Sciences					3			1					
Victorian Department of Primary Industries Marsupial Genomics										1			
Victorian Department of Primary Industries Tatura										1			
Walter and Eliza Hall Institute Structural Biology	1	1										3	
WMC Resources Technology											1		
X-Ray Technologies Ltd										1			

Table 5.3 Australian research at overseas synchrotrons, 2002–2004, supported by ASRP and AMRFP

Supported by ASRP 2003-04

Principal Investigator	Others	Institution	Topic
Australian National Beamline Facility at Photon Factory, Tsukuba, Japan			
Dr N Armstrong	W Kalceff, P Lynch	University of Technology, Sydney	Characterisation of Nanoparticles Using Bayesian/Maximum Entropy Methods Applied to Synchrotron Diffraction Data
Dr A Berry	H O'Neill, D Scott	The Australian National University	The Oxidation State of U in Basaltic Melt at 1400°C
Dr S Best	M Bondin, T Behrsing	The University of Melbourne	Redox Initiated Structural Change in Iron-Sulfur Compounds (continuation)
Prof S Bhargava	D Akolekar	RMIT University	Interaction Dispersion of Noble Metal Nanoparticles on the Catalytic Support Materials: An EXAFS Study
Dr A Buckley	S Goh	The University of New South Wales	Interfacial Characterisation of Electrochemically Oxidised Aluminium
Dr P Dastoor	L Thomsen, B Watts	The University of Newcastle	Molecular Alignment of Organosilanes on Surfaces Studied by X-ray Absorption Spectroscopy
A/Prof R De Marco	A van Riessen, G Parkinson, S Bailey, N Kirby, A Rohl	Curtin University of Technology	In Situ Electrode Kinetic and Grazing Incidence X-ray Diffraction Studies of Technologically Important Electrochemical Systems
Dr G Edward	J Ma, P Zhu	Monash University	Morphology and Orientation Resulting from Polymer Processing
Dr C Glover	R Albion, C Bullen	The Australian National University	Local Atomic Structures of Semiconductor Nanocrystals
Dr P Halley	P Sopade	The University of Queensland	Structural and Organisational Changes in Starch Granules During Heat-Moisture Treatment Under Isothermal Conditions: X-ray Diffraction Studies
Dr G Heath	A Edwards, S Best, M Bondin	The Australian National University	Redox State Modulation of Metal-Metal Bonding (continuation)
Dr B Kennedy	C Howard, Q Zhou, L Li	The University of Sydney	Structures and Phase Transitions in Metal Oxides and Halides
Dr C Kepert	K Chapman, C Weeks	The University of Sydney	Reversibility of Negative Thermal Expansion in the $MM'(CN)_6$ Family
Dr C Kepert	K Chapman	The University of Sydney	Negative Thermal Expansion in Co^{III} Prussian Blue Analogues
Dr P Kluth	B Johannessen, M Ridgway	The Australian National University	Ion Irradiation Induced Preferential Amorphisation of Metallic Nanocrystals in Silica Measured with EXAFS
Prof P Lay	A Levina, H Harris, Ming-Chu Cheng, I Mulyani, J Aitken	The University of Sydney	XAFS Studies of Bioinorganic Systems
A/Prof I M Low	U Mahmood, M Tan	Curtin University of Technology	Depth Profiling of Phase Composition and Texture in Human Teeth
Dr A Nikulin	A Darahanau	Monash University	Non-Destructive Characterisation of Nanostructures Using PRXRD Technique
Dr J Overgaard	D Hibbs	The University of Sydney	Charge Density Studies of Drug Molecules and Their Metal Complexes
Dr A Peele	K Vora	The University of Melbourne	LIGA for Lobster and CXRL
Dr M Ridgway	S Kluth, Z Hussain	The Australian National University	Amorphous Compound Semiconductors – Formation and Relaxation
Dr M Riley	G Schenk, G Hanson, L Gahan	The University of Queensland	XAS of Binuclear Metalloenzymes and Model Complexes
Dr S Schmid		The University of Sydney	Ceramic Materials with Modulated Structures
Dr A Stampfl		ANSTO	Understanding Bio-Glue from an Electronic Perspective
Dr V Streltsov	J Varghese, K Barnham	CSIRO	X-ray Absorption Studies on Structural Consequences of Metal Binding to the Amyloidβ-peptide
Dr N Tran		The University of New South Wales	Structural Order of Residual Oxygen in GaN Films Grown by Single Source Chemical Vapour Deposition
Dr K Wallwork	M Chauvet	ANSTO	Protein-Mineral Interactions with Calcium Oxalate Crystals
Dr Z Zhang	C Howard, G Lumpkin	ANSTO	Phase Diagram for the Perovskite System $SrTiO_3$-$La_{2/3}TiO_3$

BioCARS Beamline at Advanced Photon Source, Chicago, USA

Dr T Garrett		Walter & Eliza Hall Institute	Structural Analysis of the Human Leukemia Inhibitory Factor Receptor (LIFR)
Dr L Guddat		The University of Queensland	Branched Chain Amino Acid Biosynthesis or Acetohydroxyacid Synthase
Dr M Guss		The University of Sydney	Structure of Human Purple Iron Phosphatase (Uteroferrin)
Dr M Parker		St Vincents Med Res Inst	Inflammatory Protein A
Dr M Parker		St Vincents Med Res Inst	Human Growth Hormone Receptor
Dr P Ramsland	W Farrugia	Austin Research Institute	Engineering Immune System Glycoproteins into Uniform Crystalline Lattices
Dr J Rossjohn		Monash University	Coral Pigment
Dr J Whisstock		Monash University	Serine Proteinase Inhibitors

ChemMat CARS at Advanced Photon Source, Chicago, USA

Dr J Cao	J Wright	Swinburne University	Seeking Correlation Between the SAXD Patterns of Human Hair Keratin and Donors' Biological Characteristics
Prof G Edward	P Zhu, R Knott	Monash University/ANSTO	The Influence of Processing on Polymer Morphology and the Consequent Solid State Material Behaviour
Dr C Garvey	R Knott	ANSTO	SAXS Study of the Structure of Polymaleic Acid Aggregates
A/Prof A Gerson	J Addai-Mensah, Huixin Li	University of South Australia	X-ray Scattering from Supersaturated Caustic Aluminate Solutions
Prof E Gray	T Blach	Griffith University	In-situ XRD Study of the Kinetics of the α-to-β, Phase Transformation in the $LaNi_5$-H System
Prof R Lamb	H Zhang, N Tran	The University of New South Wales	Investigation of the Fractal Structure of In Situ Silica/ Fumed Silica/PDMS3-Component System and Its Correlation with the Film Morphology
Dr A Neufeld	R Taylor	CSIRO Manufacturing & Infrastructure Technology	Critical Parameters which Influence the Kinetics of Controlled Electro-Wetting of Reactive and Noble Metals
Dr D Sutton	T Hanley, R Knott	ANSTO/University of New South Wales	A Study of the Nucleation Characteristics of Polymer Crystallisation under Shear
Dr P Turner	B Skelton (UWA), J McKinnon – (UNE)	The University of Sydney	Specialist Crystallography at the Advanced Photon Source (SCrAPS2003)

XOR-CAT at Advanced Photon Source, Chicago, USA

Dr C Dillon	P Lay, J Aitken	The University of Sydney	Micro-SRIXE and Micro-XANES Analyses of Chromium Compounds in Lung Cells:
Dr P Donnelly	J Aitken, W Reade	The University of Sydney	Synchrotron studies of Chocolate-on-White Ware: SA Levantine Ceramic from the Levant Dating from c1550 to 1450 BC
Prof T Hambley	R Alderden, T Failes, M Hall	The University of Sydney	Monitoring Hypoxia Selective Agents in Tumors and Tumor Models
Prof E Harvey		CRC MicroTechnology	Fabrication of Two-Layered Structures with Alignment for a Micropump
Prof P Lay	C Dillon, J Aitken	The University of Sydney	Micro-SRIXE and Micro-XANES Investigations of the Intracellular Distributions and Forms of Indoleamine 2,3-deoxygenase (IDO)
Prof K Nugent		The University of Melbourne	Coherent X-ray Optics and X-ray Imaging
Dr M Ridgway	C Glover, G Foran	The Australian National University	Electronic Structure and Interface Effects of Ge Nanocrystals Embedded in a SiO_2 Mixture
Dr C Ryan	B Etschmann	CSIRO Minerals	Selective X-ray Bragg Spectrometry: Optimizing Fluorescence Microprobe Sensitivity for Precious Metals
Dr R Welberry	D Goosens, A Heerdegen	The Australian National University	Diffuse Scattering from Crystals Containing Flexible Organic Molecules

Supported by AMRFP, 2003-04

Facility	Principal Investigator	Others	Institution	Topic
APS	Dr C Chantler	Z Barnea, N Rae, M de Jonge, L Young, S Southworth	The University of Melbourne	High Precision Measurement of Imaginary Component of Atomic Form Factor at Intermediate Energies for Silicon
APS	A/Prof B King		The University of Newcastle	Surface Analysis Using a Free Electron Laser
BESSY II	Dr J Riley	A Tadich, L Broekman, E Huwald	La Trobe University	Angle Resolved Photoelectron Spectroscopy of Alloy Systems

Elettra	A/Prof A Gerson	C Piantadosi, R Jones	University of South Australia	Surface and Bulk X-ray Photoelectron Spectroscopic Analysis of Metal Sulfide Minerals
Elettra	Dr K Siu	M Morgan, T Beveridge	Monash University	Glioma Detection in a Rat Model Using Diffraction Enhanced Imaging
ESRF	Dr J Bartlet		ANSTO	Mechanism for Silica and Zirconia Nanoparticle Growth and Final Size in compartmented Salt-Free Catanionic Nanoreactors
ESRF	Dr A Berry	H O'Neill, S Sommacal	The Australian National University	Effects of Composition, Oxygen Fugacity, Pressure and Cooling on the Sulfur Speciation in Quenched Silicate Melts by µXANES
ESRF	Dr I Grey	E Silvester, C Macrae	CSIRO Minerals	Redox Reactions of Chromium During Ilmenite Alteration
ESRF	Dr J McKinnon		University of New England	Non-Linear Optical Properties of Molecular Materials: An Innovative Approach Using High-Resolution X-ray Diffraction Data
ESRF	Dr P Turner		The University of Sydney	Single Crystal Diffraction Data Collections (3 experiments)
Hasylab, DESY	A/Prof T Finlayson		Monash University	X-ray Sensitive Polymer Films
SPring-8	Prof R Lewis	K Sui, M Kitchen	Monash University	A Novel Method of Diffraction Enhanced Imaging (DEI) that Permits Imaging of Dynamic Processes by the Simultaneous Acquisition of Refraction and Absorption Images
SPring-8	Dr A Nikulin	A Darahanau	Monash University	High Resolution Tomographic X-ray Phase Retrieval
SPring-8	Dr K Pavlov	J Gillam	Monash University	A New Multi-Wave Diffraction Enhanced Imaging Technique: Laue Diffraction Case
SRS Daresbury	Dr E Gilbert		ANSTO	Parallel SAXS and DSC Investigation of Incommensurate Modulated Structures in Phase Separating Binary Paraffin Mixtures
Swiss LS	Dr V Streltsov		CSIRO Health Sciences & Nutrition	Structural Studies of Complexes of Interleukin-6 and its Receptors
Swiss LS	Dr J Varghese	V Steltsov	CSIRO Health Sciences & Nutrition	Structure of Interleukin-6 Signalling Complexes

Supported by ASRP 2002–03

Principal Investigator	Others	Institution	Topic
Australian National Beamline Facility at Photon Factory, Tsukuba, Japan			
Dr G Azevedo	B Johannessen	The Australian National University	Characterisation of Nanocrystal Formation in SiO_2 with EXAFS
Dr A Berry	H O'Neil, D Scott	The Australian National University	The Effect of Composition on Cr and Fe Oxidation States in Silicate Glasses and Melts
Dr A Berry	H O'Neill, S Sommacal	The Australian National University	The Oxidation State of U in Silicate Glasses
Dr S Best	M Bondin, S Borg	The University of Melbourne	Redox Initiated Structural Change in Iron-Sulfur Compounds (continuation)
Dr S Best	S Borg, M Bondin	The University of Melbourne	Redox Initiated Structural Change in Iron-Sulfur Compounds (continuation)
Dr S Best	M Bondin, G Heath, A Edwards	The University of Melbourne	Redox State Modulation of Metal-Metal Bonding
Dr J Brugger	W Liu, B Etschmann	SA Museum	Structure of Fe(III) and Cu(I) Chloro-complexes in Hypersaline Solutions
Dr R Corkish	Dr A Nikulin, E-C Cho, J Xia	The University of New South Wales	Structural Studies of Si/SiO_2 Interface Prepared by High Temperature Oxidation of SOI Wafer
Dr R De Marco	A van Riessen, A Lowe	Curtin University of Technology	An In-Situ Synchrotron Radiation-Grazing Incidence X-ray Diffraction Study of the Surface Chemistry of the Iron Electrochemical Sensor
A/Prof G Edward	G Simon, J Ma	Monash University	Processing Effects on Polymer Morphology and Orientation
Dr G Edward	J Healy, P W Zhu	Monash University	Morphology and Orientation Resulting from Polymer Processing
Dr B Etschmann	W Liu	CSIRO Exploration and Mining	Structure of Cu(I) Chloro-complexes in Hypersaline Solutions
Dr C Glover	P Kluth	The Australian National University	EXAFS Measurements of the Local Structure of Ferromagnetic GaMnAs Alloys
Dr T Hambley	M Hall, C Underwood	The University of Sydney	Investigations into the Rate of Biotransformation of Inorganic Chemotherapeutics
Dr R Hart	A van Riessen, K Winters	Curtin University of Technology	Defect Density, Size, Size Distribution and Strain in Kaolins

Dr M James	T Boecking	ANSTO	Investigation of Long Range Order in Ultra Thin Organic Monolayers on Silicon
Dr B Kennedy	Q Zhou, C Howard	The University of Sydney/ANSTO	Structures and Phase Transitions in $Ba_{1-x}Sr_xBi_2Nb_2O_9$
Dr B Kennedy	L Li	The University of Sydney	Valence Transitions in $Ba_2PrRu_{1-x}Ir_xO_6$
Dr B Kennedy		The University of Sydney	High Temperature Phase Transitions in the Perovskite $SrRhO_3$
Dr B Kennedy	Q Zhou	The University of Sydney	High Temperature Phase Transitions in the Layered Bismuth Oxide $Bi_4Ti_3O_{12}$
Dr B Kennedy	C Howard	The University of Sydney/ANSTO	High Temperature Phase Transitions in the Double Perovskite Cryolite Na_3AlF_6
Dr C Kepert	K Chapman	The University of Sydney	Negative Thermal Expansion in the $M^{II}Pt^{IV}(CN)_6$ Family
Dr P Kluth	B Johannessen	The Australian National University	Structural Properties of Metallic Nanocrystals Formed by Ion Implantation into SiO_2 Measured with Temperature Dependent EXAFS
Dr K Latham		RMIT University	A Preliminary EXAFS Study on the Incorporation of Iron into the Crystalline Lattice of Zeolite LTL
Prof P Lay	J Aitken, A Levina, I Mulyani	The University of Sydney	XAFS of Cr Dietary Supplements and Genotoxic Chromium Complexes
A/Prof J Low	Z Oo, B Stauble	Curtin University of Technology	Depth-Profiling of Near-Surface Composition in Vacuum-Treated Aluminium Titanate
Dr A Masters	R Syna, S McNiven	The University of Sydney	Mo EXAFS as a Probe of Molybdenum Speciation in the Production of Pharmaceuticals
A/Prof T Masters	R Syna, S McNiven	The University of Sydney	Mo EXAFS as a Probe of Molybdenum Speciation in the Production of Pharmaceuticals
Dr A Nikulin	A Benci, C Langer	Monash University	Characterisation of SiGe:C Alloys Near Absorption Edge of Ge II
Prof G Parkinson	M Loan, A van Riessen	Curtin University of Technology	Understanding Nanoscale Materials with Short-Range Order: Ferrihydrite
Dr K Pavlov	M Tabuchi, S Mudie	Monash University	Investigation of In Segregation in InGaN Heterostructures by Methods of Statistical Diffraction Theory (Reciprocal Space Mapping)
Dr K Pavlov	S Mudie, M Tabuchi	Monash University	Characterisation and Comparison of a Novel Reciprocal Space Mapping Routine, Utilising Image Plates as the Detector
Dr M Ridgway	W Wesch	The Australian National University	EXAFS Measurements of Structural Relaxation in Amorphised Compound Semiconductors
Dr M Ridgway	B Johannessen	The Australian National University	Irradiation Induced Preferential Amorphisation of Semiconducting and Metallic Nanocrystals in SiO_2 Measured with EXAFS
Dr B Singh,	A Tong, B Kennedy	The University of Sydney	Interaction of Copper, Iron, Lead, Chromium with Synthetic Kaolinite
Dr D Sutton	T Hanley	ANSTO/University of New South Wales	Structure Development in Nanocomposite Materials
Dr S Thomson	V Luca, C Griffith	ANSTO	EXAFS Experiments on a New Titanium Mesoporous Oxide (TOM) Support Material
Dr A van Riessen	R Hart, K Winters	Curtin University of Technology	Mimicking Biomineralisation of Calcium Carbonate Polymorphs
Dr L Vance	G Thorogood, M Carter	ANSTO	X-ray Spectroscopy and Diffraction of Hollandites
Dr C Weeks	C Kepert, K Chapman	The University of Sydney	XAFS Study of Negative Thermal Expansions in $Zn^{IV}(CN)_2$ and $Zn^{II}Pt^{IV}(CN)_6$
Dr Z Zhang	C Howard, G Lumpkin	ANSTO	Phase Diagram and Structures in the Perovskite System $SrTiO_3$-$La_{2/3}TiO_3$
Dr Z Zhang	C Howard	ANSTO	Phase Diagram for the Perovskite System $SrTiO_3$-$La_{2/3}TiO_3$

BioCARS Beamline at Advanced Photon Source, Chicago, USA

Dr Paul Carr	Samir Hamdan, James Murphy	The Australian National University	Probing the Active Site of the Epsilon SubUnit of DNA Polymerase III
Dr Luke Guddat	Jennifer McCourt	The University of Queensland	Branched Chain Amino Acid Biosynthesis
Dr B Kobe		The University of Queensland	Crystal Structure Determination and Peptide Recognition of the FHA Domain from the Yeast Protein Kinase Dun1
Dr M Lawrence	Jenni Carmichael	CSIRO	Insect Hormone ReceptorI
A/Prof Jenny Martin	C Gee, F McMillan, B Heras	The University of Queensland	Structural Studies on Medically Relevant Protein Targets

Dr Michael Parker	Julian Adams, Geoff Kong	St Vincents Med Res Inst	Human Class Pi Glutathione Transferase: Structural Basis for Substrate Binding
Dr G Polekhina	Michelle Dunstone, Geoffrey Kong	St Vincents Med Res Inst	Stuctural Studies of Intermedilysin, APP and Siah in Complex with its Binding Partners
Dr J Rossjohn		Monash University	Coral Pigment
Dr J Rossjohn		Monash University	Immune Receptors
Dr J Whisstock		Monash University	Serine Proteinase Inhibitors
A/Prof M Wilce		University of WA	Structural Analysis of SH2 Domains

ChemMat CARS at Advanced Photon Source, Chicago, USA

Dr Chris Garvey	Robert Knott	ANSTO	An ASAXS Study of the Structure of Polymaleic Acid Aggregates
Dr Jinan Cao	Jon Wright	Swinburne University	Correlation between X-ray Diffraction of Human Hair Keratin and Biological Characteristics
Dr Ian Gentle	Jeremy Ruggles, Ben O'Driscoll	The University of Queensland	Molecular Recognition between Metalloporphyrins and Solubilized Cations at the Air-Water Interface
Dr Ian Gentle	J Ruggles, G Foran	ANSTO	Studies of Interfacial Structure of Porphyrins and Silicates by X-ray Reflectivity
A/Prof V James	M Read, G Corino	The Australian National University	A Study of Changes in the Diffraction Patterns of Human and Baboon Hair with Disease
Dr Robert Knott	Tracey Hanley, David Sutton	ANSTO	Polymer Crystallisation and the Effects of Shear
Dr Kay Latham	John White	RMIT University/The Australian National University	Small-Angle X-ray Scattering Studies on the Earliest Stages of Crystallisation of Zeolite Molecular Sieves from Clear, Homogenous Solution Using SR

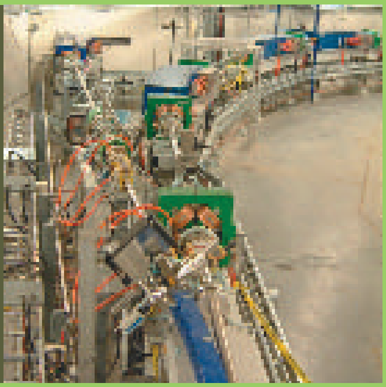
SRI-CAT at Advanced Photon Source, Chicago, USA

Dr A Buckley	Siew Wei Goh	The University of New South Wales	Oxygen K-edge XAS of Surface Oxide Layers on Aluminium
Dr A Buckley	Siew Wei Goh	The University of New South Wales	Threshold S KLL Auger Spectroscopy and XAS of Metal Sulfides
Dr P Dastoor	J Quinton, L Thomsen, B Watts	University of Newcastle	Molecular Alignment of Organosilanes on Surfaces Studied by X-ray Absorption Spectroscopy
Dr P Donnelly	Jade Aitken, Wendy Reade	The University of Sydney	Synchrotron Studies of Chocolate-on-White Ware: A Levantine Ceramic from Jordan and the Levant Dating from c1550 to 1450 BC
Dr M Ghantasala	Errol Harvey	Swinburne University	LIGA Fabrication Studies Using SU8 Resist with Aligned Structures for Making a Micropump
Dr M Ghantasala		Swinburne University	Fabrication of Two-Layered Structures with Alignment for a Micropump
A/Prof T Hambley	Mr M Hall, Ms R Alderden	The University of Sydney	Investigation Into the Mechanism of Action of Platinum Anticancer Complexes in Tumour Cells
Prof P Lay	Jade Aitken, C Dillon	The University of Sydney	Micro-SRIXE and XANES Investigations of the Intra-cellular Distributions and Forms of Indoleamine 2, 3-deoxygenase (IDO)
Dr A Mancuso	Keith Nugent, Andrew Peele	The University of Melbourne	Recovering Phase in the Presence of Scattering
Prof B O'Connor	A Van Riessen, Matthew Rowles	Curtin University of Technology	Dependence of Si and Al Radial Density Distributions on Chemical Composition in Alkali-Activated Aluminosilicate Polymers
Dr Tim Payne	P Milham	ANSTO/UWS	Cadmium Distribution in Sydney Basin Agricultural Soils by Synchrotron X-ray Fluorescence
Dr M Ridgway	C Glover, G Azevedo	The Australian National University	Local Structural Characterisation of Amophised and Annealed InP and GaP
Dr Chris Ryan	B Etschmann	CSIRO	Synchrotron – Nuclear Microprobe Energy: Towards Real-Time, Quantitative SXRF Elemental Imaging
Dr J Thornton		DSTO	Finding the Pair Distribution of Pristine and Degraded Thermal Barrier Coating Zirconia
Dr N Tran	R Lamb, H Zhang	The University of New South Wales	Structural Order of Residual Oxygen in GaN Films Grown by Single Source Chemical Vapour Deposition
Dr N Tran	R Lamb, H Zhang	The University of New South Wales	Structural Order of Residual Oxygen in GaN Films Grown by Single Source Chemical Vapour Deposition

Supported by AMRFP, 2002-03

Facility	Principal Investigator	Others	Institution	Topic
ALS, USA	Dr J Martin		The University of Queensland	Structural Studies on PNMT, Mouse Latexin, Insect Ferritin
APS, USA	Dr A Berry		The Australian National University	(i) Copper Speciation as a Function of Temperature in Fluid Inclusions (ii) Micro-XANES Determination of the Oxidation State of Fe in Natural Melt Inclusions
APS, USA	Prof V James		The Australian National University	A Study of Changes in the Diffraction Patterns of Hair with Disease
APS, USA	A/Prof B King		University of Newcastle	Surface Analysis Using a Free Electron Laser
BESSY II, Germany	Prof R Leckey	E Huwald, A Tadich	La Trobe University	Electronic Structure Determinations Using an Advanced Toroidal Spectrometer
BESSY II, Germany	A/Prof J Riley	A Tadich	La Trobe University	Observations of Mn Layers on GaAs Using Angle Resolved Photoemission
BESSY II, Germany	A/Prof J Riley		BESSY II Germany La Trobe University	Development of a Toroidal Spectrometer and Observations of Mn Layers on GaAs Using Angle Resolved Photoemission
Centre for Advanced Microstructures and Devices, USA	Dr M Ghantasala	C Davenport	Swinburne University	Fabrication of High Aspect Ratio Structure Micro-components for Microfluidic Applications Using Synchrotron Radiation
Elettra, Italy	Dr K Siu		Monash University	Extending the Applications of Diffraction Enhanced Imaging DEI: Dosimetry and Contrast Agent Studies
ESRF, France	Dr J McKinnon		University of New England	Non-Linear Optical Properties of Molecular Materials: An Innovative Approach Using High-Resolution X-ray Diffraction Data
ESRF, France	Dr M Ridgway	G Azevedo	The Australian National University	Structure of Metal-Decorated Nanocavities in Si
NSLS, USA	Ms V Peterson		University of Technology, Sydney	Investigation of Tricalcium Silicates
Pohang, Korea	Dr Deenapanray	M Petravic	The Australian National University	Structural Characterisation of (In)GaAsN Epitaxial Layers by Photoemission Spectroscopy
Pohang, Korea	Prof R Lamb	N Tran, E Lee	University of New South Wales	Structural Order of Ultra-Thin Films Grown by Single Source Chemical Vapour Deposition
Pohang, Korea	Dr A Nikulin	I Svalbe, R Horney	Monash University	Experimental Studies in Quantitative X-ray Phase Retrieval
Pohang, Korea	Dr J Russell	M Hill, R Lamb	University of New South Wales	Crystallographic Orientation of ZnO Films on Optical Fibres
Pohang, Korea & APS, USA	Dr M Petravic	P Deenapanray, V Coleman, M Fraser	The Australian National University	(i) Synchrotron-based Photoemission Studies of Composition Changes on III-N-V Surfaces Under Low Energy Ion Bombardment (ii) FEL-based Resonance Ionisation Spectrometry of Impurities from Semiconductor Surfaces
SLAC, University Stanford	Dr B Begg		ANSTO	Actinide Incorporation in the Zirconolite Polytypes
SLAC, University Stanford	Dr M Guss	S Graham	The University of Sydney	Structures of Metalloproteins and Metalloenzymes
SLAC, University Stanford	Dr M Maher		The University of Sydney	Multiple Wavelength Anomalous Dispersion MAD Data Collection from Metalloprotein Crystals
SLAC, University Stanford	Dr M Ridgway		The Australian National University	EXAF Characterisation of Implanted-Induced Disorder in Compound Semiconductors and Structural Perturbations in Elemental Nanocrystals
SLAC, University Stanford	Dr C Young	C Doonan, D Nielsen	The University of Melbourne	Metal and Sulfur XANES and EXAFS Studies of Molybdo Enzyme Models
SPring-8 Japan	Prof R Lewis		Monash University	An Investigation into the Nature of the Speckle Pattern Seen in Images of Lung Tissue
SPring-8 Japan	Dr A Nikulin		Monash University	Fundamental Studies of 90 Degree Bragg Reflection
SRRC, Taiwan	Dr A Buckley	N Tran, B Holzschuh	University of New South Wales	Structural Order of Residual Oxygen in GaN Films Grown by Single Source Chemical Vapour Deposition

Source: ASRP annual reports



06

The Australian Synchrotron in the international context

IMAGE: Canadian Light Source booster ring, showing extraction region.
Printed with permission from Canadian Light Source.

Photographer: Sandra Ribiero, CLS

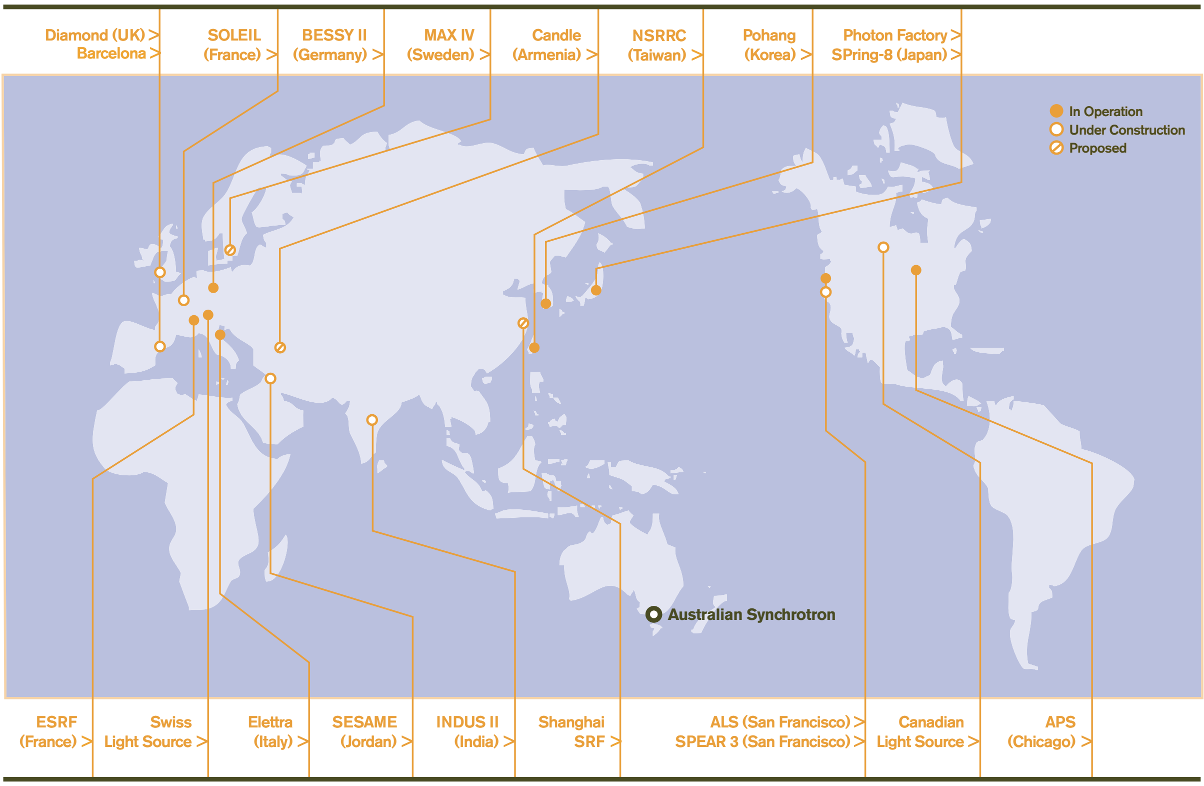
Chapter 06

The Australian Synchrotron in the international context

Synchrotrons originated in the 1940s and have evolved progressively; the first serious exploitation of synchrotron light was in the 1960s. As scientists became aware of its great potential as a tool for conducting a wide variety of leading edge experiments, development accelerated dramatically – particularly over the past fifteen years – with the building of a number of second generation and, from the mid 1990s, third generation facilities. At present there are about 50 facilities worldwide[1]. Most scientifically developed countries have a local facility, including countries such as Brazil and India. Japan has eight major installations (with a number of others privately operated), Germany seven and Sweden two.

The design objectives for the Australian Synchrotron, which were established in early 1999 following a feasibility study[2] and widespread community consultation both in Australia and overseas, were:

- an energy of 3 GeV to provide the best balance between energy range and cost
- a performance competitive with other third generation facilities currently under construction
- adequate beamline and experimental stations to satisfy 95% of the research requirements of an expected Australian community of 1,200 different scientists



GLOBAL PERSPECTIVE Third Generation Synchrotrons with Energies > 1.5 GeV

Figure 6.1. *Showing the installation of third generation synchrotrons around the world. Those already operating are solid and those under construction are open.*

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[1] Lists of world's synchrotron facilities at http://spring8.or.jp/ENGLISH/other_sr and at http://www-ssrl.slac.stanford.edu/SR_SOURCES.html

[2] Prepared for the Australian Government by J.W. Boldeman, 1998.

- provision of facilities and an environment to cater for all demands of Australian industry for synchrotron analytical requirements
- a sufficiently competitive performance to attract a potential international research community of at least 300 researchers
- a robust design to allow relatively easy construction and commissioning.

With these design objectives a full proposal[3] for an Australian synchrotron was prepared and submitted to the Australian Government in December 1999 by the ASRP.

The design of the Australian Synchrotron ring (known as the 'lattice') is the result of four years of intensive effort led by Prof. John Boldeman in collaboration with Prof. Dieter Einfeld of the Forschungszentrum Kahlsruhe[4]. The lattice has been evaluated in detail at two meetings of the International Machine Advisory Committee and by independent specialists at a design workshop in October 2002 at the Lawrence Berkeley Laboratory. During the period 2000 to 2003, the proposed design was also submitted to international scrutiny at many international conferences and workshops. The conclusion of all of these meetings is that the lattice is a particularly robust design with a very high performance satisfying the requirements of the Australian research and industrial community. The design specification has been confirmed at numerous workshops in Australia over the past two years as being optimal for Australian scientific needs. Details of the lattice design are included in appendix 2.

The medium energy 3 GeV capability adopted for the Australian synchrotron is widely regarded as providing the best value-for-money design of synchrotron. It covers the energy range needed for most experiments and has the flexibility to accommodate most foreseeable developments in synchrotron science.

The 6.1 shows the extended performance characteristics compared with three world class third generation 3 GeV synchrotrons currently under construction in the UK (Diamond), Canada (Canadian Light Source) and the USA (SPEAR III).

In the regional context, the Australian Synchrotron will complement low energy synchrotrons in Singapore (0.7 GeV) and Taiwan (1.5 GeV), which are better suited to the ultraviolet and soft x-ray part of the spectrum. It is likely that reciprocal access arrangements will be made with these facilities.

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[3] J.W. Boldeman, The Boomerang Proposal Parts I–VII, prepared for the Australian Synchrotron Research Program, December 1999.

[4] J.W. Boldeman et al., The Australian Synchrotron: A Progress Report, paper presented at the ANA Conference, November 2003; J.W. Boldeman & D. Einfeld 'The Physics Design of The Australian Synchrotron Storage Ring – Boomerang', NIM, 2003, in press.

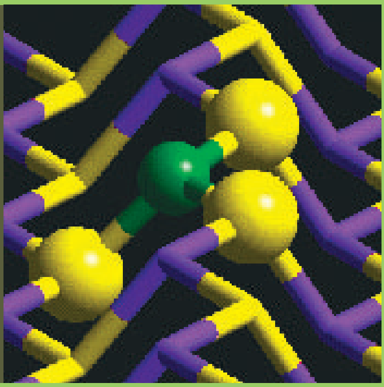
Table 6.1. Comparison of the Australian Synchrotron with others currently under construction in the UK, Canada and the USA

Parameter	Australian Synchrotron[2]	Diamond (Chilton, UK)[3]	Canadian Light Source	SPEAR III (Stanford, USA)
Lattice energy	3.0 GeV	3.0 GeV	2.9 GeV	3.0 GeV
Useable straights[1]	12	22	10	14
Circumference	216.0 m	561.6 m	170 m	234 m
Current[4]	200 mA	300 mA	200 mA	500 mA
Emittance[5]	7 nmrad	2.7 nmrad	18.1 nmrad	18 nmrad
Lifetime at max. current	~ 17 h	10–20 h	N/A	~50 h
Beam size in straights (height × width)	340, 13 μm	123, 6.4 μm (5 m str.) 178, 12.7 μm (8 m str.)	420, 29 μm	510, 40 μm

Notes:

1. The number of useable straights determines how many high performance insertion devices can be installed on the facility.
2. Australian Synchrotron has a dispersion level of 0.2 m.
3. Diamond has straights of two different lengths – 5 m and 8 m.
4. Most facilities will start up with 200 mA but some have plans to increase the current after several years of operation. This option is also available for the Australian Synchrotron.
5. The emittance specifies the size of the electron beam in the straight sections. The smaller the number the higher the brightness of the photon beams. The emittance of the Australian Synchrotron is smaller than that for the CLS and SPEAR III but not as small as Diamond.

07



Economic benefits of the Australian Synchrotron

IMAGE: Sphalerite

Structure of copper-activated sphalerite during froth flotation, elucidated by synchrotron EXAFS.

Chapter 07

Economic benefits of the Australian Synchrotron

Wealth generation and growth in GDP is highly correlated with national R&D activity.

In Feldman and Florida's discussion of the convergence of technological infrastructure, innovation and economic benefit, they recall that "in his classic work on innovation and capitalism, Joseph Schumpeter (1954) argues powerfully that economic growth requires innovation"[1].

All major OECD countries have now invested or are investing in synchrotron facilities.

International Reviews

There have been many economic assessments of the benefits that flow to a community following the exploitation of a national synchrotron. Clearly there would not be as many synchrotron facilities in the world were this not the case[2]. Extracts from several international reviews are presented below.

The BESAC report (1997) (USA)

The BESAC report (1997)[3] evaluated the impact of the advent of synchrotron radiation on technology in the United States with a view to determining the appropriate level of funding support that the Department of Energy should give to the four DOE National facilities in the US. This review concluded that:

> *"Synchrotron radiation research has evolved from an esoteric endeavour practised by a small number of scientists primarily from the fields of solid state physics and surface science to a mainstream activity that provides essential information in the materials and chemical sciences, the life sciences, molecular environmental science, the geosciences, nascent technology and defence related research among many fields."*

Canadian Light Source proposal

The proposal prepared for the Canadian Government supporting the installation of the Canadian Light Source[4] concluded that:

> *"Countries are not building synchrotrons solely to support basic research, significant as that research has been and doubtless will be. They are building them because of the diversity, importance and potential of high-technology, industrial applications."*

Business Case for Diamond (UK)

The Business Case for the installation of Diamond in the United Kingdom[5] claimed that:

> *"[failure to install Diamond] would be an erosion of the UK's international presence in key areas of research, notably structural biology and materials research. This would lead to a significant loss of capability to carry out research in these and related areas and migration of funds and expertise to non-UK research institutions. This would have a severe negative impact on the UK's science base.*
> *There is also the risk that industrial users requiring synchrotron radiation, such as pharmaceutical companies, would relocate their activities overseas."*

National Synchrotron Light Source (USA)

Suffolk County in the USA, which had the National Synchrotron Light Source within its borders, evaluated the impact the NSLS had on the local economy[6]. Their assessment was that NSLS had contributed between $US1b and $US2b over the life of the project.

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[1] M.P. Feldman & R. Florida, 'The geographic sources of innovation: technological infrastructure and product innovation in the United States', Annals of the Association of American Geographers, 84(2) (1994) pp 210–229, citing J. Schumpeter, Capitalism, Socialism and Democracy, 1954, Harper & Row, New York.

[2] List of world's synchrotron facilities at http://www.spring8.or.jp/ENGLISH/other_sr and at http://www-ssrl.slac.stanford_edu/SR_SOURCES.html

[3] Report of the Basic Energy Sciences Advisory Committee (BESAC) on DOE Synchrotron Radiation Sources and Science, Washington, D.C., 1996.

[4] Canadian Light Source, The Proposal for Construction of a National Synchrotron Light Source for Canada, Sept 1996 (SAL). Submission to Natural Sciences & Engineering Research Council (NSERC) of Canada.

[5] P.R. Woodruffe, Business Case for the Diamond Synchrotron, Office at Science and Technology, Version 2.0 p 23

[6] See OECD (1995) Megascience Policy Issues, The Megascience Forum, OECD, Paris.

Assessments of Potential Economic Benefits to Australia

There have been four assessments of the economic benefits that an Australian based synchrotron facility would contribute to the national economy.

Boomerang Proposal

The Boomerang Proposal Part IV (1999)[7], the original proposal for an Australian synchrotron, included an analysis of economic benefit by considering scenarios in the areas of:

- biotechnology and, in particular, structure-based drug design
- micromachining – nanostructured products
- environmental management
- scientific instrumentation
- diagnostic medical services
- mineral and oil assays
- high technology materials.

The new procedure of structure-based drug design where new drugs are developed through an analysis of target structures rather than through extensive trial and error clearly depends on knowing the structure of the target molecule, and it is apparent that this is dependent on synchrotron access. To access the economic consequences involves a number of assumptions not the least of which is the level of funding support – investment that will be available in Australia to take the intellectual property (IP) generated in a synchrotron study all the way to a marketable product. The maximum conceivable revenue can be assessed.
The Boomerang Proposal suggested:

"The installation of Boomerang would provide the opportunity for Australia to compete on a level playing field as a pharmaceutical supplier in the 21st century. It could be expected that products based on the generation of IP by Australian researchers at Boomerang could generate annual revenue of as much as $2b."

Of course as stated previously, to capture the full benefit of the IP would require major investment in development and drug trials.

With respect to micromachining, the assessment predicted possible revenue of $60–120m per annum.

Centre for Strategic Economic Studies

The Centre for Strategic Economic Studies (CSES) also carried out an evaluation in 1999 of the impact of a national synchrotron light source on the Australian economy[8]. They also used a scenario-based analysis but were able to introduce the data into a well respected economic model. Their summary analysis of the impact of the facility concluded:

"The establishment of a national synchrotron light source facility in Australia will provide a key link in emerging product and process developments that will be critical to the very industries that are now at the core of the local economy and those industries likely to form the engine for growth in the 21st century."

Other more specific conclusions were:

"Input-Output analysis of the direct, indirect and induced effects of the synchrotron reveals that it will generate a total of $687 million in additional output and $367 million additional value added, create a total of 441 additional jobs and generate tax revenue of almost $83 million over the 25 year life of the project."

"Those industries that are direct and potential users of synchrotron light-based research in Australia currently account for 2.7 million jobs or 32% of total employment: more than $187b or 28% of total industry gross product; more than $61b or fully 78% of our industry attributable merchandise exports and more than $3b or 77% of industry attributable R&D expenditure."

"A possible pharmaceutical industry development scenario could see the introduction of an Australian synchrotron facility contribute towards $1.3b per annum in additional industry revenue by 2010 and 3,200 additional jobs."

"If each extraction, processing and remediation benefited from synchrotron-based research as much as assays analysis, then up to $1b of mining production over the next 20 years would be directly attributable to synchrotron research."

"A possible induced investment scenario could see cluster development involving additional investments of $170m per annum by 2010, rising to $355m per annum by 2020; creating 850 new jobs by 2010 rising to 2,000 new jobs by 2020; and a potential $1.8b per annum in additional exports by 2010 rising to $4b per annum by 2020."

The delay in installing the facility relative to the assumptions in the CSES report means, of course, that these analyses are all delayed by three years.

Centre for International Economics

A separate report from the Centre for International Economics focussed more on the user demand and did not adopt any scenario analyses[9]. Some comments from this report are listed below:

"Royalties from a single successful drug delivery have been demonstrated to vastly exceed the threshold benefits (i.e. the total cost over the life of the facility) required for the synchrotron investment."

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[7] J.W. Boldeman, prepared for the Australian Synchrotron Research Program, 1999.

[8] Report for the Victorian Government by The Centre for Strategic Economic Studies, Victoria University (Melbourne), 1999.

[9] Centre for International Economics (CIE). The Net Benefits of a National Synchrotron Investment. Report prepared for The Steering Committee for the Australian Synchrotron Research Program, 20 October 1999, CIE, Canberra and Sydney, 1999.

"Synchrotron applications in microtechnology are likely to be at the very top end of the value adding spectrum."

"In the important mining and minerals sector, even very small unit cost savings that might be derived through synchrotron applications will translate into large dollar boosts to sectoral output value."

PricewaterhouseCoopers Feasibility Study

The National Synchrotron Steering Group established by the Federal Government as a consequence of the submission of the Boomerang Proposal commissioned PricewaterhouseCoopers to conduct a feasibility study and strategic business plan for a national synchrotron facility[10]. Their evaluation of the potential economic benefits arising from the establishment of the facility include:

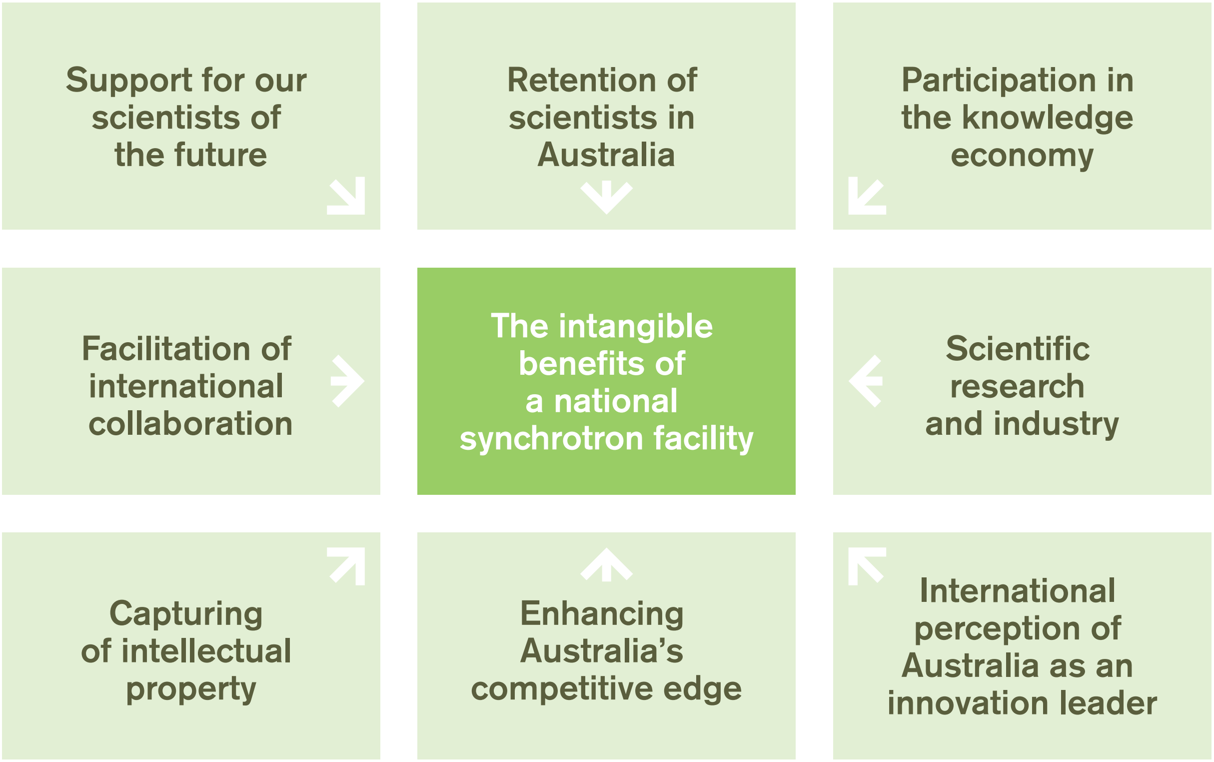
"Net national benefits – the core quantitative contribution of this investment cost to the Australian economy is the improvement in productivity that research can create. It is known that the synchrotron will be relevant to key sectors of the Australian economy such as biotechnology and mining. From foreign experience, synchrotron technology plays a critical role in R&D in some of these sectors. As a result, quantitative estimates can be provided to show how reasonable the expectations of a net national benefit might be.

- *The synchrotron need only contribute to output improvements of 0.03% for the mining, chemical and agricultural sectors to recoup its costs.*
- *Indicative scenario modelling using the MONASH model showed improvements in GDP of $640m per year after ten years when minor productivity improvements were applied to just a few key parts of the mining, chemicals and agricultural sectors of the economy. The improvement is permanent as it places the economy on a higher investment and growth path overall.*

Such an improvement would normally be associated with a corresponding boost in tax receipts to the Commonwealth and State Governments of up to $450m per annum."

Why do we need a Synchrotron?

The intangible economic benefits



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[10] PricewaterhouseCoopers, Feasibility Study and Strategic Business Plan for a National Synchrotron Facility. Report prepared for the National Synchrotron Steering Group, October 2000.

08

Status and timetable of the project

IMAGE: (left to right) Prof Peter Darvall, (former) Vice Chancellor, Monash University, Hong Lim MP, Member for Clayton and the Hon John Brumby MP, Minister for Innovation, inspect the site for the Australian Synchrotron

Chapter 08

Status and timetable of the project

The indicative schedule for completing the machine, the building and the proposed initial suite of beamlines is shown in table 8.1. Shading indicates the stages of design, including recruitment of personnel, construction, commissioning and user operation, which is then ongoing.

External Building and Synchrotron Machine

The contract for design and construction of the building has been let and site works have commenced. Details of final machine design are included in appendix 2. Current activities (at November 2003) include:

- injection system – preferred tenderers have been short-listed
- magnets and vacuum systems – call for registration of interest has been issued
- ongoing recruitment of staff for the design and engineering of the facility.

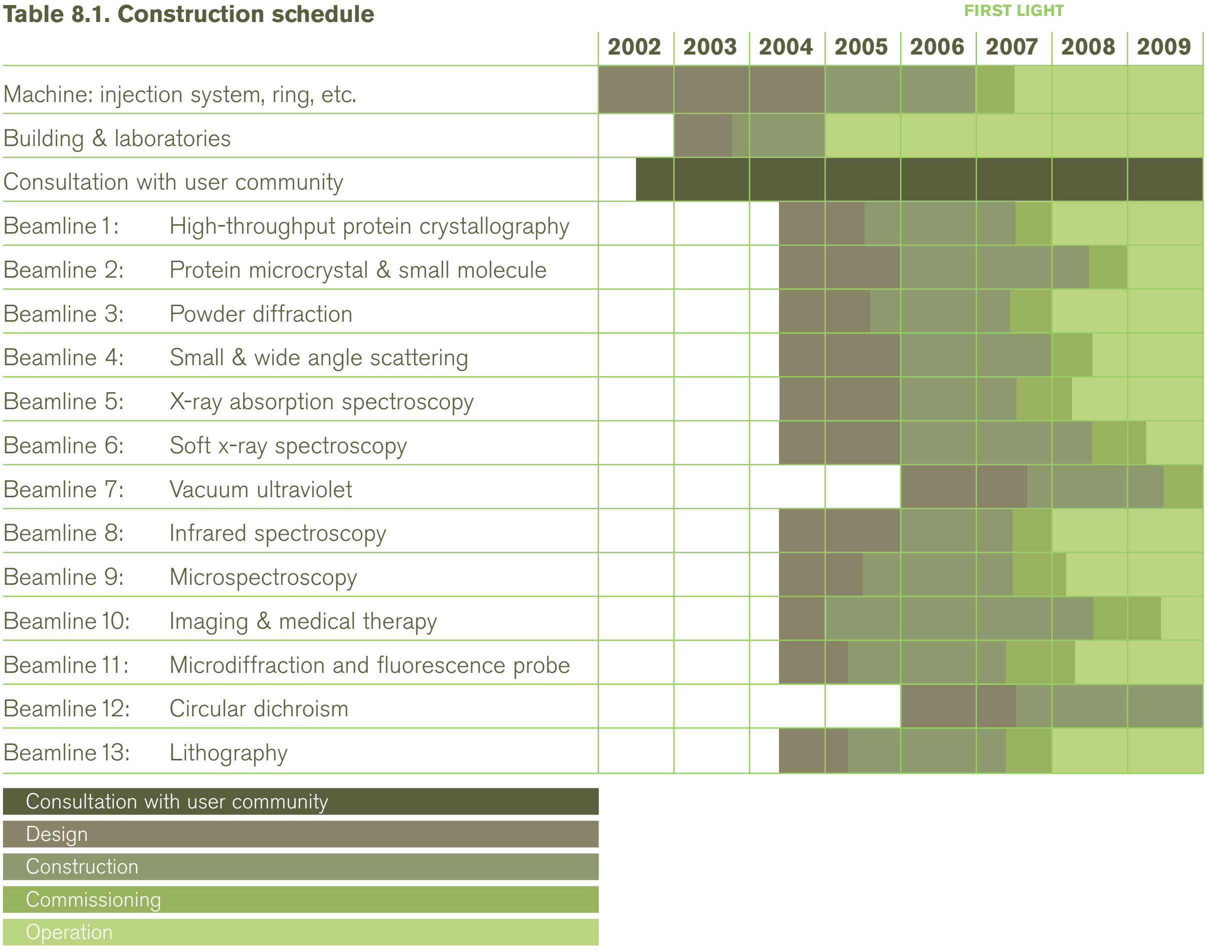
Beamlines

Development of beamline proposals in conjunction with the potential user community has been underway since mid 2002, and will continue throughout the life of the facility.

It is assumed that sufficient funding for the beamlines will be guaranteed by mid-2004 to enable the beamline design phase to commence.

Beamline schedules will be refined as designs proceed.

Table 8.1. Construction schedule



09

Management of the facility and principles for access to the beamlines

IMAGE: Entrance to the Australian Synchrotron (artist’s impression).

The Australian Synchrotron will provide core infrastructure for science and industry. It will stimulate research and enhance international collaboration.

Courtesy Architectus/Thiess

Chapter 09

Management of the facility and principles for access to the beamlines

The Australian Synchrotron is a national facility to be used by researchers from around Australia and New Zealand, as well as regional and international scientists. Therefore governance, access and operations issues can only be finalised in consultation with key national stakeholders in the full knowledge of the scientific and funding requirements of the facility. The governance model should take account of the breadth of available international experience and draw on the experience of bodies such as ISAC. To that end a considerable amount of consultation has already occurred and will continue as the National Science Case is carried forward.

Without limiting the possibilities that might be discussed and developed during consultation with potential partners, a *possible* model, based on international experience, is discussed.

Ownership

Under this possible model, the Australian Synchrotron would be established as an incorporated entity structured as a company limited by shares or by guarantee. A corporate structure is a common international model (for example, the European Synchrotron Radiation Facility – France, BESSY II – Germany, Advanced Photon Source – USA, Canadian Light Source – Canada) and facilitates investment by the private sector and potential overseas stakeholders. One model would allow for the owners of the company to be the initial 'investors' in the project.

Management

To manage the facility an independent, expert Board could be appointed by 'the owners'. The Board would need to have the required set of scientific, technical and commercial skills and experience to ensure that this national facility is operated to the highest international standards. In addition to their financial oversight and other corporate governance responsibilities set by the owners, the duties of the Board would include decisions on how the facility will be managed and operated (see below), setting a broad policy and operating framework.

A number of advisory committees could be established to make recommendations to the Board and to the Management of the facility. They may comprise:

- a **Scientific Committee** to advise on the strategic direction and design specifications of the Australian Synchrotron;
- an **Access Committee** to advise on the allocation of beamtime to users (this Committee could be supported by relevant expert committees, as used at the European Synchrotron Radiation Facility in Grenoble, France); and
- a **User Committee** to advise on the requirements and concerns of the user community.

Operations

It is important that the operator has a national focus, a sound reputation in financial management and the ability to run large, highly sophisticated scientific infrastructure. To ensure the provision of an environment conducive to good science, the operator must maintain a firm focus on user needs, ensure that equipment is maintained as leading edge, and strive for reliability of service.

The options for operation of the facility are:

- operation directly by the Board
- contracting out to an operator approved by the Board.

In contracting out operations, the Board could conduct a 'capability' tender to assess interest and competence of existing scientific organisations (e.g. ANSTO, CSIRO, universities) or the private sector. This approach may assist in attracting and retaining staff as part of a larger parent organisation. Importantly, it would provide clarity in determining whether the optimal operating approach would be to establish an in-house operating team or to contract an external operator.

Establishment of the Core Beamlines

International advice received by the Australian Synchrotron has been to advocate the establishment of a core set of beamlines meeting critical needs of Australian science and industry as is proposed in this document. This is the approach that is taken at many of the overseas synchrotrons; a very successful example is the ESRF, which has seventeen participating owner countries.

The model requires 'establishment' partners to agree as a group to contribute to this generic set of beamlines rather than to fund specific portions of individual beamlines. These beamlines would be owned, built and operated by the Australian Synchrotron.

Access to the Core Beamlines

Users of the core beamlines would be either non-proprietary (typically, researchers from universities or research institutions) who, while retaining ownership of intellectual property generated, normally place their research outcomes and intellectual property in the public domain, or proprietary (typically, industry or researchers funded by industry) who retain control over any intellectual property they generate while using the synchrotron. Users would apply for either merit-based access or priority access.

The model envisages that experiment time on the core beamlines could be allocated principally by a merit assessment process but with potential for funding contributors to gain access to additional reserved time allocation, again merit based. There could also be a priority system for 'proprietary' users.

Merit-based access

Merit-based access would involve periodical calls for applications for beamtime allocations. Applicants would develop proposals setting out their research, identifying the beamline(s) capable of meeting their research requirements, and estimating the time needed on that beamline.

Merit assessment of proposals would follow international norms and occur through a process of peer review by an Access Committee which would be responsible for the selection assessment process. Depending on the strategic priorities, the merit assessment criteria could be focussed on scientific excellence, or expanded to encompass a broader range of benefits. See table 9.1.

Table 9.1 Criteria options for determining merit

Criteria based strictly on scientific merit

- Scientific excellence
- Technical feasibility of the research
- Capability and track record of the research team
- Availability of resources
- Need to use a synchrotron to conduct the research

Additional criteria for a broader view of merit

- Potential for collaboration
- Potential economic/social benefits arising from the expected outcomes of the project

Priority access

A priority access mode would be needed to accommodate users requiring rapid access, and to enable the synchrotron to develop its user base. Priority access could be provided by setting aside a proportion of available beamtime or scheduled on an ad hoc basis and rescheduling other users or a combination of both.

Consideration should be given to ease of access for researchers who are not located close to the synchrotron. It is noted that the ASRP and AINSE models provide useful guides for enhancing access for these researchers.

Pricing of Access to the Core Beamlines

Development of pricing models for access is expected to be a key area of future discussions with funding partners. For general research, international experience indicates a model where operating funds are directly provided to the facility from national science funding sources with researchers provided with beamtime on the basis of the merit of their applications and the results of their work being openly available. NSAC strongly recommends that this should be the model adopted for the Australian Synchrotron. Consistent with international practice, commercially based access charges could be directly applied in the case of users where the project results are used for commercial gain, or where the user seeks a priority position in the queue for a certain beamline.

Non-core Beamlines

The model envisages that once the core beamlines are established, stakeholders could be offered the opportunity to finance the construction of additional 'non-core beamlines'. Access rights for non-core beamlines would be related to the contribution that, in addition to funding a new beamline or instrumentation, could include operating the beamline, building a new user community, or engaging in education or outreach.

Internationally, providers of beamline funding are granted 25–75% of the available beamtime for a period of 3 to 5 years. The majority of the remaining beamtime is allocated to other users according to the merit of their applications. The precise details of the conditions for installing a non-core beamline would be negotiated with the management of the Australian Synchrotron.

Issues such as the impact of the new beamline on the efficiency of the operation of the whole facility, compliance with facility standards (particularly with respect to safety) and compatibility with other equipment for ease and efficiency of maintenance will be major items for consideration during the negotiations.

User Support

Many users of the Australian Synchrotron will not be expert in synchrotron technology, especially in the early years of operation. A major role of the expert permanent scientific and technical staff will be to make using the synchrotron as user-friendly as possible, and in certain cases to provide full service including, for example, protein crystallisation, data analysis and the opportunity to operate the system remotely. It will be important therefore that expert permanent scientific and technical staff should have the time and capability to assist researchers with experimental design, operation of the beamlines and interpretation of data.

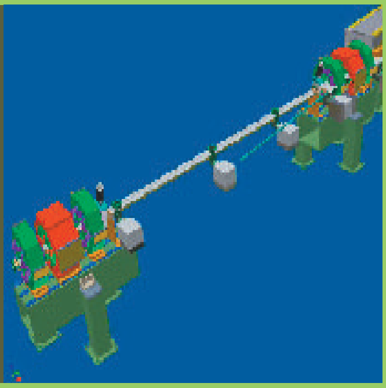
It will also be important that rigorous induction and regular education programs are provided for users covering all aspects of accessing the synchrotron, including safety.

Industrial users and researchers who undertake synchrotron research infrequently and have little expertise in the techniques may particularly value comprehensive service provision. It is envisaged that full service provision might be important in beamlines 1, 3, 4, 5, 6 (second station), 8, 9, 10, 11 and 12 (see table 9.2).

Table 9.2. Beamlines where full user support may be needed

Beamline	Applications that may require full user support
1. High-throughput Protein Crystallography	■ Protein crystallography, structural biology
3. Powder X-ray Diffraction	■ Minerals, advanced materials, pharmaceuticals
4. Small and Wide Angle X-ray Scattering	■ Protein secondary structure, structural biology, food science, agricultural industry, functional polymer manufacture
5. X-ray Absorption Spectroscopy	■ Environment, toxicology, forensics, minerals
6. Soft X-ray Spectroscopy (second station)	■ Minerals, materials and device manufacturing (surfaces), corrosion investigation
8. Infrared Spectroscopy	■ Forensics, archaeology and museum studies, pharmaceuticals
9. Microspectroscopy	■ Nano and bio-materials development & manufacture, drug development
10. Imaging & Medical Therapy	■ Small animal imaging for medical research
11. Microdiffraction and Fluorescence Probe	■ Minerals, agriculture
12. Circular Dichroism	■ Drug design

10



Beamline summaries

IMAGE: Computer Aided Design (CAD) render of a beamline emerging from a section of the Australian Synchrotron storage ring.

The Australian Synchrotron has the capacity for more than 30 beamlines to service a vast range of scientific disciplines.

Chapter 10

Beamlines 1 and 2: crystallography of macro- and small molecules

01/02

Potential Research Fields

Beamline 1

Life sciences

- Biological research and drug design
- Biotechnology and bio-sensors
- Plants and crops

Physical sciences

- Agricultural technology
- Food technology

Beamline 2

Life sciences

- Biological research and drug design
- Biotechnology and bio-sensors

Physical sciences

- Sustainable environment
- Advanced materials
  - Functional polymers
  - Nanomaterials and composites
  - Biomaterials
- Earth sciences
- Oil and gas production and distribution
- Food technology
- Chemical reactions and catalysts

Introduction

In the first phase it is proposed to construct two beamlines to characterise biological macromolecules. Beamline 1 will be designed for high-throughput protein crystallography. Beamline 2 (Protein Micro-crystal & Small Molecule X-ray Diffraction), will also be capable of characterising small molecules via a separate end station.

This is deemed the most cost-effective start-up approach, but it is anticipated that the user base for both requirements will expand rapidly and in the next suite a dedicated beamline for small molecule studies will be justified, leaving beamline 2 solely for protein crystallography.

Protein Crystallography

The major activity on beamlines 1 and 2 will be protein crystallography, where single crystals are analysed by x-ray diffraction using the multiple wavelength anomalous dispersion (MAD) technique. As described in chapter 3, protein crystallography provides the primary structural information on the complex macromolecules that drive biological processes. The scale of this activity worldwide is very large, because of the enormous number of different proteins expressed by the genome, as well as many viruses and nucleic acids.

It is envisaged that beamline 1 will be able to be used by researchers who are not specialists in crystallography. It will be best suited to larger protein crystals and for initial assessment of more complex crystals which might then be further investigated on the fine-focus beamline 2.

Beamline 2 will provide high flux and brilliance and improved beam focus. The characteristics are important for obtaining diffraction data from extremely small and weakly diffracting protein micro-crystals (10–30 micron size, which are, in general, difficult to grow and diffract weakly) – an area of research that is predicted to grow rapidly in the next few years. It will be a fine focus beamline (80 micron beam size) with slits capable of reducing the spot size to as little as 5 microns. It is intended to be used by specialist protein crystallographers.

A key feature is to make user access as friendly as possible, and in certain cases to provide full service at beamline 1, including crystallisation, data analysis and the ability to operate the system remotely.

User Community

Currently, there are about 45 protein crystallography groups in Australia and New Zealand and this number is growing steadily. The larger laboratories are centred around the State capitals and Auckland, and at a number of smaller laboratories elsewhere in both countries. Australian laboratories currently access overseas synchrotrons, principally the BioCARS facility at the Advanced Photon Source, near Chicago, through the Australian Synchrotron Research Program (ASRP).

The specialist protein crystallography community from its beginning in the late 1970s has formed a cohesive and cooperative group with good communications between the chief investigators.

By 2007 it is expected that there will be a much larger community that will include non-specialist protein crystallography users, who would use the beamlines for routine structure determination and view the beamlines as a routine analytic tool for biology.

Research Applications

Macromolecular research applications

The new field of proteomics has emerged that involves the systematic characterisation of the gene products of entire organisms. A key component of proteomics is the three-dimensional structural elucidation of proteins, termed structural genomics, which is being undertaken by worldwide public and commercial consortia. Once the structures of complexes of multiple proteins are solved and large proteins are broken down into their functional domains, it is possible to study their mechanisms or ligand binding properties at atomic resolution.

Small Molecule Diffraction

A second end station on beamline 2 will determine three-dimensional small-molecule (and macromolecular) structures to resolutions from normal to high (3 to 0.4 Angstroms) of weakly diffracting crystals and of crystals for charge density studies.

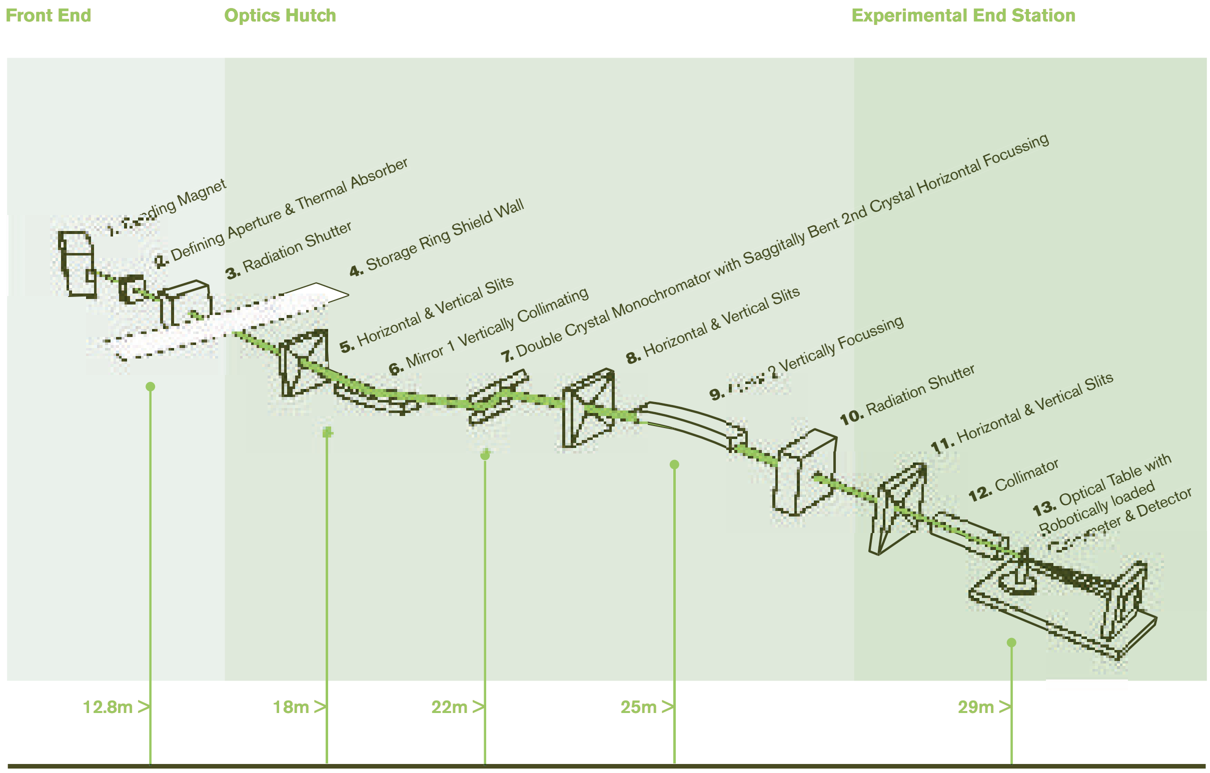
The use of the brilliant, highly collimated and tunable x-ray radiation from the synchrotron will either enable structural studies that are impossible with conventional laboratory sources, or provide improved precision and accuracy. Unlike any other x-radiation source, synchrotron light is tunable and this will provide contrast between isoelectronic species and also sensitively discriminate between oxidation states.

Applications of the small molecule facility will include the structure determination of micro-crystals with dimensions of a few microns or less. No other technique has the ability to assign unambiguously atom-to-atom connectivity, stereochemistry, absolute configuration, and charge density distributions.

Moreover, the facility will allow the resolution of disorder, and thus an understanding of its relation to physical properties, the identification of super-structure and structures under change (for example, pressure), which is not possible with laboratory x-ray sources. This will allow the structure elucidation of the ever increasing complexity of molecules/materials, for which it is difficult to grow large crystals for conventional x-ray studies.

User Community

The use of synchrotrons for small molecule studies is in its infancy in Australia and New Zealand, and it is difficult to predict the user community for 2007 reliably. The number of research groups in the small molecule community who use single-crystal x-ray diffraction data



BEAMLINE 1 High throughput Protein Crystallography

Figure BL1.1 *Schematic of the high throughput protein crystallography beamline* for molecular structure determinations is conservatively estimated to be at least 100, and so the number of potential users of the synchrotron is certain to be significantly greater than 100.

Currently the level of awareness in the small molecule community of the powerful capabilities of a synchrotron is relatively low. International experience suggests that once the synchrotron is fully operational, the community's appreciation and use of synchrotron light will increase dramatically. Demand for the dedicated single-crystal facility at SRS, UK, is over-subscribed by more than a factor of two. The new UK synchrotron under construction (Diamond) will have a dedicated small molecule single-crystal facility, reflecting a recognition of the importance of synchrotron investigations of small molecule structure for the benefit of UK science, industry and the economy. The same benefits would be provided by small molecule studies at the Australian Synchrotron. Small-molecule structure elucidation supports a wide range of chemical, geochemical, material science and medical R&D activities in Australia and New Zealand.

Beamline Design

Beamline 1 will be sourced from a bending magnet and will be operational on first light from the synchrotron. Beamline 1 is intended to be a highly automated work-horse with crystals robotically loaded and centred and to be capable of being operated remotely. Because of the very large scale on which proteomics research will be conducted, it is expected that throughput will need to be high It will use the MAD technique, in which the wavelength of the x-ray beam is scanned over a range of frequencies close to the x-ray absorption edge of certain of the metallic atoms in the protein crystals. In addition, emphasis will be placed on rapid automatic data collection and interpretation. The data will be automatically handled by sophisticated software to provide detailed crystal structure information in real time.

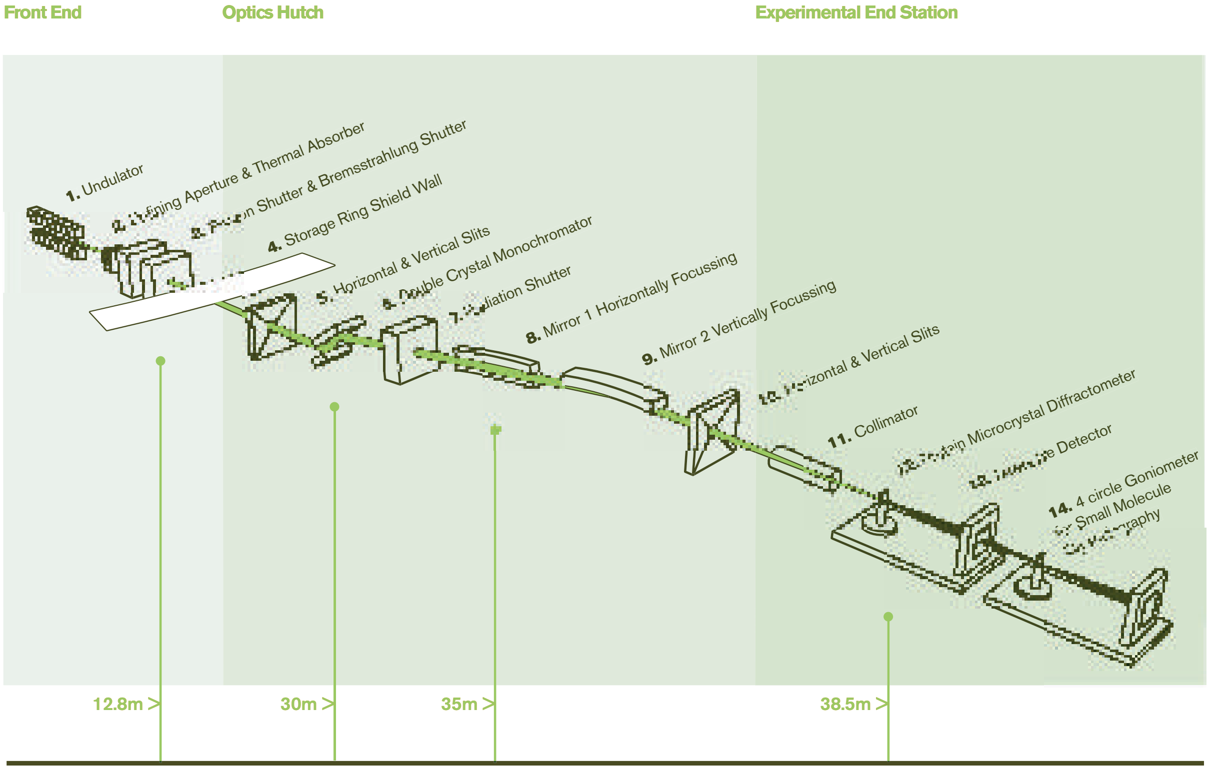
At a later stage, consideration will be given to sourcing the beamline from an undulator, to provide higher flux at the sample.

Beamline 2 will be driven from an undulator to produce the high brightness that is required for a highly focussed beam. Like beamline 1 it will have robotic loading and centring of the crystals and will also have MAD capability.

A second end station will be installed in a separate hutch on beamline 2 that will be able to collect high resolution, low signal-to-noise data from large protein complexes and virus crystals (the maximum unit cell size of biological materials to be studied is planned to be about 1,200 Å) as well as small molecules.

The design of the two beamlines has been developed according to the following principles:

- As far as possible the beamlines will use common elements and equipment to reduce cost and for efficiency of maintenance. The small molecule end-station, in particular, would use well-established and essentially 'off the shelf' technology.



BEAMLINE 2 Protein Microcrystal & Small Molecule X-ray Diffraction

Figure BL2.1 *Schematic of the protein microcrystal and small molecule x-ray diffraction beamline*

- Requirements for beam spot size and divergence will vary depending on the crystals to be analysed, so flexibility will be built into the beam optics.
- The designs will be based on the current international best practice, particularly the beamlines at the Swiss Light Source.
- Each line will commence operations with a flat panel detector to ensure rapid start-up. Once each beamline is fully operational the flat panel detector will be replaced with a single pixel type. This will be staged so that the flat panel from beamline 1 will be used to start up beamline 2.
- The beamlines will be automated and made as user friendly as possible, recognising that the users are unlikely to be specialists in these synchrotron based techniques.
- Provision will be made to enable remote operation of the facility, and for rapid interpretation of the data. Robotic operation will be added after initial commissioning.

It is envisaged that at commencement both functions on beamline 2 will be housed in the same end station, but later, as demand for small molecule studies increase, they will be housed in separate end stations for greater experimental flexibility.

The combination of small molecule crystallography with protein micro-crystallography will provide equipment and personnel benefits for both applications. Both fields have convergent detector needs – wide solid-angle, linearity, high dynamic range and low noise. Small molecule studies require a four-circle kappa goniometer, and although not the conventional choice it provides recognised benefits for protein data collection. A four-circle goniometer provides full diffraction sphere coverage, and this has been shown to facilitate and accelerate the determination of protein structures. Precision studies of small molecules require shorter wavelengths than would normally be used by protein crystallography. Shorter wavelengths minimise absorption and additionally charge density studies are now beginning to be extended to proteins; this is likely to have a significant impact on rational drug design programs.

Ancillary equipment will include cryostats providing a temperature range of at least 15 K to 1000 K and diamond anvil cells for high pressure studies.

BEAMLINES 1 & 2

Beamline 1 – High-throughput Protein Crystallography	
Source	Bending magnet
Energy range	2–23 keV
Resolution	$<1 \times 10^{-4}$
Nominal beam size at sample (horizontal × vertical)	300 × 200 microns
Features	Robotic loading, MAD capability

Beamline 2 – Protein Micro-crystal and Small Molecule X-ray Diffraction	
Source	In-vacuum undulator
Energy range	5.5–20 keV
Resolution	$<1 \times 10^{-4}$
Nominal beam size at sample (horizontal × vertical)	80 × 30 microns
Features	Robotic loading, MAD capability, 2 end stations

03

Beamline 3: Powder diffraction

Potential Research Fields

Life sciences

- Biological research and drug design
- Plants and crops

Physical sciences

- Sustainable environment
- Forensics
- Advanced materials
  - Ceramics
  - Nanomaterials and composites
  - Metals and alloys
  - Biomaterials
- Engineering
- Mineral exploration and beneficiation
- Earth sciences
- Agricultural technology
- Food technology
- Chemical reactions and catalysts

Introduction

The design and optimisation of new materials and/or mineral processing methodologies is dependent on obtaining precise structural information, especially under non-equilibrium conditions. Such information can be obtained either by single-crystal or powder diffraction techniques. In most laboratories the production of diffraction-quality crystals may be months (or years) behind new discoveries (e.g. high temperature superconductivity). Researchers must then rely on powder diffraction studies. In certain cases, for example in mineral processing or in the study of materials under extreme conditions, powder diffraction can be the optimum method for research.

Advantages of a Synchrotron Source

Laboratory-based powder diffraction techniques are inherently resolution-limited – in the range of observations (d-range), the signal to noise ratio, and the shape and width of observed reflections. Synchrotron-based instruments are the only means whereby these limitation can be overcome to give the resolution required to determine and refine precise and accurate structures of even moderately complex materials from powder samples.

Another advantage of synchrotron light is that it enables the use of anomalous dispersion to be used to obtain information on specific elements, as discussed in chapter 2.

User Community

The past decade has witnessed a staggering growth in the use of synchrotron powder diffraction. The Australian powder diffraction community has made a significant contribution in this area and has an outstanding international reputation.

Powder diffraction plays a key role in the study of nanomaterials, and one of the flagship instruments at the Brookhaven National Laboratory Center for Functional Nanomaterials (USA) is the powder diffractometer at its National Synchrotron Light Source.

The current Australian Synchrotron powder diffraction community exceeds 23 independent research groups from 13 institutions. The total number of Australians using synchrotron powder diffraction methods, including postgraduate research students, is estimated to be greater than 50. The 23 research groups indicate that if beam time and funding limitations were removed they would require 160 days per year for existing programs. This demand is sufficient to use all the time available on a dedicated beamline on the Australian Synchrotron.

The Australian National Beamline Facility at the Photon Factory (Japan) boasts one of the best x-ray diffractometers in the world. Australian scientists are also intimately involved in the development of a diffractometer as part of the ChemMatCARS consortium at the Advanced Photon Source (USA). Australian scientists have also been regular users of similar equipment at many international synchrotron facilities including ESRF (France) and SPring-8 (Japan).

Approximately 25% of all experiments funded by the ASRP utilised the powder diffraction technique. Therefore the installation of a powder diffractometer is a high priority to ensure that this is a world competitive instrument to retain Australia's standing in this fundamental application of x-rays.

Research Applications

The powder diffraction beamline is expected to be used for studies in the following key areas.

Oxide based materials

The majority of advanced materials used in magnetic, conductivity, superconductivity, ferroelectric, catalytic and battery applications are solid metal oxides. This is a very high priority research area in Australia. Metal oxide chemistry is dominated by classes of materials having crystal structures derived from simpler parent structures such as perovskite or rutile. Small lattice distortions, which are critical to the key electronic and physical properties of these oxides, usually lead to lower symmetries and superstructures. These distortions are characterised by subtle peak splittings and the appearance of weak superlattice reflections in diffraction data. Typical examples include polar distortions in bismith oxide ferroelectrics, Jahn-Teller distortions in manganese oxide battery materials and valence ordering in colossal magneto-resistance materials (CMR). The detection and understanding of such distortions requires the high resolution afforded by synchrotron radiation. For more on this, refer to chapter 3.

An underlying feature of many of the most interesting materials is the strongly correlated behaviour of the electrons and coupling of the electronic charge and spin degrees of freedom with those of the electron orbitals and the lattice. The greatest potential for functionality is in materials at the edge of a structure and/or electronic instability where small changes in chemical or physical conditions lead to a major change in properties. Success here requires rapid data collection, which is only possible on a high brightness synchrotron radiation source.

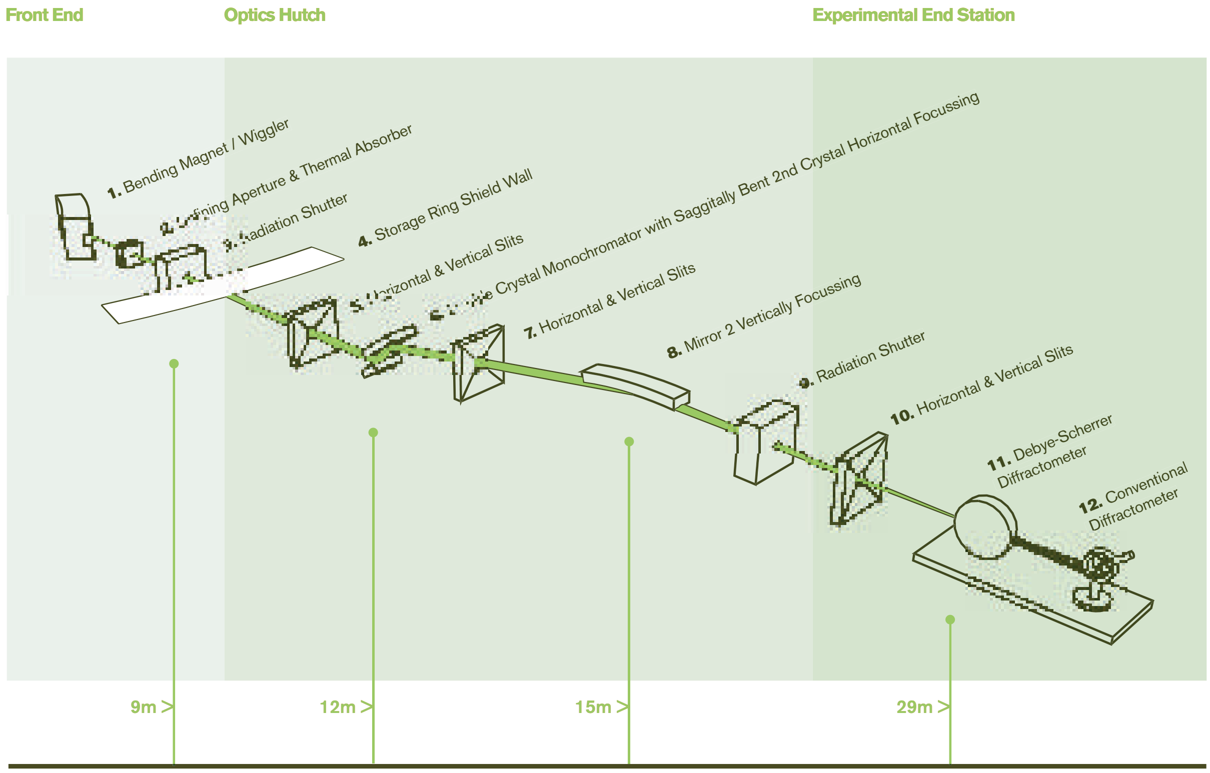
Microporous and framework materials

Detailed knowledge of the crystal structure of microporous materials such as zeolites is required in order to understand their properties and improve their use of catalysts, sorbants and micro-reactors. These materials typically have large unit cells and it is common to observe complex patterns because of low symmetry or subtle distortions. In many cases a very high x-ray flux as delivered by a synchrotron source is the only way these problems can be studied.

Another application is in the study of a novel class of cyanide-bridge coordination framework solids that display negative thermal expansion behaviour. These have diverse potential applications in high precision and low thermal shock materials where the positive thermal expansion exhibited by the vast majority of materials is a hindrance. The ability to access low d-spacing – possible with synchrotron radiation – is critical in the study of the amplitude of such processes.

Mineral processing and soil sciences

Powder diffraction has been applied widely for analysis in the mineral processing industries. Laboratory techniques have traditionally been used; however, as ore grades



BEAMLINE 3 Powder Diffraction

Figure BL3.1. *Schematic of the powder diffraction beamline* become lower with increasing complexity in the mineralogy, improved peak resolution and peak-to-background ratios are required to conduct full characterisation. The synchrotron-based powder diffraction technique provides the inherent high resolution, high sensitivity and high speed capability that is critical in such studies.

This high speed capability will be used in studies where the sample environment emulates the processing conditions found in industry. The availability of a range of sample environments, including high temperatures and pressures, will be a key feature of this instrument. Some examples are provided in chapter 3.

Strain, texture and phase mapping

Powder diffraction has important applications in mechanical engineering, particularly in the mapping of residual strain fields, the detection of phases that degrade the material properties, mapping texture of the material, and determining grain size and the degree of cold work. High-energy synchrotron radiation (60 keV, which will be available from the wiggler source) enables measurement in the depth range of 0.01–1 mm. This depth range is very important as it is where most of the degradation of mechanical components originates. It also covers the thickness range of many protective coatings (e.g. thermal barrier coatings) and surface engineering treatments (e.g. laser shot peening).

The large flux of high energy x-rays available from insertion devices enables the two-dimensional mapping of strain, texture and phase in practical times. At each point of a map, a large area two-dimensional position-sensitive detector collects the rings of the diffraction pattern. Increasing the sample to detector distance provides information on cold work and grain size. Such maps are important in most areas of mechanical engineering (e.g. aerospace and power generation) and enable the integrity of newly developed procedures (e.g. welds) or aged components (e.g. turbine blades) to be assessed.

Furthermore, techniques are now being developed, with spiral or conical post sample collimators, to produce full three-dimensional maps of strain. Coupling the two- or three-dimensional mapping data with imaging data from beamline 10 (imaging and medical therapy) will increase the power of both the mapping and imaging techniques. Thus flaws can be located using beamline 10 and the associated strain fields mapped using beamline 3. Similar synergies may also be possible with other beamlines.

Pharmaceuticals

Powder diffraction has a key role to play in structural studies of pharmaceuticals and their interaction with low molecular weight peptides. Already powder diffraction patterns play a key role in unequivocally establishing the crystalline form of a pharmaceutical in a manufactured drug. Where the data has sufficient resolution, these methods will aid in understanding the solubility and dissolution of these forms.

To ensure that powder diffraction is available on the synchrotron at first light, this beamline will be sourced initially from a bending magnet. Specific techniques can be refined during this start-up period. However, as soon as the electron beam is sufficiently stable, the beamline will be moved to a wiggler source. This will enable an increase in flux and extension of photon energy to 65 keV, so that the capability of this beamline rivals the best in the world.

Beamline Design

Optics

The preferred optics for the beamline are conventional, and consist of a mirror and monochromator. All the optical components should be incorporated into a separate hutch. The first mirror provides vertical collimation and removes high-order harmonics. A double crystal monochromator consisting of two Si (111) crystals is required. At this stage provision has been made for a second mirror in the optics hutch to allow for a future upgrade of the beamline to permit the beam to be focussed (see figure BL3.1).

End stations

Two powder diffractometers on a single beamline are proposed, the first being a relatively compact Debye-Scherrer camera having a large area detector. The second diffractometer would include a large two-dimensional position-sensitive detector for strain and texture measurements capable of being mounted to collect transmitted or reflected diffraction data, as well as being equipped with an array of analyser crystals coupled with scintillation detectors for very high resolution studies.

A positioning table will enable strain, texture and phase mapping and will be able to accommodate moderately large (20 cm) and heavy (5 kg) mechanical components or samples on standard mounting plates. The standard mounting plates will be interchangeable with those on beamline 10 and will facilitate the accurate co-alignment of the sample or component to better than 0.01 mm.

Both diffractometers will be configured to enable an array of environmental conditions to be studied, including high pressure, high and low temperature, and variable atmosphere.

A compact mechanical test machine will also be available to calibrate the strain data in situ to obtain the stresses, and also to load or fatigue the sample or component in situ.

Beamline 3 – Powder X-ray Diffraction	
Source	Bending magnet, then wiggler
Energy range	4–65 keV
Resolution $\Delta E/E$	$<1 \times 10^{-4}$
Beam size at sample (horizontal × vertical)	2 × 5 mm

Beamline 4: Small and wide angle scattering

Potential Research Fields

Life sciences

- Biological research and drug design

Physical sciences

- Forensics
- Advanced materials
- Functional polymers
  - Ceramics
  - Nanomaterials and composites
- Earth sciences
- Oil and gas production and distribution
- Agricultural technology
- Food technology
- Chemical reactions and catalysts

Introduction

Studies of the structure and dynamics of large molecular assemblies in environments such as solutions are key to understanding living organisms and complex materials such as polymers, colloids and emulsions. For this reason, small angle scattering (SAXS) and wide angle (WAXS) diffraction, normally combined on one beamline, are recognised as two of the most important synchrotron applications.

At the Advanced Photon Source, nine of the twenty-five undulator beamlines are capable of performing small angle scattering, and the situation is similar in most synchrotrons around the world.

Advantages of a Synchrotron Source

A major advantage of a synchrotron source is the ability to study processes that are changing with time because of the extremely high beam intensities. Dynamic processes are of enormous interest in both the life sciences and physical sciences, and they represent an area where synchrotron sources are contributing valuable knowledge, unobtainable by other experimental techniques.

User Community

There is an active community of researchers using small angle scattering in a number of fields. Currently in Australia there are several laboratory-based SAXS instruments. Access to synchrotron SAXS is available primarily to Australian users through the ASRP to the newly-commissioned instrument at Sector 15 at the Advanced Photon Source (ChemMatCARS) in Chicago. This instrument has not been available for long and already demand exceeds supply as researchers take advantage of the benefits of SAXS on a third generation source.

X-ray and neutron scattering methods complement one another, and the simultaneous refinement of data produced using a combination of both methods on the one system is very powerful. A small angle neutron scattering instrument to be built at the Replacement Research Reactor at Lucas Heights will augment and complement the Australian Synchrotron SAXS/WAXS beamline. The major benefit of such analysis is the removal of potential ambiguity in the interpretation of data.

Research Applications

SAXS/ WAXS studies have broad applicability across a range of materials and biological sciences. Examples of fields of science and technology that can benefit from these methods are:

- polymers
- mesoporous materials
- self-assembled systems
- food science
- fibres
- colloids
- composite materials
- proteins in solution
- membranes
- crystallisation studies

Biological sciences

Small angle scattering (SAXS) can now determine the shapes of macromolecules in solution, and provide information on the assembly of protein components in functional units. This information is being used to determine what changes in association are relevant to the function of these complexes. This has been useful in understanding biochemical regulation by providing insights into domain reorientation and protein–protein interactions in cellular signalling. The shapes of these assemblies can then be used to construct atomic models based on the structure of the individual components, or used in phasing crystallographic data on these complexes.

The dynamics of many important biological processes, such as protein folding, are studied by SAXS. For example, several folding intermediates have been detected in the re-naturation of apo-myoglobin and lysozyme.

The dynamic processes involved in conformational diseases such as prion diseases and neuro-degenerative disorders are important in the understanding of how these diseases arise. In prion diseases such as bovine spongiform encephalopathy (mad cow disease) an ‘infectious’ form of the prion protein causes nucleation of toxic oligomers of normal protein by altering the conformation of normal proteins. This process is also thought to take place in Alzheimer’s and other neurodegenerative diseases. Time resolved SAXS is one of the few techniques that can provide direct information on the rate and mechanism of protein oligomerisation during conformational transformation.

Nanotechnology

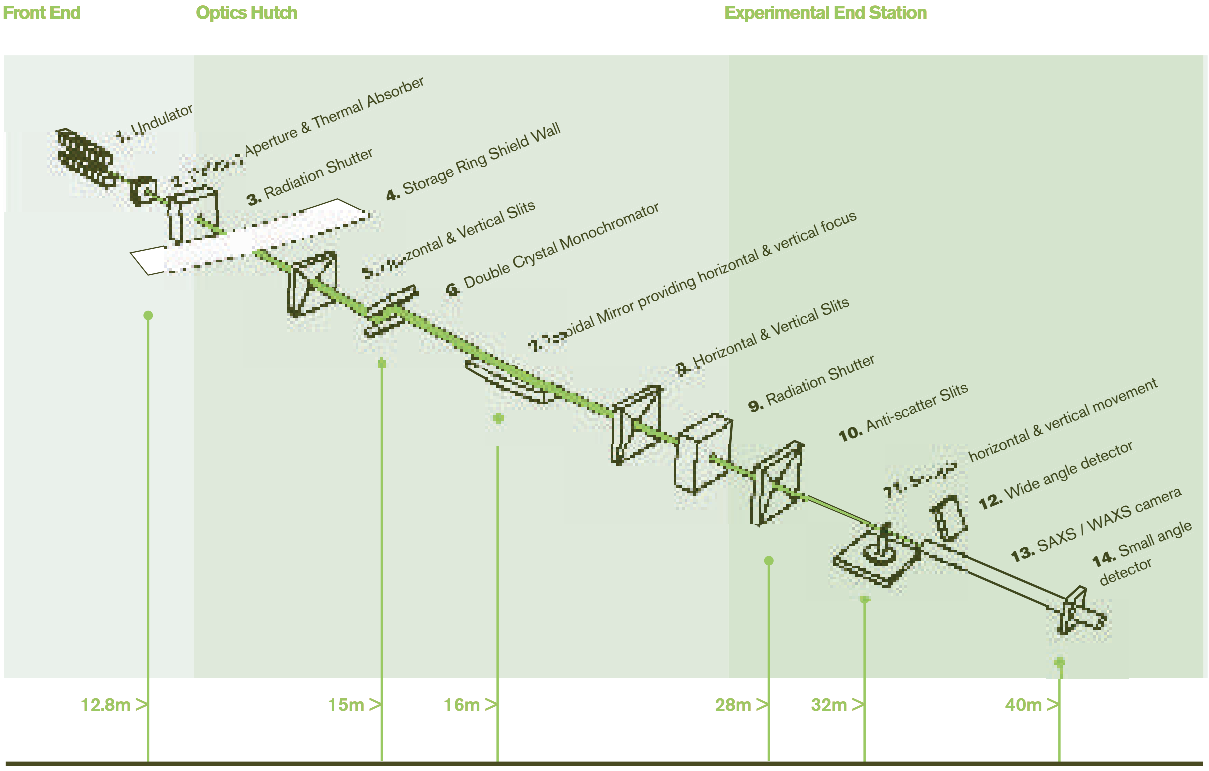
The application of biomolecules to nanotechnology, for example in biomaterials, also relies on an understanding of the basic structures and dynamics of large assemblies, for example the behaviour of liposomes, which is likely to grow in importance for controlled drug delivery. Such systems can be readily studied using SAXS, in a far more direct way than any other method. Self-assembled systems are an important way of manufacturing nanomaterials, for example the clustering of fullerene C60 and higher fullerenes, which has implications in their purification and in building up novel materials. SAXS and WAXS are important techniques for studying the hierarchy of interplay of the components and the formation of complex arrays.

Fibres have a wide range of applications in nanomaterials depending on their degree of entanglement and alignment. For example, the interplay of carbon nanotubes in building up materials with novel function, which again is best studied by SAXS/WAXS techniques.

Micromolecular assemblies and protein folding and unfolding are growth areas in structural biology.

Polymer science and engineering

Polymers are long chain molecules that play an important role in biology, medical applications, new materials, biotechnology, and nanocomposites. The final properties of the polymeric materials are determined by their nanostructure. Australian scientists are at the forefront of many areas of polymer science.



BEAMLINE 4 SAXS / WAXS

Figure BL4.1. *Schematic of the SAXS/WAXS beamline*

An area in which SAXS will contribute greatly is that of polymer blends. Most commercial blend systems contain a polymeric surfactant, or compatibiliser, between the two phases of the blend. These are formed by the in situ reaction of the two components. This affects the chemistry and hence the phase behaviour and crystallisation.

Food science

The melting of gel structures is an important part of the food industry where gels such as amylopectins are used as stabilisers and bulking agents. Recent work has been directed at exploring the mesoscopic structure of starch granules, the impact of biochemical changes in the enzymatic pathways involved in starch deposition in the plant on the internal granule structure and the consequences for breakdown during gelatinisation and other processing treatments.

Other polysaccharide gels need to be further characterised and their melting properties compared to their rheological parameters. In particular, by carrying out x-ray rheology experiments as a function of temperature, it should be possible to quantify the strength and number of the crystalline junction zones as they break down under shear. As rheology is frequently used to characterise food gels, but without the means of unambiguously moving from this information to an understanding of structure, this capability will be invaluable.

Beamline Design

The SAXS/WAXS beamline should make use of the best collimated beam possible with the highest possible flux at the sample position. It will be driven from a 22 mm period in-vacuum undulator.

It will have a useful working energy range of 5.5–20 keV and can be easily tuned.

The beamline will be capable of measuring data at low and high angles simultaneously, and rapidly enough for time-dependent studies. The design will enable incorporation of a USAXS (Bonse-Hart) instrument for ultra small angle x-ray scattering, and allow for the incorporation of additional focussing elements with little or no modification to the underlying optics.

The end station should provide for the ability to change camera length quickly and for rapid flight path evacuation. A hutch large enough to allow in situ measurements of processes, such as extrusion of polymers or food gels, is important.

Beamline 4 – Small and Wide Angle X-ray Scattering	
Source	In-vacuum undulator (22 mm period)
Energy range	5.5–20 keV
Resolution $\Delta E/E$	$< 10^{-4}$
Beam size at sample (horizontal × vertical)	200 × 100 micron (or smaller)
Q range	0.001Å^{-1} – 12.0 Å^{-1} (SAXS); 5 Å^{-1} (WAXS)

Beamline 5: X-ray absorption spectroscopy

05

Potential Research Fields

Life sciences

- Biological research and drug design
- Biotechnology and bio-sensors
- Plants and crops

Physical sciences

- Sustainable environment
- Forensics
- Advanced materials
  - Ceramics
  - Micro-electronic and magnetic materials
  - Biomaterials
- Mineral exploration and beneficiation
- Earth sciences
- Oil and gas production and distribution
- Agricultural technology
- Chemical reactions and catalysts

Advanced manufacturing

- Production of micro-devices

Introduction

X-ray absorption spectroscopy (XAS) is a well-established, quantitative analytical technique used by both academia and industry to obtain atomic-scale structural and chemical state information for a wide range of systems in both liquid and solid form. XAS probes both the short- and medium-range order of a sample and as such is complementary to x-ray diffraction.

An XAS spectrum is typically separated into XAFS (extended x-ray absorption fine structure) and XANES (x-ray absorption near edge structure) regions. Analysis of XAFS yields structural information such as bond length, coordination numbers and disorder. In closer proximity to the absorption edge, analysis of the XANES yields chemical information such as the local coordination geometry and oxidation state of the absorbing atom.

XAS is a sufficiently well established and broadly used technique for it to be commonly offered as a commercial analytical service by both synchrotron facilities and private companies.

Advantages of a Synchrotron Source

An XAS experiment is the measurement of the absorption coefficient of a sample as a function of incident photon energy. In multi-elemental samples, this commonly necessitates the careful examination of multiple absorption edges and thus XAS measurements are not practical on a laboratory-based system.

XAS measurements need an intense, tunable source of photons afforded only by a synchrotron. XAS beamlines are thus available at synchrotrons worldwide and are used by scientists from the biological, biochemical, chemical, earth, environmental, materials and physical sciences and engineering. The maturity of the technique in experimental performance and data analysis is such that non-specialists now comprise a significant fraction of the user base.

Synchrotron facilities with an energy range comparable to the Australian Synchrotron typically have multiple beamlines dedicated to this technique. For example, at the Photon Factory, Japan, XAS measurements comprised 23% of all experiments over all beamlines performed in 2001.

User Community

The Australian XAS user base currently exceeds 70 practitioners with an anticipated increase to 150 when a domestic facility is operational. XAS users comprise the largest fraction of the Australian synchrotron science community and XAS experiments comprise the largest fraction of Australian synchrotron science measurements. At present, Australian access to XAS capabilities is facilitated by the ASRP at the Australian National Beamline Facility (ANBF) at the Photon Factory, Japan. At this single multi-purpose beamline, XAS measurements represented 42% (70.5 days) of all experiments performed in 2001. Flux limitations from the bending-magnet source at the ANBF inhibit XAS experiments on dilute samples. For such measurements, Australian XAS users seek access to alternative synchrotron facilities worldwide. In 2001, this accounted for an additional 50 days of XAS experiments performed by Australian scientists. Total Australian XAS usage in 2001 was ~120 days/year with an estimated demand of ~180 days/year. Demand for XAS measurements in 2001 was thus sufficient to utilise all available time on a dedicated wiggler-based beamline at any synchrotron facility worldwide.

Research Applications

Historically, Australian XAS research has been characterised by both diversity and excellence. The former is demonstrated by the breadth of disciplines represented in the user community, while the latter is apparent from the level of ARC funding accorded synchrotron-based research proposals.

A dedicated XAS beamline at the Australian Synchrotron will further these traits. Research applications are widespread and some examples are discussed below.

Biological sciences

Therapeutic target site identification: metal (Cu, Zn and Fe) binding to amyloid ß-peptide, the latter found in all biological fluids, may be responsible for some of the pathological effects of Alzheimer's Disease. A determination of the metal-binding site yields a potential therapeutic target site. This specific example demonstrates the complementary nature of biological XAS and protein crystallography and the common necessity of using both techniques for a structural solution.

Biochemical sciences

Carcinogens: to characterise the structures of a range of reactive Cr complexes with biological reductants. This research will provide important new insights into metal-based toxicology.

Anti-cancer technologies: investigations of cobalt (Co) and platinum (Pt) anti-cancer drugs with the aim of developing new technologies that enable the determination of the oxidation state in situ in different regions of tumours and in models of hypoxic tumours.

Anti-inflammatory drugs: characterisation of new drugs in the solid state, and in solution, pharmaceutical formulations and biological fluids. This research has been essential in determining the stability of the drugs in pharmaceutical preparations and in understanding the pharmacology.

Chemical sciences

Transition metal complexes: elucidation of the molecular details of the chemistry associated with enzyme catalysis. This research aims to understand the influence of redox or charge state on the electronic and molecular structure of metal complexes or clusters in order to anticipate (and ultimately control) the reactions and reactivity of transition metal catalysts.

Earth sciences

Ore metals: identification of the metal complexes involved in the transport of ore-metals (Cu, Au, Ag) by supercritical hydrothermal solutions to form economically important ore deposits. Interest is focussed on the partitioning of Cu between coexisting brine and vapour phases during boiling, as this process may explain the relationship between different ore types in a common geological setting. An improved understanding of the formation of these major economic deposits may aid in predictive exploration.

Magma oxidation: determination of the oxidation state of elements in magmas (silicate melts). The abundance of elements in the mantle relative to those in meteorites that are thought to have condensed from the primitive solar nebula can be used to help constrain models for the differentiation and evolution of the Earth. Australian scientists have recently used XAS measurements performed at high temperature to show that approximately half the chromium (Cr) in a mid-ocean ridge basalt (the most common rock on the surface of the Earth) at 1400°C is Cr^{2+} even though this oxidation state has never been identified in a terrestrial material.

Environmental sciences

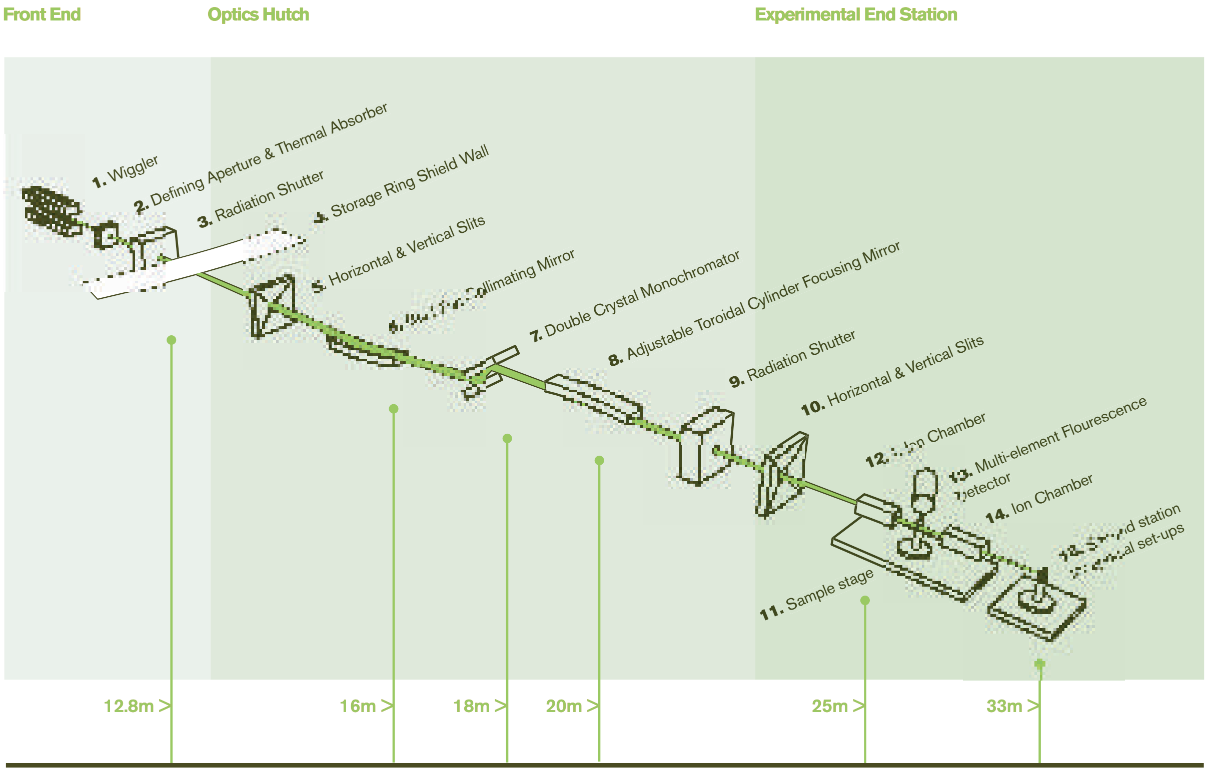
Radionuclides in the marine environment: investigating the solid state redox speciation of metals in particles suspended in marine water. Redox speciation changes of Fe and Mn play an important role in the formation and growth of natural particles and the sorption and release of radionuclides and trace elements in the marine environment. Using XANES to define the extent and dynamics of these redox changes is important to elucidate basic mechanisms and establish sorption and transport models.

Materials sciences

Semiconductor device fabrication: characterisation of ion-implantation-induced disorder in semiconductor substrates with application to both electronic and photonic device fabrication. The ion implantation process is one of several basic building blocks used in the production of all modern semiconductor devices and the form and extent of residual ion-implantation-induced disorder ultimately governs device performance. These studies are of a fundamental nature with both scientific importance and technological relevance.

New science

Nanoscience: XAS is an ideal technique to yield insight into the novel properties exhibited by materials at the nanometre scale. XAS studies have been initiated by Australian scientists to study both semiconducting and metallic nanoparticles in a variety of matrices for application to photonic devices and chemical catalysis, respectively.



BEAMLINE 5 X-ray Absorption Spectroscopy

Figure BL5.1. *Schematic of the x-ray absorption spectroscopy beamline*

Ultra-dilute measurements: New developments in photon production and detection incorporated in the XAS beamline will make measurements at the ultra-dilute level possible. This will enable pioneering experiments in a variety of fields including biochemistry and engineering.

Fast-scanning/time-resolved measurements: fast-scanning XAS will be used to develop methodologies for determining the structures of intermediates in enzymatic processes using standard stopped-flow and other mixing technologies. This will provide new insights into biochemically important pathways that were not assessable previously.

Electron-beam ion trap: a new and novel device that can be coupled to the XAS beamline and enable a new generation of fundamental experiments to reduce uncertainties on tests of quantum electrodynamics in the x-ray regime by an order of magnitude. Though a similar proposal is under consideration at an American facility, this represents another opportunity for Australian scientists to be world leaders.

Beamline Design

Because of the current usage and demand, a dedicated wiggler-based XAS beamline is proposed for the Australian Synchrotron. The combination of wiggler, collimating mirror, double-crystal monochromator and focussing mirror is recommended by the Australian XAS community and international experts.

It will be a user-friendly beamline appropriate for both novices and seasoned practitioners.

Table BL5.1 Beamline operating modes

Energy	Operating Mode
<~10 keV	The wiggler will operate at K = 10 and will yield excellent harmonic rejection to < 5 keV.
>10 to ~20 keV	The combination of the wiggler spectrum for K = 20 will provide good intensity in the 10–20 keV range and very good harmonic rejection at 30–60 keV.
>20 to ~35 keV	The wiggler will operate at K = 20 or higher, depending on the photon energy required. A higher index set of monochromator crystals will be utilised.
>35 keV	Higher photon energies will exceed the critical energies of the mirrors so the beamline must be able to operate with both mirrors withdrawn.

Notes: The combination of mirrors, mirror coatings and a variable-field wiggler enables the precise optimisation of the beamline for a given experiment. Four modes of operation are envisioned. K is the undulator factor and defines the opening angle of the of insertion device.

Sample size and type will be varied and include both solid and liquid samples. Measurement capability at temperatures from ~10–1273 K (e.g. a cryostat and furnace) will be necessary.

Detectors including ion chambers, Stern-Heald-Lytle detectors and a multi-element solid-state detector are necessary. Recent innovative designs including log spiral and pixel array detectors also warrant consideration.

Two hutches in tandem – the first to house the standard XAS measurement station and a second to accommodate experiments that necessitate prolonged set-up time (for example, an ultra-high vacuum deposition chamber) are required.

A wiggler source is necessary to achieve the desired combination of energy and flux. The flux from a 2 T, 16 cm period advanced variable-field, multi-pole wiggler not only satisfies the needs of the Australian XAS community but provides the flexibility to optimise the beamline for specific experimental requirements of energy range, energy resolution, flux and harmonic content.

Improved energy resolution will be achieved with a collimating mirror (a bent flat).

A fixed-exit-height, double-crystal monochromator able to withstand the full power output of the wiggler is required. The first crystal will therefore have in excess of 2 kW of power impinging upon it. The capability of exchanging crystals must be rapid and multiple crystal sets will be needed to cover the energy range of the beamline.

Beamline 5 – X-ray Absorption Spectroscopy	
Source	Wiggler (3 T)
Energy range	4–30 keV, with option for up to 65 keV
Resolution $\Delta E/E$	$<10^{-4}$
Beam size at sample (horizontal × vertical)	~0.2 × 1 mm
Photon flux	$>10^{12}$ photons/sec at sample

06

Beamline 6: Soft x-ray spectroscopy

Potential Research Fields

Life sciences

- Biotechnology and bio-sensors

Physical sciences

- Forensics
- Advanced materials
  - Functional polymers
  - Ceramics
  - Nanomaterials and composites
  - Metals and alloys
  - Micro-electronic and magnetic materials
  - Biomaterials
- Mineral exploration and beneficiation
- Earth sciences
- Agricultural technology
- Chemical reactions and catalysts

Advanced manufacturing

- Production of micro-devices

Introduction

Soft x-rays are generally understood to be x-rays in the energy range 100–3,000 eV. They have insufficient energy to penetrate the beryllium window of a hard x-ray beamline but have energies higher than that of extreme ultraviolet light. Soft x-rays cover an energy range of importance for spectroscopic studies of many elements in the periodic table. They are well suited to characterising surfaces and near-surface interfacial layers.

The soft x-ray beamline will be set up primarily for XAS of low atomic number elements and x-ray photoelectron spectroscopy (XPS), although there are other significant research applications such as photo-desorption and threshold x-ray excited Auger electron spectroscopy (XAES).

There will be two end stations to enable experimental flexibility, with the second end station capable of XPS and XAS mapping of samples in special atmospheres at pressures of up to 20 torr.

User Community

Australian and New Zealand researchers carry out their synchrotron soft x-ray spectroscopy wherever they can obtain beam time, including Taiwan, Korea, Japan, Germany, USA, Sweden and France. Much of the research is carried out as part of an individual collaboration, and not necessarily funded through the ASRP or even the Access to Major Research Facilities Program. Thus, to some extent, current demand is not fully visible nor fully satisfied.

All soft x-ray beamlines are currently oversubscribed, and very few end-stations available to Australian researchers meet their requirements. Australians are carrying out some cutting edge work, but at present, progress is limited by insufficient access to suitable beamlines.

If only the main user groups currently seeking access to beam time at synchrotrons are considered, it is estimated that the proposed soft x-ray beamline equipped with the ASRP end-station that is currently under construction for initial installation for use on the Taiwan synchrotron would be fully utilised from the outset. The current user base primarily consists of approximately 15 user groups. The limited size of this user base largely reflects the absence of soft x-ray spectroscopic facilities. It is estimated that with better access the potential user base would consist of 30 groups from 18 universities, several CSIRO Divisions and ANSTO, with industry working in association with some of these groups.

Research Applications

Synchrotron soft x-ray spectroscopy provides distinctive information for numerous research areas ranging from fundamental studies in solid state physics and nanotechnology to applied chemical problems in catalysis and coal combustion.

Earth and environmental sciences

Synchrotron soft x-ray techniques are already opening up new ways to address the complex problems arising from earth resource utilisation, and this contribution is expected to increase in areas such as environmentally sustainable ore extraction, mineral processing, coal combustion and soil use.

The surface chemistry of metal sulfides is of major importance in the separation of the valuable and unwanted components in base metal ores, in the hydrometallurgical processing of a concentrate to produce the corresponding metal from the sulfide, and in the leaching of rejected material in waste heaps. Since the application of synchrotron XPS to mineral fracture surfaces, the importance of surface chemical states arising from relaxation of the outermost layer following fracture has become evident.

The enhanced surface sensitivity provided by synchrotron XPS, as well as the ability of angle-dependent x-ray absorption near edge structure (XANES) to reveal orientation, have also assisted elucidation of the mechanism by which flotation reagents interact with the surface of minerals.

Determination of the chemical forms of heteroatoms, such as nitrogen, in a large molecular weight or complex material such as coal is a case where soft x-ray absorption spectroscopy is used to complement conventional XPS for low atomic number non-surface chemical characterisation. This information is sought in research to minimise the generation of undesirable species such as NOx in coal combustion.

The ambient mapping facility on the second end station will enable measurements to be made at pressures of up to 20 torr with high spatial resolution. It will provide maps of surfaces when exposed to a variety of atmospheres including water, oxygen, helium and nitrogen. Thus, for instance, it will be possible to follow mineral oxidation, hydrolysis or collector adsorption in real time.

Physical and material sciences

A niche area in which Australia has been successful to date is the development of thin film materials for electronic and optoelectronic devices. Thin films of materials with particular chemical and/or physical properties such as piezoelectricity are typically deposited onto an appropriate substrate by one form of chemical vapour deposition, and during the development phase for both precursor and deposition conditions, the physical and chemical properties of the film must be determined. Variable-angle XAS from a synchrotron source can augment initial conventional XPS analysis to reveal the orientation of film crystallites.

Chemical and biochemical sciences

In many chemical, biochemical and earth science-related systems it is essential to obtain information about a species while it is in contact with an aqueous or other liquid environment and while it is at a particular electrochemical potential. A wet cell for non-microscopic XAS will be of considerable interest to researchers in a number of fields. In particular, with silicon nitride cell windows, the carbon K-edge near 0.3 keV can be studied, and the region between the carbon K-edges and the oxygen K-edge near 530 eV is often referred to as the ‘water window’. It is expected that it would be possible to investigate solid electrode surfaces and even particulate slurries, with the electrochemical potential established by redox reagents in the liquid flowing through the cell.

For materials that can be investigated under ultra high vacuum, XAS is able to provide chemical information that is difficult to obtain by non-synchrotron techniques such as conventional XPS.

For biological samples that need to be kept in damp conditions, or where it is desired to study the action of catalysts in special environments, the ambient mapping facility will be used.

Beamline Design

Energy range

In order to achieve an x-ray beam of adequate stability and energy resolution, it is considered that the energy range sought should be restricted to 100–2500 eV.

The insertion device will be a variable polarisation undulator, capable of supplying linear vertical, linear horizontal, left and right circularly polarised light. The device will work in the 1st, 3rd and 5th harmonics. Limited tapering of the undulator is desirable for producing a broader range of energies in the harmonic peak, but is not essential. It is expected that it will be an ‘Apple’ type, as fast switching of polarisation is not needed. The device may have either a single period or consist of two modules of different periods to cover the entire energy range required. A design study of the insertion device will provide quantitative data for deciding the preferred specification.

Such an insertion device will meet the needs of the x-ray absorption community by allowing the measurement of linear and circular dichroism without the necessity to rotate the sample.

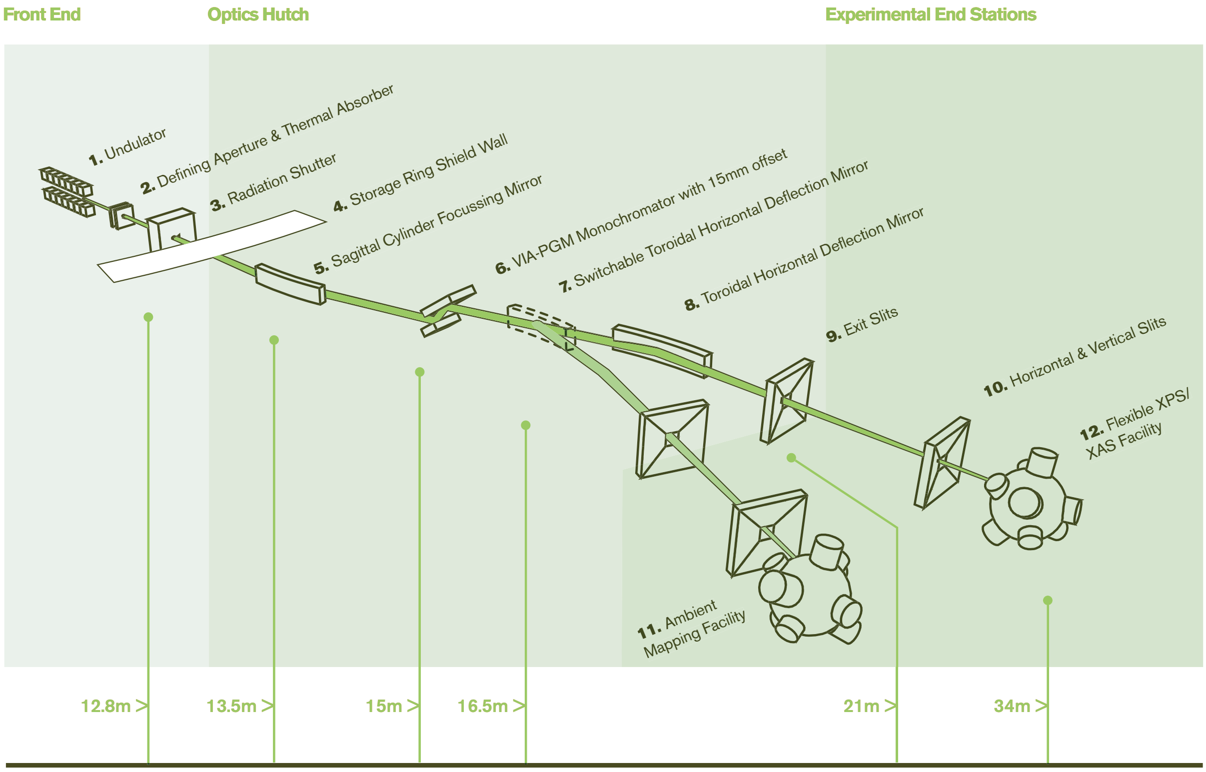
Elliptically polarising undulators are currently the most advanced general-purpose insertion devices. The provision of circularly polarised light ensures that the beamline will be sufficiently flexible to cater for future developments in the scientific areas of interest to the Australian user community.

The resolving power will be 20,000, which is relatively easy to achieve with modern monochromators. In addition there will be provision for lower dispersion gratings with reduced resolution but correspondingly higher flux for experiments that require maximum flux at moderate resolution.

Special features

A soft x-ray beamline and end-station must be maintained under a clean, ultra high vacuum (UHV).

There must be vacuum continuity between the analysis chamber and the synchrotron ring. Therefore, the vacuum in the beamline and end-station must be comparable with that in the ring, in terms of both pressure and quality. It is important that the UHV in both the beamline and end-station be as carbon-free as possible, not only to maintain the reflectivity of the optical components at higher photon energies, but also to facilitate XAS at the carbon K-edge.



BEAMLINE 6 Soft X-ray

Figure BL6.1. *Schematic of the soft x-ray spectroscopy beamline*

The necessity to work under clean UHV conditions means that synchrotron soft x-ray spectroscopy is more demanding and time-consuming than hard x-ray spectroscopy. As a consequence, typical beam access periods are longer, and fewer users can be accommodated. The strategy proposed to address this problem is to have two end-stations, in a branched rather than in-line configuration, sharing one monochromator. The two end-stations proposed are the ASRP soft x-ray spectroscopy end-station, and the other an XPS/XAS end-station optimised for industrial (especially minerals) research. A mirror could switch the radiation between the two end-stations, so that measurements could be made in one end-station while specimen preparation or vacuum recovery was taking place in the other.

In addition, allowance will be made for the ability to connect specialist end-stations in the future.

The soft x-ray spectroscopy end stations

The ASRP soft x-ray spectroscopy end-station is currently being built in Germany at a cost of ~$A1m, and is scheduled to be completed by August 2004. It will be used at the NSRRC in Taiwan until the Australian Synchrotron is operational, when it will be transferred to Australia. Thus, a fully commissioned end-station would be available, at minimal cost in addition to the beamline itself, as soon as beamline 6 becomes operational. This end-station has been designed, and is being constructed, to meet the stringent clean vacuum requirements noted above. In particular, the vacuum system will be as carbon-free as possible, and the end-station will allow the investigation of specimens that must be maintained at a low temperature while they are under vacuum, in order to retain moderately volatile material that might otherwise sublime or desorb.

The ASRP end-station has also been designed to accommodate a cell for the XAS of systems that need to be investigated in their wet environment. A conceptual design for this cell has been developed.

The second soft x-ray spectroscopy end-station will be a modified version of an ambient XPS facility at the Advanced Light Source (Berkeley, USA). The design is a result of collaboration by a consortium consisting principally of the University of South Australia, the Victorian and South Australian Governments, the University of Western Ontario, the Canadian Light Source and researchers at the Advanced Light Source.

Beamline 6 – Soft X-ray Spectroscopy	
Source	Undulator (75 mm period), variably polarising
Energy range	0.1–2.5 keV
Resolution $\Delta E/E$	10^{-5}
Special features	Ultra high vacuum

07

Beamline 7: Vacuum ultraviolet spectroscopy

Potential Research Fields

Life sciences

- Biological research and drug design
- Plants and crops

Physical sciences

- Advanced materials
    - Nanomaterials and composites
    - Metals and alloys
    - Micro-electronic and magnetic materials
    - Biomaterials
- Chemical reactions and catalysts

Introduction

A high resolution beamline for a range of vacuum ultraviolet (VUV) spectroscopic studies of solids, atoms and molecules – covering photon energies from 10 eV to 350 eV – holds particular promise as a generator of significant new fundamental science, and strategic work of future technological importance. A particular strength of the proposed beamline is the potential to bring several powerful surface science techniques to bear on a particular problem under the same conditions.

Advantages of a Synchrotron Source

A synchrotron radiation source is essential for the proposed VUV experimental techniques because they use all the features of synchrotron light, namely the tunability, the circular and linear polarisation, the coherence and the single- and multi-bunch timing modes. These combined features enable the coincidence detection of physical and chemical reaction particles and their time development. The proposed studies are not possible without a synchrotron.

User Community

The number of users with existing synchrotron experience in the VUV area in Australia is significant (at least eight groups) but not large in comparison with other synchrotron techniques. Access to VUV beamlines has not been available through the ASRP to this time. The groups are, however, distinguished by their extensive experience and an advanced capability in terms of both synchrotron and end-station instrumentation.

Due to the ultra high vacuum nature of VUV beamlines, and the essential requirement to prepare atomically clean single crystal samples in situ, a typical beamline visit is of 2–3 weeks duration for solid state experiments. For gas phase experimentation, custom built end stations are commonly required with possible consequences in terms of time lost changing instrumentation. Experiments involving coincidence techniques are particularly time intensive.

Using Germany's BESSY facility as a model, eight user groups can be offered two 2-week periods per year. On this model, an Australian VUV beamline would already be over subscribed.

Research Applications

Existing synchrotron facilities dedicated to the VUV region include comparable beamlines in operation at BESSY (Berlin), Elettra (Trieste) and ALS (Berkeley). A wide range of spectroscopic and microscopic techniques is in evidence at these facilities, with several of them having unique Australian components that have made them world leaders. These features, and new developments, will be established in the VUV beamline of the Australian Synchrotron.

Angle resolved photoemission spectroscopy

Angle resolved photoemission spectroscopy is the pre-eminent technique for the elucidation of the electronic structure of crystalline solids.

Solid state studies

Although the photoemission technique has many applications at higher energies, it is in the VUV region of the spectrum that angle resolved data is essential for providing a sufficiently detailed view of the electronic band structure of crystalline solids.

By 2007, state of the art instrumentation will require energy resolution of a few meV coupled with angular resolution significantly better than 1 degree. Instrumentation will be required to resolve fine structure in many materials of technological value and to investigate electronic structure beyond the one-electron approximation.

The availability at synchrotron sources of circularly polarised radiation that can be rapidly switched between both helicities enables a suite of magnetic circular dichroism experiments to be undertaken. These can reveal spin-orbit interactions in the conduction band to derive the electronic structure of magnetic materials.

Applications include understanding the properties of shape memory alloys, of colossal-magneto-resistance alloys and of strongly correlated materials such as the cobaltates and high temperature superconductors.

Photoemission from the valence band is very attractive for studying chemisorption on semiconductor surfaces.

The study of low binding energy core lines of vacuum fractured, conducting (or small band gap) mineral single crystals, in conjunction with detailed valence band studies can illuminate interrelationships between crystal and electronic structure, bulk vs surface states and, in the end, the reactivity of such materials.

Novel inner shell Auger photoemission coincidence spectroscopy (APECS) has a unique ability to disentangle signals originating from different sites within a solid and/or from overlapping spectral features, such as surface alloys in metallic systems that intermix only in the first layer and then can influence the underlying electronic structure. APECS shows an enhanced surface sensitivity compared to non-coincidence photoemission.

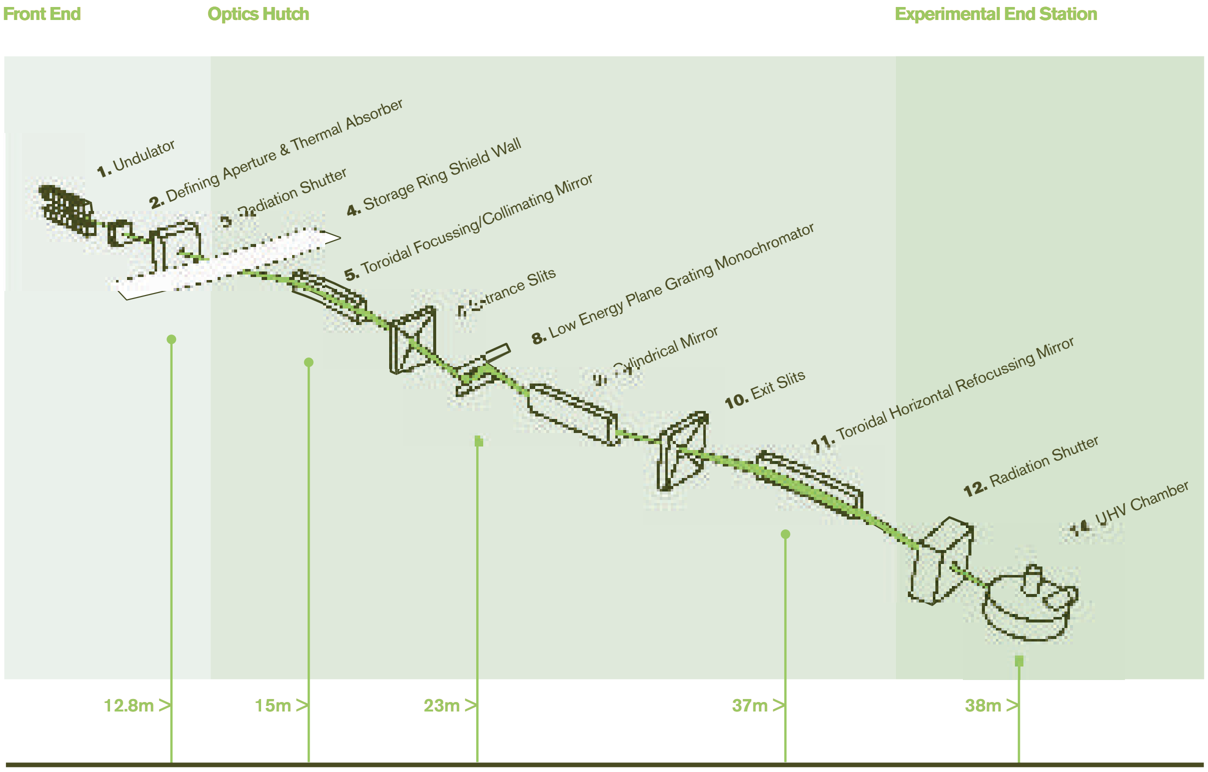
Gas phase studies

Angle resolved photoemission measurements have traditionally been used to validate molecular orbital calculations of both stable and transient molecules. Synchrotron VUV gas phase studies allow investigation of electron correlations in bound and continuum states, electron exchange and spin-orbit effects, interference and coherence, orbital and magnetic dichroism effects and relativistic effects.

New techniques, such as angle-resolved photo-electron-photo-ion coincidence spectroscopy now make possible, for the first time, the study of electron-ion momentum vector correlations and reveal intermolecular scattering and associated interference. Exploration of the dynamics of the photo-excitation of free molecules and the high resolution VUV spectroscopy of atmospheric molecules are examples of topics of strong current interest.

Double photo-ionisation, studied using coincidence angular distribution techniques, may be used to investigate the important question of coherence in atomic physics.

A recently developed technique with great promise involves the investigation of the intrinsic width of selected atomic states via fluorescent, rather than photo-ion emission. This technique also has particular merit for the optimisation and the determination of the resolution of VUV beamlines.



BEAMLINE 7 Vacuum UV Spectroscopy

Figure BL7.1. *Schematic of the VUV beamline*

Pulsed multi-bunched operating modes of the synchrotron enable an extensive list of time-of-flight spectroscopies, including rotational-vibrational, fragmentation modes and lifetimes of molecules as well as inner-shell effects.

Adsorbate studies

Synchrotron-based angle resolved VUV photoemission will enable studies on the identity and bonding of the successive surface-intermediates in various chemical vapour deposition (CVD) processes; the bonding of amino acids with metal surfaces; and the characterisation of carbon nanotubes, gallium nitride nanowires and silicon quantum-wire arrays.

Biosystems

Surface science has recently been increasing in prominence in the biomedical area, based on the fact that many biological reactions occur at surfaces. Thus any fundamental understanding of the biocompatibility of a medical device must take into account the properties of proteins and cells at interfaces, and the characteristics of local biological reactions. Principles worked out in surface science laboratories are likely to become the basis for ways of improving the function and durability of materials featured in a wide range of medical products.

The electronic properties and interactions of matter at an atomic level in biological environments are largely unknown. Yet the detailed understanding of these systems is crucial to the successful development of many new technologies that have direct impact in our community. Applications include medical implants, delivery systems (for example of radiopharmaceuticals), bio-sensors and chips for diagnostics, biomimetic materials (such as the construction of artificial skin or organs), and novel artificial photosynthetic devices.

VUV light is able to probe the valence and low-lying core states of many elements in the periodic table. The interaction of such states ultimately controls the complex interactions and properties observed in biological systems. The high flux and small spot size produced by the VUV beamline will allow for many ground-breaking experiments and studies to be performed on biosystems from a sub-Angstrom to micron scale.

As most biosystems are made of several functioning parts, small spot microscopy on objects as tiny as only a few nanometres to as large as several microns in size would be of tremendous importance in order to determine accurately the electronic state of each part.

Studies will initially focus on more traditional (but still as yet not understood) systems such as the electronic properties and structure of amino acids (essential building blocks) on various surfaces. Techniques such as high-energy resolution valence band and core level mapping as well as ‘photon-in/photon-out’ and ‘photon-in/electron-out’ scattering techniques will be used. One significant new direction would be the study of liquid–solid interfaces and multi-layered systems.

Beamline Design

The beamline would be matched to a long-period variable-polarisation elliptical undulator as source.
A design study is currently being prepared by staff at the BESSY synchrotron facility in Berlin. It is expected that this undulator will deliver both linearly polarised and circularly polarised radiation and that the plane of linear polarisation can be rotated through 90 degrees from horizontal to vertical. Such capabilities are considered particularly important as they open up many possibilities relating to magnetic effects in solids and chirality effects in the gas phase.

The optical components of the proposed plane grating monochromator (PGM) beamline operate in glancing incidence reflection mode. All sections of the beamline must be maintained under UHV conditions ($<10^{-10}$ torr), in common with the end stations. A full description of the optical design is available[1], but for present purposes it is sufficient to point out that the final mirror causes the beam to be focussed to a spot of approximately 220 microns (horizontal) by 10 microns (vertical) at a position 1 metre behind the final mirror. The photon resolving power will be greater than 10,000.

Beamline 7 – Vacuum Ultraviolet (VUV)	
Source	Undulator (185 mm period), variably polarised
Energy range	10–350 eV
Resolution $\Delta E/E$	10^{-4}
Beam size at sample (horizontal × vertical)	220 × 10 micron
Special features	Ultra high vacuum (pressure $<10^{-10}$ torr)

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[1] R. Follath. A collimated PGM for the U125 operating at 3 GeV. Bessy report. Berlin 2003.

08

Beamline 8: Infrared spectroscopy

Potential Research Fields

Life sciences

- Biological research and drug design
- Biotechnology and bio-sensors
- Biomedical and medical imaging

Physical sciences

- Sustainable environment
- Forensics
- Advanced materials
  - Functional polymers
  - Ceramics
  - Nanomaterials and composites
  - Micro-electronic and magnetic materials
  - Biomaterials
- Mineral exploration and beneficiation
- Earth sciences
- Oil and gas production and distribution
- Food technology
- Chemical reactions and catalysts

Introduction

This beamline will cover the infrared spectrum. The absorption of near infrared light by samples provides information about the chemistry and structure of materials in a non-contacting, non-destructive manner by probing the molecular vibrations.

Developments in Fourier Transform (FT) techniques in the latter part of the twentieth century led to the introduction of infrared microscopy and very high resolution instruments.

Infrared vibrational spectroscopy is very widely used in Australia. Every reputable research or analytical laboratory (chemistry, physics, materials, biochemistry and microbiology) would possess an infrared system. Many industrial production facilities use the techniques for quality control.

Advantages of a Synchrotron Source

Laboratory based instruments are driven by black body sources such as globar. Synchrotron light, which is highly collimated, polarised, tunable and much more intense (at least 100 times more intense), will vastly increase the potential of the techniques, especially in microspectroscopy, in the far infrared and at high resolution. Time-dependent studies of fast reactions will be possible, higher spatial resolution of three-dimensional images can be obtained, and it will be possible to image biological cells chemically without using fluorescent tagging.

The high intensity will enable very fast throughput of large numbers of mineralogical samples.

Australian User Community

Infrared spectroscopy is a relatively new technique for a synchrotron – the first line was built at the National Synchrotron Light Source, Brookhaven, USA, in 1994. Demand from US researchers has been heavy, and access to the beamlines for non-US researchers has been minimal, so there has been very limited opportunity for Australian researchers to gain experience in this field to date.

Initial biospectroscopic studies using infrared by Australian scientists were carried out at SRS (Daresbury, UK). Access has recently become available for Australian researchers to the SRRC (Taiwan) through the Australian Synchrotron Research Program, and this will stimulate the growth of the user community.

A Synchrotron Radiation Infrared (SRIR) Users Group has been formed in Australia. The range of interests represented by members of the SRIR Users Group is very wide. The current membership comprises 15% industry, 25% Australian Government institutions, and 60% universities and academic research institutions. A relatively large proportion of the academic research is also industry related.

Interest has also been expressed by a number of researchers from New Zealand and the size of the SRIR User Group is expected to grow. Based on the ASRP and overseas experience, it is anticipated that the user base could be more than 200 by 2007. This beamline is thus the start of what should be an extended program.

Research Applications

When combined with other synchrotron techniques, particularly diffraction, vibrational spectroscopy is highly effective for characterising the structure, composition and state of samples – from minerals through to biological tissue.

In Australia infrared spectroscopy and microspectroscopy are used in:

- geology and mineralogy – detection of mineral species without complicated specimen preparation, separation of real from artificial diamonds, studies of inclusions in gemstones
- environmental science – identification of the contents of aerosol and steam-flow filters, studies of combustion processes, atmospheric monitoring, exhaust gas monitoring
- biology – monitoring the uptake of drugs into cellular structures, in particular anti-cancer drugs; identification of tumours; following in real time the conformational changes of proteins (this complements protein crystallography studies)
- medicine – monitoring and researching biopolymers and implants
- beer and wine production – understanding the subtleties of yeast and fermentation
- materials science – in situ studies of corrosion at surfaces, development of materials to protect metal surfaces, studies of aging mechanisms in high performance polymers and fibres
- national security – identification of drugs (recreational and narcotic) from police raids and/or customs
- forensic science – study of fibres, dyes, paints, pigments and gunshot residue; measuring the rate of aging of fibres to establish the time of a crime
- museums and the National Trust – in situ studies of antiques (e.g. paintings, manuscripts, textiles and statues), studies of inks to understand how best to store manuscripts or identify fakes, measuring the degradation of film and photo negatives
- semiconductor physics – band-gap studies of new classes of semiconductor materials and large scale deficiencies in the manufacturing process
- engineering – study of the build-up of deposits on pistons in engines.

Beamline Design

A very wide range of techniques and applications can be met with the Infrared Spectroscopy Beamline, which will provide users with access to:

- infrared (IR) microscopy to the diffraction limit
- confocal IR imaging of biological samples, composite materials and surfaces
- high resolution gas-phase spectroscopy.

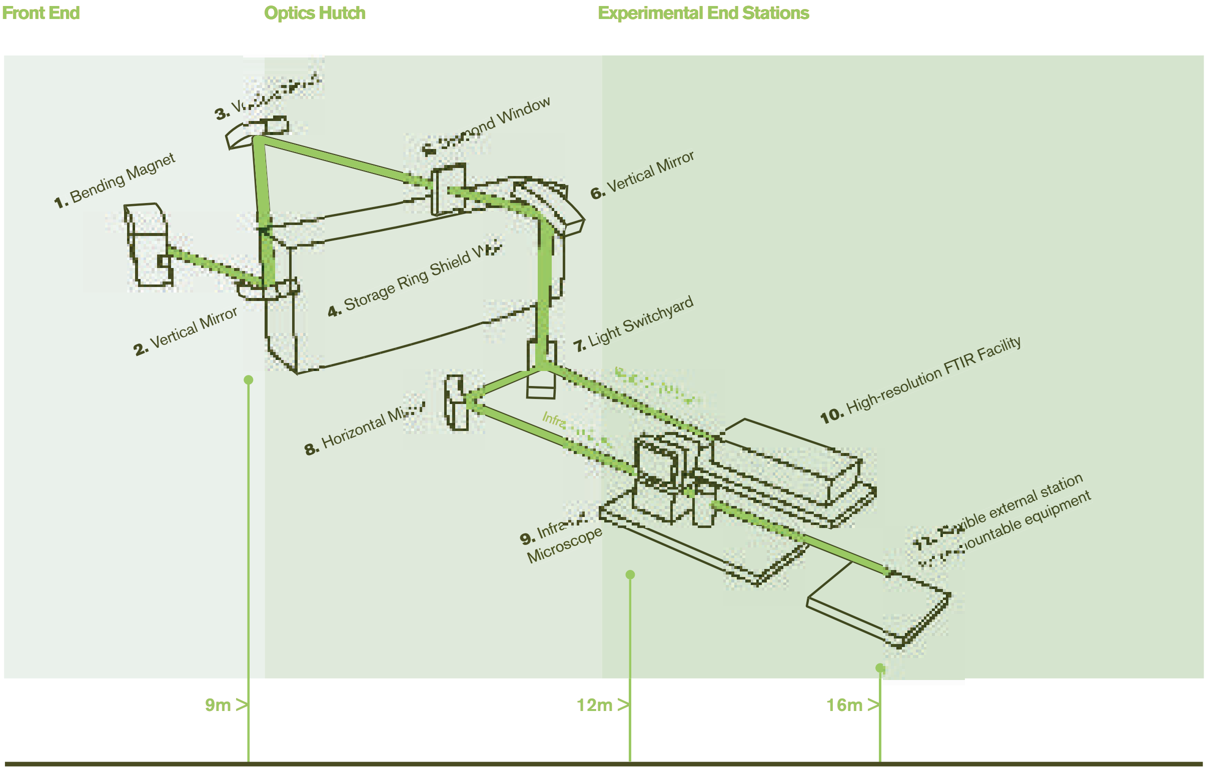

Figure BL8.1. *Schematic of the infrared spectroscopy beamline*

At least two beamlines will be required to satisfy eventual user demand. The first beamline will be designed for mid IR microscopy and high resolution spectroscopy. The second line, to be built later and not included in the initial suite of beamlines, should be for further IR microscopy and also specialised for terahertz (THz) technology. Because it is anticipated that the use of synchrotron-based infrared spectroscopy will grow dramatically, a third window will be reserved for later.

The first beamline will be designed to accommodate conventional commercially available FT spectrometers based on Michelson-Morley interferometers, to scan the spectrum of absorbed radiation from samples under test.

The photon source for the beamline will be from a bending magnet and cover the energy range from 0.001 to 1 eV, 2–10,000 cm^{-1}. The flux will be the maximum possible. This involves collecting as large an angular beam spread as possible from the dipoles – apertures of 70 × 17 mrad^2 are envisaged.

The exit window will be diamond, and the first mirror will be water-cooled silicon carbide. This mirror will be as close as possible to the exit aperture of the storage ring and within the radiation shielding walls. It should reflect the light upwards, to be reflected again along an evacuated beamline. It will have a facility for beam splitting and will feed two large dust-free end stations.

The hutches will be set up to give maximum flexibility in the types of experiments that can be undertaken. Provision will be made for spectrometers to be moved to the beam ports as required, and it will be possible for researchers to bring in specialised equipment.

It is envisaged that the second beamline will make use of electron beam binding techniques in the ring to maximise THz radiation.

Beamline 8 – Infrared Spectroscopy	
Source	Bending magnet
Energy range	0.001–1 eV (2–10,000 cm^{-1})

Beamline 9: Microspectroscopy

09

Potential Research Fields

Life sciences

- Biological research and drug design
- Biotechnology and bio-sensors
- Biomedical and medical imaging

Physical sciences

- Sustainable environment
- Forensics
- Advanced materials
  - Ceramics
  - Nanomaterials and composites
  - Metals and alloys
- Mineral exploration and beneficiation
- Earth sciences
- Oil and gas production and distribution
- Chemical reactions and catalysts

Introduction

This beamline will incorporate the most advanced technologies for focussing the x-ray beam, and will be able to achieve a minimum beam size on a sample approaching 0.1 microns for medium to hard x-rays.

It will be a world class instrument of elemental composition and chemical oxidation states using the two-dimensional mapping μ-XRF, μ-XANES and μ-XAFS providing techniques. It will be the only beamline in Phase I to solve scientific problems requiring micron to sub micron resolution. The spatial resolution is not limited to micron and sub-micron spot sizes and the beamline will be a powerful source for samples of up to 1 mm at sub-micron resolution. This beamline will be of particular importance for the emerging area of nanoscience.

Advantages of a Synchrotron Source

Microprobes using electrons, protons, heavy ions and laboratory based x-rays are in wide spread use. Each of these provides unique and complementary information.

Synchrotron microprobes extend the capabilities of these microfocus techniques with synchrotron light having several distinct advantages, including:

- high brightness, leading to very high photon fluxes on the samples, thereby enabling time-dependent processes and reactions to be followed in real time
- ability to focus the light to very small spot sizes while retaining high brightness that enables high spatial resolution and thus ‘imaging’ of elemental distribution and structure on a sub-micron scale
- tunable beam excitation energy, which means that individual elements in the sample can be selected for analysis and imaging with total discrimination possible against more energetic K or L x-rays. In the case of this beamline the energy range covers the absorption edges of elements from Ti upwards. This is particularly appropriate for the detection of trace elements in samples, and when coupled with the high brightness of the beam it is possible to analyse down to parts per billion level.

User Community

Australian science has been prominent in the use of all microprobe techniques. A pioneering experiment in 1965 used a microfocus proton beam from a van de Graaff accelerator at AINSE to study oxygen concentrations in small spots on the surface of αTi-O alloys[1]. This established the concept of proton microprobe research, which is now a versatile analytical tool with dozens of facilities throughout the world and a dedicated international conference on its applications. The interest in proton microprobe research continued to develop in Australia. Over the last twenty years or so, researchers at Melbourne University have been recognised internationally as leaders in the development and application of proton microprobes[2]. In fact they have marketed their technology internationally, selling focussing quadrupoles and microprobe systems for analysis worldwide. Similar facilities at CSIRO have focussed on solving issues related to mining and exploration industries and has a world class reputation in this area[3].

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1 J. R. Bird, T. M. Sabine, Nature 211 (1966) 739.

2 G.J.F. Legge, P.M. O'Brien. R.M. Sealock, G.L. Allan, G. Bench, G. Moloney, D.N. Jamieson and A.P. Mazzolini, Nucl. Instr and Meth. B30 (1988) 252–259

3 C.G. Ryan, D.J. Jamieson, W.L. Griffin, G. Cripps, R. Szymanski, Nucl. Instr. and Meth, B181 (2001) 12–19

Ion microprobe technology has also been extended to heavy ion beams. One of only three dedicated heavy ion microprobes in the world is located on the tandem accelerator ANTARES at ANSTO[4] in Sydney.

This strong interest and expertise in microprobe analysis has been carried over to microfocus spectroscopy on synchrotron facilities.

The ASRP has joined the APS in Chicago where one of the sectors includes a dedicated high-performance microprobe beamline. Thus Australian scientists have been able to combine high performance micro-x-ray techniques on international synchrotrons with nuclear reaction analysis and heavy ion elastic recoil spectroscopy on national facilities to become world leaders in microprobe applications. However, access to the microprobe facilities at the APS is currently limited to about three days per month and thus demand has outstripped supply, and is increasing rapidly due to the growing importance of micron and sub-micron technologies within Australian research priorities.

There are currently 64 known potential Australian users for the micro/nanofocus beamline on the Australian Synchrotron, representing nineteen universities and research organisations (including three from industry and two government agencies). Organisations with the largest number of identified potential users are ANSTO, CSIRO and the Universities of Sydney and Melbourne. Therefore to satisfy this growing demand, a world class facility is required. There has been widespread discussion in this research community and there is consensus that the proposed beamline will satisfy all their research interests.

Research Applications

Sub-micron technology

Beamline 9 will be an important part of the 'toolkit' required for leading edge research in the emerging field of micron and sub-micron technology. It will be particularly powerful for spectrographic analysis of individual particles and microcrystals of sub-micron size, and will be complemented by the small molecule and powder diffraction beamlines (beamlines 2 and 3) to provide comprehensive characterisation of composition and structure.

Biotechnology

In biotechnology synchrotron microprobes can be used for simultaneous elemental and chemical mapping of tissues, cells and other biological samples providing:

- a better understanding of diseases and immune processes, as well as toxin and heavy metal uptake down to a sub-micron cellular level
- a better understanding of the functionality of a large number of metallo-proteins through the study of the spatial distribution and chemical properties of such species in cells and tissues
- mapping of the distribution and biotransformations of anti-cancer and other drugs in cultured cells and tissues in order to gain a better understanding of drug pharmacology and pharmacokinetics for improved drug design and delivery
- two-dimensional scanning of chromatography gels in which all of the proteins of an organism or an organ are separated. This would enable all of the metallo-enzymes to be mapped, especially those containing Se. XANES and XAFS can be used to determine the local environment about the absorbing atom(s) in order to identify the type of metallo-protein or the sulfur donors in a protein
- a better understanding of the distribution, uptake and metabolism of metal-containing pharmaceutics in cells and tissue for the development of better and safer drugs. Micro-XAS can provide structural chemical information regarding the intracellular biotransformation of the drugs
- gene maps obtained by attaching different metal oxides to DNA and RNA sequences and scanning them by a sub-micron x-ray beam.

Geoscience

Micron resolution is essential in the earth sciences in order to deal with typical sample sizes of relevant structures found in nature. The major analytical techniques such as electron probe, laser ablation ICPMS (inductively coupled plasma mass spectroscopy) coupled and ion probes such as PIXE and SHRIMP also have micron-scale resolution. The ability to produce not only an element map of a sample, but also to determine the oxidation state, as well as how a particular element is bound or coordinated, is the scientific quantum leap offered by the synchrotron microprobe over all other microprobe techniques. It leads in particular to:

- increased efficiency of mineral processing through a better understanding on the micron scale of mineral formation, porosity, chemistry and trace element partitioning in rocks
- more efficient management of mine wastes and mine rehabilitation through a more detailed knowledge of toxicity, chemistry and oxidation states of metals and other mine waste forms
- predictive mineral exploration tools based on a better understanding of ore-forming processes
- determinations of the oxidation state of magmas by XANES to improve our understanding of the geological conditions leading to the release of sulfur as the emission of sulfur during volcanic eruptions can have a profound effect on the Earth's climate
- analysis of tiny inclusions of melt trapped in zircon crystals more than 4 billion years old for chemical indicators of the hydrosphere and atmosphere, with a view to ascertaining when conditions suitable for life first appeared on Earth, and providing a better understanding of weathering processes
- the understanding of the relative abundance, chemical state and distribution of trace elements as indicators of geological processes

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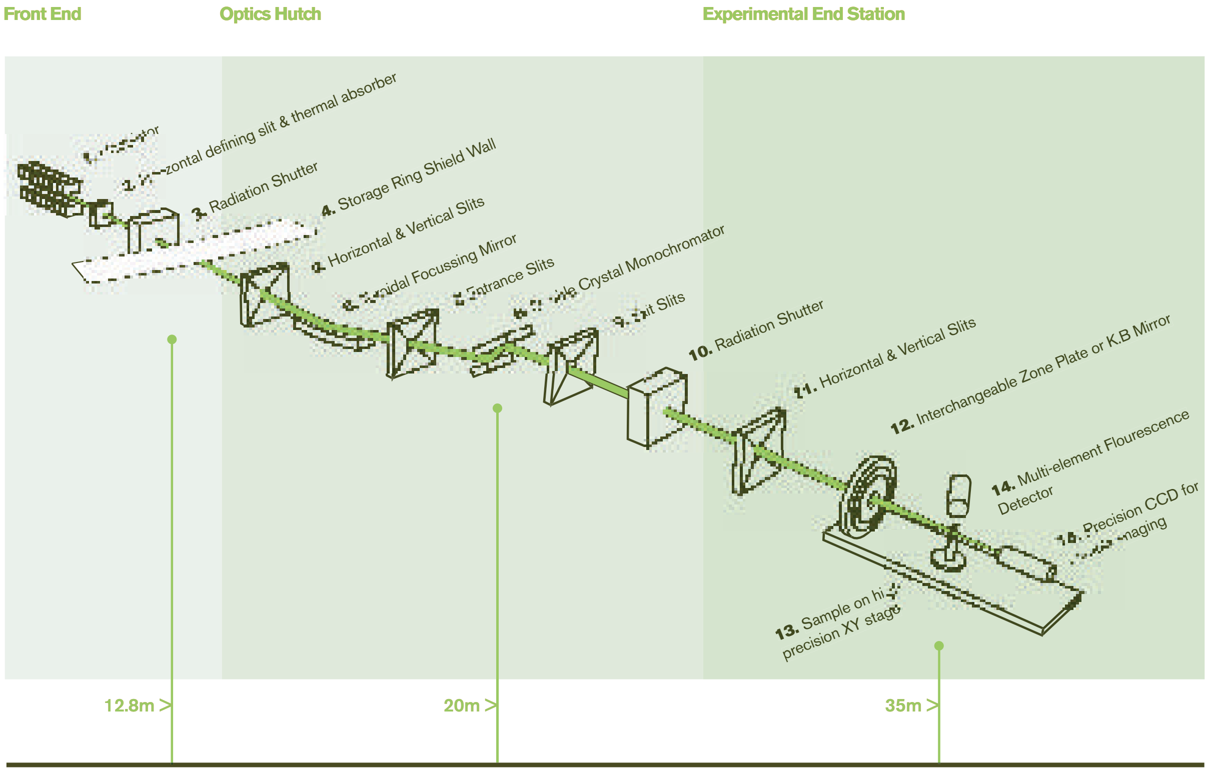
[4] R. Siegele, David D. Cohen, Nucl. Instr. and Methods B158 (1999) 31



BEAMLINE 9 Microspectroscopy

Figure BL9.1. *Schematic of the microspectroscopy beamline*

- the analysis of extraterrestrial material (dust particles, meteorites, future samples to be returned from Mars) for information on the evolution of the planets and solar system.

Environment

Increasingly the study of toxins in the environment and their pathways requires sub-micron resolution as well as the ability to determine their oxidation state. In particular:

- Increased understanding, on the micron scale, of plants and bacteria that can break down or accumulate toxins or elemental waste, the pathways of the waste and the mechanisms involved can all help optimise processes for waste recovery.
- The transport, origin, chemistry and health hazards associated with micron and sub-micron particulate matter in air and water pollution can be analysed individually by synchrotron radiation induced x-ray emission.

Materials

The high sensitivity, nanoscale resolution and ability to obtain information about chemical binding on a microscale, which will be possible with this beamline, will have many applications in materials research. For example the beamline will be useful for:

- the study of surface corrosion, micro-pitting and wear mechanisms of materials to minimise economic losses and improve the effectiveness of lubricants
- a better understanding of the chemistry and interaction processes of impurities and contaminants in materials and their effects on possible recycling processes
- a better understanding of de-bonding and delamination processes, particularly related to composite materials, involving changes in chemistry and elemental distribution on a micro scale
- a better understanding of polymer crystallisation and seeding of polymers for industry to produce consistent quality and reduce refuse and the study of metal implantation of polymers
- study of grain boundaries, impurities, charge transport and collection efficiency, lifetime, recombination, band gap in photovoltaic materials to improve efficiency in photovoltaic materials
- a better understanding of the structure, porosity and composition of fuel cell electrodes as well as their poisoning, impurity distribution and oxidation to improve the performance and durability of fuel cells.

Beamline Design

The beamline will provide sub-micron spatial resolution (around 0.1 micron) with the highest flux possible and a tuning range of 5.5–25 keV.

The very small beam spot sizes will be achieved by using an insertion device that produces a beam with a high brightness. An undulator (possibly 22 mm period) using the 3rd, 5th and 7th harmonics is the most appropriate choice.

The monochromator will be an adaptation of a large commercial silicon double-crystal unit. The first silicon crystal would probably be cryogenically cooled to operate at the temperature where the expansion of silicon is zero.

The beamline will be designed to accommodate both a zone plate for high resolution microscopy as well as a set of Kirkpatrick-Baez (KB) mirrors. Both will be easily and quickly interchangeable for different applications. Zone plates are intended for high resolution applications (0.1–2 microns), while the KB mirrors are required for chromatic focussing for applications such as EXAFS.

To enable two-dimensional mapping of micro-XRF and XAS data, the end station will have an *XYZ* target mounting stage with sub-micron precision, possibly with a cryo-cooling facility, mounted on a vibration-free optical table. A high resolution CCD camera and light microscope will allow precision placement and monitoring of the samples.

Appropriate x-ray detection systems would be solid state, energy dispersive Ge and Si arrays. An ionisation chamber with high speed capabilities would also be provided.

The multiple detectors will require a multi-parameter high speed data acquisition system as a fast data analysis technique. Data acquisition will include sample XY coordinates and the monochromator settings for μ-XAFS.

Beamline 9 – Microspectroscopy (sub-micron XAS, XANES, XRF)	
Source	In-vacuum undulator (22 mm period)
Energy range	5–20 keV
Resolution $\Delta E/E$	$<10^{-4}$
Minimum beam size at sample (horizontal × vertical)	0.1 × 0.1 micron
Brightness	10^{18} photons/s/mrad^2/mm^2/0.1% band width

Beamline 10: Imaging and medical therapy

Potential Research Fields

Life sciences

- Biological research – small animal imaging
- Biomedical and medical imaging
- Medical therapy
- Plants and crops

Physical sciences

- Forensics
- Advanced materials
  - Functional polymers
  - Ceramics
  - Nanomaterials and composites
  - Metals and alloys
  - Micro-electronic and magnetic materials
  - Biomaterials
- Engineering
- Mineral exploration and beneficiation
- Oil and gas production and distribution
- Agricultural technology

Advanced manufacturing

- Production of micro-devices

Introduction

It is proposed to construct a world class beamline for developing the technology for high resolution x-ray imaging of objects of the size of small animals, and a wide range of materials science samples in the first stage. Full human and large object imaging will be possible in a later stage. The technology for the beamline will build on the pioneering work of Australian scientists based largely in Melbourne[1].

One aspect of this work relates to the development of phase-contrast imaging techniques that transcend the conventional reliance on absorption to produce contrast. A second aspect relates to the development of theory to make these imaging techniques quantitative. These developments provide the basis for major advances in x-ray imaging science that are not only relevant for synchrotron-based imaging but also for radiography with conventional sources.

The beamline will be capable not only of satisfying the demand in Australia for synchrotron-based imaging using hard x-rays, but will also have sufficient flexibility and novel features to permit the development of new techniques and take advantage of the world standing that Australian scientists have in this area. It is intended that this beamline be a facility that will attract overseas researchers and which will be a flagship for the Australian synchrotron.

User Community

Potential users of this beamline include groups from at least fifteen biomedical research institutes (linked to pharmaceutical drug developments), five Cooperative Research Centres and a number of small to medium enterprises. Also, major manufacturing companies including automotive component suppliers and a number of major aerospace companies as well as the defence industry are expected to be interested in direct or collaborative research. Most of the biomedical and medical users will be new, because this is an area that cannot practically be addressed by current overseas synchrotron access arrangements as they involve live animal or patient studies.

Research Applications

The use of a synchrotron for imaging offers some remarkable improvements over the use of conventional radiographic equipment, greatly facilitating new x-ray imaging techniques as illustrated in the images in chapter 3. The combination of fine-tunable monochromatic x-rays with high intensity and collimation makes possible enormous improvements in contrast and resolution. Moreover, the use of new contrast mechanisms based on phase measurements, coupled with being able to choose the optimal monochromatic energy for the particular situation, results in very significantly lower tissue doses than the wider-spectrum x-rays of conventional x-ray sets. A very significant added advantage is that the beam energy can be tuned to energies that correspond to

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[1] S.W. Wilkins, T.E. Gureyev, D. Gao, A. Pogany, and A. Stevenson, Nature (1996) 384, 335–8, K.A. Nugent, D. Cookson, D. Paganin & Z. Barnea, Phys. Rev. Letts. 77, (1996) 66, 2961–4; Lewis R. Medical applications of synchrotron radiation X-rays. Phys. Med. Biol. 42 (7): 1213–43, 1997.

absorption by individual elements. As a result it is possible to image specific chemical elements with high sensitivity and micron, or even sub-micron, scale resolution.

The power of these imaging techniques is particularly suited to the study of living processes, as well as in situ materials processes such as solidification and precipitation phenomena in alloys[2]. The proximity between the Australian Synchrotron, Monash University, CSIRO, The University of Melbourne and the Monash Medical Centre will bring together a set of expertise and facilities that will enable this to be only the third beamline in the world especially configured for work on a wide range of live animals. The study of live animals for medical research is an area that is impractical under overseas access programs, and so relates to an essentially new and numerous Australian Synchrotron user class that has not been served in the past.

The properties of the proposed beamline, in particular the high energy capability, will also enable the study of novel methods of radiation therapy that cannot be achieved with any other type of x-ray source. Some of these methods show great promise for the treatment of cancer.

There are numerous applications for a facility such as this and the following represents just a small sample to illustrate the possibilities.

Biomedical imaging

Despite being by far the most popular medical imaging modality, lack of soft tissue contrast is a significant problem in both medical and biomedical conventional x-ray imaging. The relatively small variations in density and composition of soft tissues means that their x-ray attenuation characteristics are very similar. Conventional radiography produces images through the differential absorption of x-rays, and so provides very little soft tissue contrast unless high doses are employed as in computed tomography. Synchrotron-based imaging techniques, however, can also produce high resolution images using differences in the refraction and scatter of x-rays as they pass through tissue. Genuine soft tissue contrast with micrometre-scale resolution is possible with synchrotron x-ray imaging.

The collimation and monochromaticity of the imaging and medical therapy beamline will allow high resolution images to be recorded at a far lower dose than required by conventional equipment. This then will allow longitudinal studies (serial imaging) to be performed for investigations where the dose required by conventional imaging would confound the experiment. A large area of application for the beamline is in the area of small-animal imaging in relation to medical research and the development of new pharmaceuticals.

One of the problems at present is that animals are often sacrificed in order to obtain anatomical information at high resolution. The present beamline will allow in vivo imaging of small animals and so provide the major advantage of allowing longitudinal studies to be carried out. This has the significant advantage of following the same animal through the process and also dramatically reducing the number of animals sacrificed in a study.

Imaging of advanced materials and manufactured products

The high contrast, high speed, high coherence and microtomography capabilities can be exploited to enormous effect in the areas of materials science, non-destructive testing and mineralogy.

Examples include:

- in situ studies of precipitation and voids in industrially important light metal alloys
- minerals studies, including sedimentation of slurries, especially relating to compressibility and permeability; Also studies of reactivity of small particles at temperature
- the study of membranes for use in advanced fuels cells
- studies of fracture in ceramics
- the use of high resolution computed tomography (CT) for the study of porosity in oil bearing rocks. By tuning to different energies it will also be possible to image the amount of residual oil left in the rock following extraction
- investigation of micro/nano structured devices by micro-CT, e.g. for use in automotive applications
- the study of advanced materials following and during various stresses, both mechanical and environmental. Many advanced materials, for example those in aerospace applications, are composed of materials that cannot be imaged with conventional x-ray techniques due to lack of contrast.

Imaging of plants

The same contrast mechanisms used to visualise soft tissues in animals can also render visible many of the structures inside plants. An enormous range of studies are envisaged but of particular interest is the study of drought- and salt-tolerant species with a view to developing more efficient crops for Australia. Phase-contrast CT techniques will be employed to study the development of root structures without removing the plant from the soil, while K edge and micro-fluorescence imaging will be used to study protein hormone flow dynamics.

Radiotherapy

In the biology of cancer, imaging and therapy are inextricably linked. The capabilities of beamline 10 are designed for excellent imaging and are also ideally suited for the study and development of novel radiotherapy techniques.

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[2] R.H. Mathiesen, L. Arnberg, K. Ramsøskar, T. Weitkamp, C. Raur, A. Snigirev. Time resolved x-ray imaging of aluminium alloy solidification processes. Metallurgical and Materials Transactions B, v. 33B, 2002 pp. 613–623; and Mathiesen, R. H. Arnberg, L. F. Mo, Weitkamp, C. Snigirev, A. Time resolved x-ray imaging of dendritic growth in binary alloys. Phys. Rev. Letts. v. 83, No 24, p 5062, 13 Dec. 1999 (full text PDF available through CSIRO e-journals; movies available at http://www.phys.ntnu.no/~ragmat/index.html)

As described in chapter 3, the major problems with radiotherapy lie in determining the extent of the spread of the disease and delivering sufficient radiation to the tumour without damaging surrounding healthy tissues. These problems are particularly acute in brain tumours where the surrounding tissue is extremely sensitive. Synchrotron radiation is able to deliver a high dose to the targeted area only, with an accuracy that is significantly better than current clinical techniques. Research will focus on three possible techniques: photon activation therapy (PAT), CT therapy, and microbeam radiation therapy.

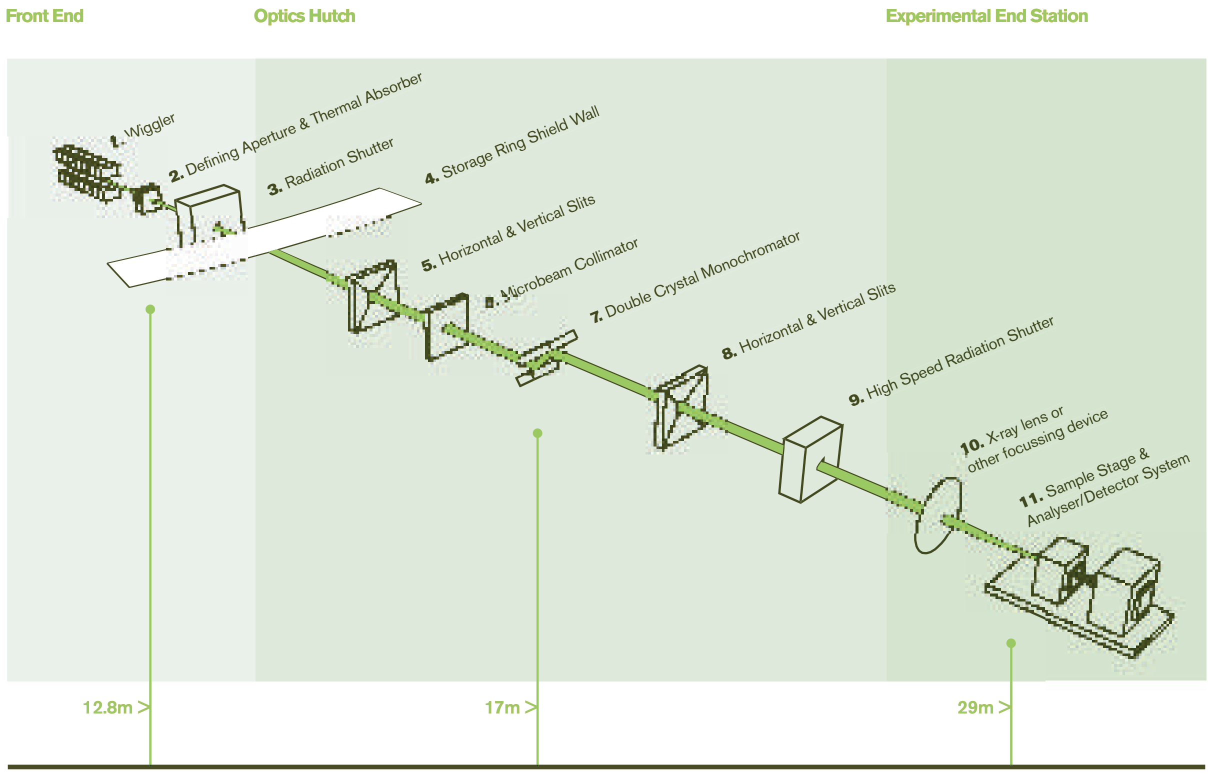
PAT and CT therapies both use specific x-ray energies that are preferentially absorbed by an element that has been delivered into the tumour. In PAT, a chemical agent (e.g. cis-platinum, which is also used for chemotherapy) is introduced and concentrates in the tumour. By choosing the correct energy, the x-ray beam interacts preferentially in the tumour and delivers a high localised dose. CT therapy also uses a contrast agent (e.g. iodine) that concentrates in the tumour, but takes advantage of beam spreading effects and stereotactic methods to spare normal tissues.

Perhaps the most exciting possibility is microbeam radiation therapy (MRT). Here extremely large radiation doses are applied to tissues in an array of micrometre-thick highly collimated x-ray beams. The extraordinary aspect of microbeam radiation is that it spares healthy tissue far better than large-area beams of the same dose and yet the tumour is still damaged. The reason for this effect is unknown, and is a fertile area for study. The method has been used with great effectiveness to deliver doses in excess of 1000 Gy to live animals. Note that 10 Gy delivered in a conventional treatment is lethal.

It is possible that therapies utilising this effect may revolutionise the treatment of some kinds of cancers, which are currently untreatable. A strong program of research into the nature of this effect together with determining the most effective way of delivering the dose will be a significant activity on this beamline.

Fundamental physics of imaging

The field of x-ray phase-contrast imaging in Australia is a very active one with world leading groups at CSIRO, The University of Melbourne and Monash University, all near the Australian Synchrotron. The establishment of the imaging and medical therapy beamline will give an enormous stimulus to further extending this line of activity and to transferring much of the fundamental research into practice. A very strong collaborative effort is envisaged between these groups, spanning algorithm, software, detector and x-ray optics developments. This will result in a world leading centre for research and applications based around this beamline. The beamline will also provide a very valuable test-bed for new ideas in the area of x-ray imaging and holography, and in the development of new and improved x-ray optics.



BEAMLINE 10 Imaging & Medical Therapy (Stage 1)

Figure BL10.1. *Schematic of the short beamline for x-ray imaging and therapy (stage 1)*

Additional benefits

The very nature of the research on this beamline will also lead to advances in machine optics, precision electronic and hydraulic movement, support and restraint devices, image acquisition, detector technology data transfer and analysis, and information technology interfaces (for interrelating image data with biological and treatment data). This can have a very large spin-off effect in the whole field of medical, industrial and biomedical imaging, a $US4 billion/year industry at the present time. The beamline will give a major boost to Australia's medical physics, biophysics and materials science communities.

Beamline Design

The beamline will be the second insertion device beamline that we are aware of to be optimised for in-line phase-contrast imaging for in vivo small animal and clinical medical applications. The beamline will incorporate the capability of using both white and pink beam modes in order to facilitate short exposure times.

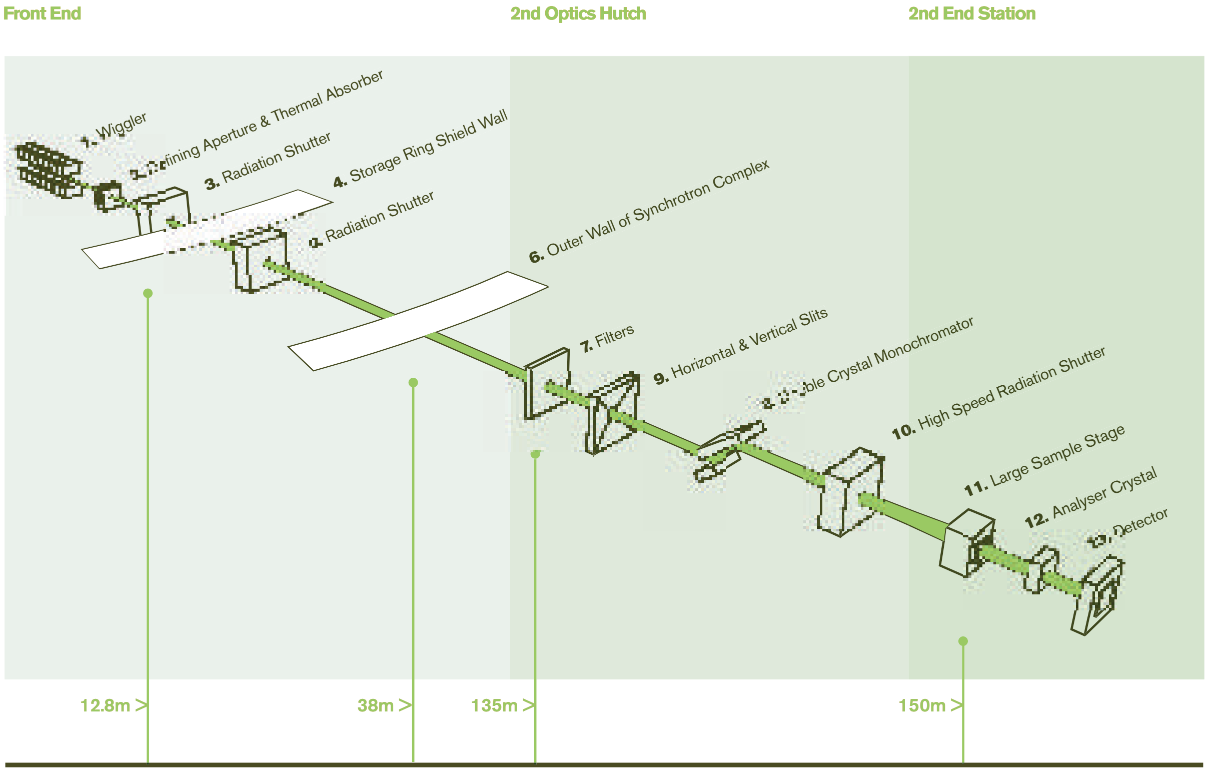
Two end stations are to be built. The first, as close as possible to the source, is to be built as part of the core initial suite of beamlines (category A, refer chapter 4). The second, a very long beamline with the sample station external to the main synchrotron building, at 150 m from the source, is a category B facility and will be built after the core suite of beamlines is established.

When both end stations are completed, two distinct modes of in-line phase-contrast imaging will be available. The first will use projection imaging from a small secondary focus 'spherical wave case' to obtain high spatial resolution (~ 100 nm), for example in microelectronics inspection, mineral grains studies or study of biomedical samples, as well as in a large class of advanced materials and manufactured products. The second mode will use a large source to sample distance (of order of 150 m) 'plane wave case', to yield a large field of view for small animal, clinical medical and large materials science studies. Other modes of phase-contrast imaging, such as diffraction-enhanced imaging, will also be possible.

Some of the advantages of the long beam line are:

- high spatial coherence (and quasi plane wave)
- potentially very high spatial resolution (now detector limited)
- large field of view due to the wide horizontal beams, especially for biomedical and clinical medical imaging applications
- low background scatter in in-line imaging applications due to the very large 'air-gap effect'
- that it will be external to the main experimental hall, so will be well suited to the establishment of a clinical/human imaging suite.

The first station will also have the capability for research on various new cancer therapies, including microbeam radiation therapy. For this work high beam energies and very high intensities are required, so that exposure time can be very short (of the order of milliseconds).



BEAMLINE 10 Imaging & Medical Therapy (Stage 2)

Figure BL10.2. *Schematic for the long beamline for x-ray imaging and therapy (stage 2)*

Beam characteristics

The energy range will cover 4–120 keV (120 keV is required for radiotherapy) with $\Delta E/E \sim 10^{-3}$ as well as a white beam option. This will require a superconducting wiggler, variable from 2 to 4 T.

A beam with high (cross-sectional) uniformity is required and this may involve special (i.e. diamond) windows and apertures, mirrors and monochromators. The optics will need to be carefully manufactured to avoid unwanted phase-contrast effects.

The beam should be broad (Station 1: 50×3 mm²; Station 2: 250×15 mm²) at sample position for many imaging applications. This might be increased by beam expansion optics if necessary.

The positional stability of the source and the mechanical stability of the long beamline will be of importance in many experiments because of the large 'lever arm' effect.

Detectors

Various detectors are envisaged for use for imaging including large area imaging plates with inbuilt scanner. Particular attention will be directed towards acquiring high performance photon counting detectors (such as pixel arrays) and energy resolving detectors, in order to give low dose and a substantial increase in information (at no greater exposure).

Beamline 10 – Imaging and Medical Therapy	
Source	Wiggler (4 T)
Energy range	10–120 keV
Resolution $\Delta E/E$	$\sim 10^{-3}$
Beam size at sample (horizontal × vertical)	50×3 mm² (Station 1); 250×15 mm² (Station 2)

Beamline 11: Microdiffraction and fluorescence probe

11

Potential Research Fields

Physical sciences

- Advanced materials
  - Ceramics
  - Biomaterials
  - Nanomaterials and composites
  - Metals and alloys
- Mineral exploration and beneficiation
- Earth sciences
- Oil and gas production and distribution
- Chemical reactions and catalysts

Advanced manufacturing

- Production and testing of microdevices

Introduction

The microdiffraction and fluorescence probe will provide rapid, simultaneous mapping of diffraction and fluorescence data. The incident x-ray beam size will be readily adjustable from several mm to 1–2 microns. With the smallest beam size the diffraction patterns measured will, in most scenarios, be indicative of single-crystal diffraction rather than powder diffraction. The innovative use of a broad bandpass incident x-ray beam will ensure that sufficient diffraction data will be obtained per incident beam position, regardless of crystalline grain size, to enable crystalline phase identification. The depth penetration of the high energy, high flux, broad bandpass incident x-ray beam will enable three-dimensional mapping of phase. In addition the provision of monochromatic radiation will enable XAS and fluorescence measurements at wavelengths selected to highlight a specific element. The definition of three-dimensional stress tensors on a grain by grain basis will be possible by the application of both broadband and monochromatic radiation.

Advantages of a Synchrotron Source

Only synchrotron light offers the possibility of simultaneous x-ray fluorescence (XRF) and x-ray diffraction (XRD) mapping at a micron scale.

In a laboratory setting a powder diffraction pattern is carried out using a monochromatic source as a function of diffraction angle but, with synchrotron radiation, diffraction data may be collected as a function of x-ray energy. In the microdiffraction and fluorescence probe, broadband Laue diffraction will be used in order to maximise the diffraction data collectable by an area detector without needing sample or detector rotation. This is not possible using a conventional x-ray source.

Because x-rays are efficient at causing excitation of inner-shell electrons, they produce low backgrounds and the samples require a minimum of preparation.

As synchrotron radiation provides white radiation, the incident x-ray energy can be selected to create maximum excitation for the element of interest. This, in addition to the high flux provided by a synchrotron x-ray source, can give rise to sensitivities in the order of parts per million. As very short wavelength x-rays are available that have a high sample depth penetration, analysis can be undertaken of melt and fluid inclusions without the necessity for destroying them.

User Community

The simultaneous XRD-XRF facility (with selected area XAS) is required for numerous scientific and industrial applications. These cover a wide range of fields and thus this instrument would serve as a basic infrastructure resource.

The beamline is likely to be used by researchers who are not expert in synchrotron techniques and so it will be designed to be simple to use and adjust. It will be supported by the necessary analytical algorithms to ensure rapid online crystalline phase identification, rapid strain mapping and calculation of stress and quantitative elemental analysis.

A significant number of industry sectors have been approached regarding their interest in using the facilities described. Letters of support have been received from the Australian Minerals Industry Research Association (AMIRA), Environmental Geochemistry International, Research Laboratories of Australia, TGR Biosciences and Rio Tinto. Mr Dick Davies, Chief Executive Officer of AMIRA, wrote:

> *… we view the possibility of being able to simultaneous map structure and composition via the VESPERS [Very sensitive Elemental and Structural Probe Employing Radiation from a Synchrotron] microprobe as highly exciting. As far as we are aware the provision of this form of rapid turn-around, on-line controlled microprobe specifically designed for industrial applications has not been attempted elsewhere. We foresee the extensive employment of this microprobe via AMIRA's member companies.*

Research Applications

Geochemical

The capacity for simultaneous XRF and XRD and complementary XAS will enable the relationship between trace elements and host phases to be established. It will also be possible to measure the diffusion and migration of elements as a function of mantle and sub-mantle conditions. Applications will include industrial mineral exploration, determination of elemental-mineral phase relationships (e.g. platinum group metals, the location of P, Si and Al in goethitic Fe-ores, and deportment of trace metals in high temperature melts and slags), process control during mineral processing, mineralogical, petrological, petrogenesis, environmental and whole-earth geochemistry research. The provision of XAS will enable the identification of elemental oxidation states as a function of crystalline phase.

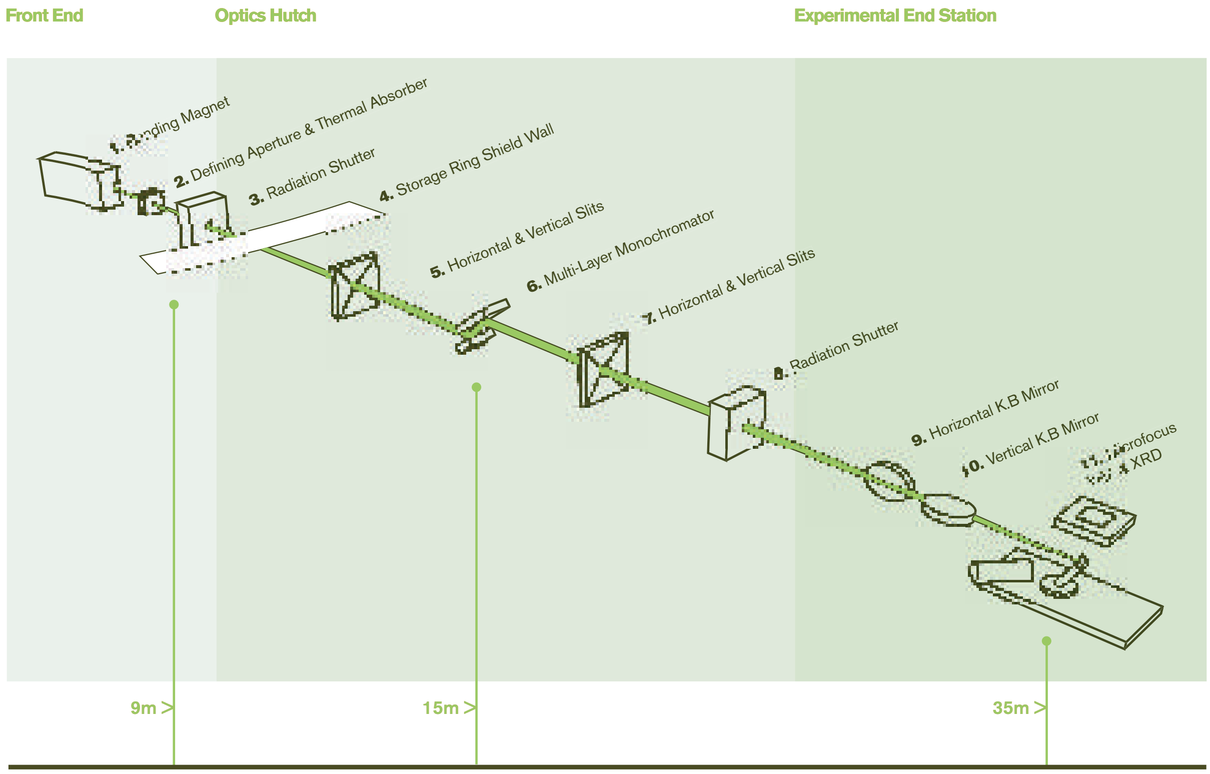
Environmental

Mineral weathering resulting in the release of acid mine drainage (AMD) is now of considerable environmental concern. It is estimated that in Australia remediation costs will be in the order of $900 million over the next fifteen years.

The dual XRF-XRD mapping facility, with XAS, will enable the identification of reaction and reprecipitation layering on mineral surfaces as a functioning of weathering. Understanding the evolution of these layers in terms of both their elemental composition and crystalline phase is important to the prediction and control of AMD. This combination of analyses will enable significant contributions to be made to the understanding of the release of toxic elements, which often accompanies AMD, and their bioavailability. The simultaneous XRF-XRD facility will also be of considerable application to other environmental concerns, for instance the identification of sources of industrial pollution.

Manufacturing

The XRF-XRD combination has many applications to the manufacturing and engineering industries. Aging of plastics and alloys to form microcrystalline domains, sometimes accompanied by elemental diffusion, is an area that could benefit from this combination of analyses.



BEAMLINE 11 Microdiffraction and Fluorescence Probe

Figure BL11.1. *Schematic of the microdiffraction and fluorescence probe*

Elemental partitioning is an area of particular importance to the microelectronics industry. The measurement of stress/strain as a function of diffusion processes that occur on corrosion, welding and annealing are also areas of application that require the combination of XRF and XRD.

The ability to map strain in metal fabrication products on a grain by grain basis at the surface will be valuable in many industrial applications, for example where surface compressive residual stress is introduced to improve fatigue performance.

Biotechnology

The combination of XRF and XRD also has biotechnological applications, for instance in the forensic sciences, for the production of bioceramics for bone implants and in the study of unwanted crystalline growths such as kidney stones.

Forensics

Typical forensic samples are small and complex matrices. Due to legal implications, the samples must be kept intact as far as possible. Non-destructive XRD-XRF mapping is an ideal analytical methodology and can be applied to materials such as metals, gunshot residues, paint, glass, soil, fibres, plastic and general polymers.

Beamline Design

The technical aims are to establish a microdiffraction and fluorescence probe that will:

- enable rapid simultaneous XRF and XRD high resolution mapping with three-dimensional resolution
- enable XAS and element-specific XRF
- be capable of mapping strain on a grain by grain basis
- require neither sample nor detector movement for collection of diffraction data
- be able to swap between white, pink and monochromatic incident x-ray modes without shifting the position of the x-ray beam incident on the samples so that XRF, XRD and XAS can all be carried out at the same point on a sample.

Beamline source

The beamline and end-station will be positioned on a bending magnet. A beam divergence of less than 2 mrad is required.

Beam focus

Grazing incidence Kirkpatrick-Baez mirrors will be used, providing a high degree of beam stability and ease of adjustment of beam size at the sample. They are applicable to broad bandpass radiation and will be insensitive to changes in wavelength, which is important when swapping the incident beam mode between white, pink or monochromatic incident radiation. Additionally the long focal length of these mirrors will enable flexibility in sample shape and alignment, and the use of robotics for sample changing.

Wavelength range and adjustment

A monochromator consisting of two graded multilayer mirrors will be required to enable the collection of sufficient data from a typical small unit cell mineral or alloy structure for single crystal diffraction analysis. Such multilayer crystals have now been designed.

To carry out XAS, strain mapping and selected element fluorescence there is also a requirement for monochromatic radiation. A Si (111) double crystal monochromator will be provided to enable these measurement modes.

Application of the Si (111) monochromator will enable the fluorescence of light elements down to approximately Na to be accessed with reasonable efficiency by using an incident x-ray energy in the region of 4 keV.

The monochromator housing will be based on a design by Ice et al[1]. This will enable rapid switching between broad bandpass, monochromatic and white beams while maintaining a static incident beam position on the sample. A spatial displacement on translation from white beam to monochromatic beam of less than 0.5 µm has been achieved.

Detectors

The optimum geometry for measurement of diffraction data is perpendicular to the plane of the storage ring. Hence it is proposed to mount a CCD camera vertically above the sample with the sample oriented at 45° to both the incident beam and the detector (i.e. 2θ of 90°). The CCD detector position will be easily changeable to enable glancing angle measurements and access to other 2θ diffraction angles.

The fluorescence spectra will be measured using an energy dispersive multi-element solid state detector. This detector will be in the plane of the synchrotron at 90° to the incident beam and 45° to the sample. Thus the footprint of the beam (when using the standard geometry) will be the same for the XRD and XRF measurement and the sample will simultaneously be tilted 45° off vertical and rotated 45° around a vertical axis. However, this will increase the footprint of the incident beam on the sample, for example a 1 µm incident x-ray beam would have a 1.4 µm footprint.

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[1] G.E. Ice, J.S. Chung, W. Lowe, E. Williams and J. Edelman, "Small-displacement monochromator for microdiffraction experiments", Rev. Sci. Inst., 71, 2001-2006 (2000)

Sample stage

The sample stage will be designed to be as compatible as possible with other instruments at the synchrotron and in the Clayton precinct. This will be important for ease of sample change between analytical facilities. Additionally, for mapping analyses a careful sample stage design will greatly facilitate the relocation of areas of interest on transferral of samples between facilities.

For detection of light elements (Ca and below) by XRF the sample and solid state detector will be enclosed by a glove bag-type arrangement with an internal positive pressure of He. Alternatively the latter section of the beamline, sample stage and detector system may be enclosed in a chamber under a moderate vacuum (0.1^{-1} torr).

Development of the concept

The microdiffraction and fluorescence probe is a new concept in beamline design. Considerable development work will be needed to prove the capability of simultaneously performing these two high precision techniques. In addition extensive research and calibration must be undertaken to derive the algorithms for interpretation of the results.

A similar beamline (VESPERS) is proposed to be commissioned on the Canadian synchrotron as part of its second suite of beamlines. A strong collaboration exists between the University of Western Ontario, the Canadian Light Source Inc. and researchers at the University of South Australia on the development and application of this beamline. This collaboration will provide a proven technical design and an experienced user base to support the establishment of the microdiffraction and fluorescence probe on the Australian Synchrotron.

Beamline 11 – Microdiffraction and Fluorescence Probe	
Source	Bending magnet
Energy range	4–37 keV
Resolution $\Delta E/E$	10^{-4}
Minimum beam size at sample (horizontal × vertical)	2 × 2 microns

12

Beamline 12: Circular dichroism

Potential Research Fields

Life sciences

- Biological research and drug design
- Plants and crops

Physical sciences

- Advanced materials
    - Functional polymers
    - Micro-electronic and magnetic materials
    - Biomaterials
- Agricultural technology
- Food technology

Introduction

Circular dichroism (CD) is a rapid and widely used technique for measuring the secondary structure (i.e shape and chain folding) of complex molecules. It is used by researchers in the biological, biochemical, chemical, pharmaceutical and crystallographic sciences to examine proteins, peptides, nucleic acids, carbohydrates, biopolymers and small chiral molecules, and to study the interactions of these molecules to form macromolecular and drug complexes.

Advantages of a Synchrotron Source

Laboratory instruments are usually sourced from a laser. Synchrotron radiation significantly extends the capability of a laboratory instrument. It provides high photon fluxes in the vacuum-ultraviolet and ultraviolet (100–300 nm) region. It is also inherently linearly polarised. The high fluxes and extended wavelength range allow the collection of CD data with unprecedented information content. Approximately 70% of pharmaceuticals target membrane proteins, about half of which are G protein coupled receptors. Conventional CD is limited in wavelength range, particularly in the presence of highly scattering and absorbing membrane systems. Protein CD spectra can routinely be measured to a lower wavelength limit of less than 168 nm and these data can be analysed to determine secondary structure content with very high accuracy. Additionally, measurements can be undertaken on compounds such as polysaccharides that do not exhibit CD in the wavelength region accessible to conventional instruments. Low noise spectra can be measured in very short time scales, with minimal sample quantities.

Synchrotron radiation is also an extremely effective source for time-resolved CD. These studies can be extended over a wide wavelength range, permitting the collection of CD spectra at millisecond time resolution, which can be analysed to determine changes in secondary structure in real time. Areas that can be investigated include:

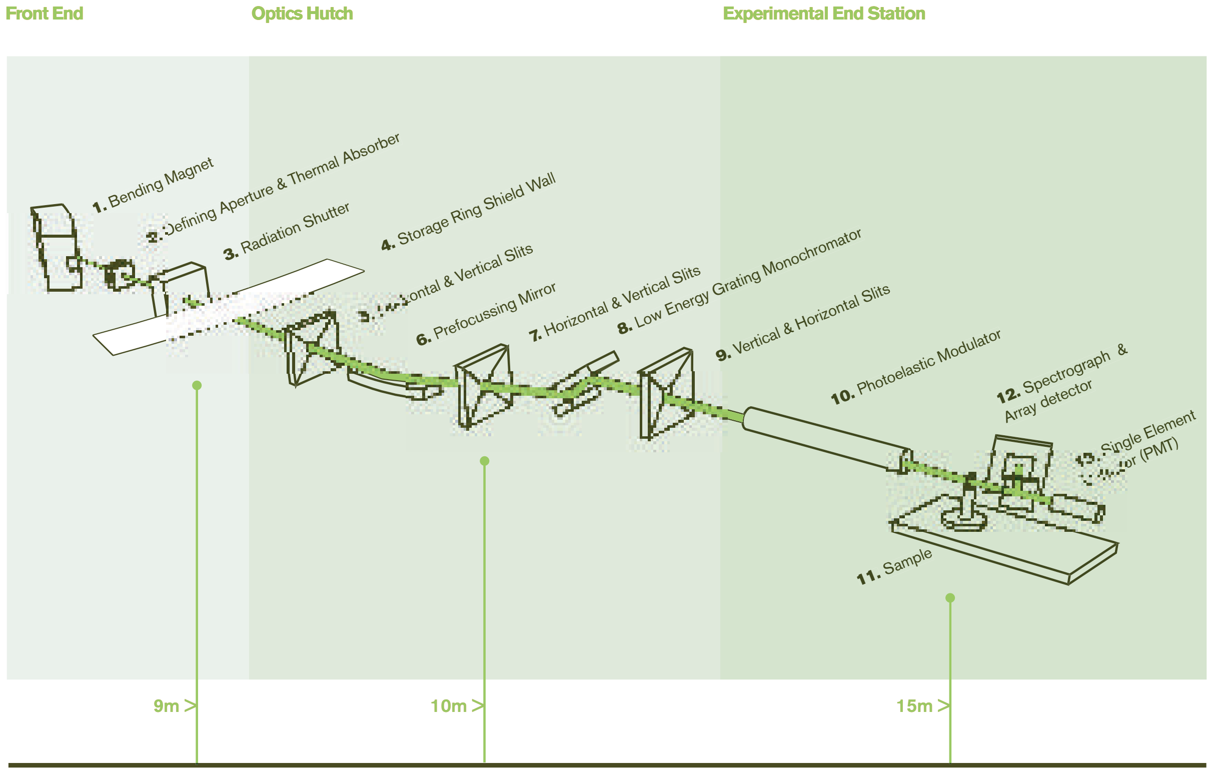
- how proteins fold, misfold and are correctly folded; protein and peptide conformation and folding in or at the surfaces of membranes
- the mutual changes in secondary and tertiary structure that occur when peptides and proteins interact with each other and with other macromolecules
- environmental effects on peptide and protein structure
- the screening of potential drug candidates
- the effects of crystallisation media on protein secondary structure.

The structural, functional and dynamics information that can be obtained by synchrotron radiation based circular dichroism (SRCD) provides information complementary to that produced by techniques such as protein crystallography PX and nuclear magnetic resonance. SRCD is therefore an essential component of any structural biology program.

User Community

SRCD is a very recent development with a rapidly expanding number of applications in a wide range of cutting edge biomedical research. To date Australian CD users have not had the opportunity to access a SRCD beamline.

More than 32 potential users have expressed interest in being able to access the CD beamline. Given the current rate of expansion of biomedical research and structural biology in Australia, and the increased capabilities and



BEAMLINE 12 Circular Dichroism

Figure BL12.1. *Schematic of the proposed beamline for circular dichroism spectroscopy*

application of SRCD compared to conventional instruments, this number could easily reach 100–150 within two years of this beamline opening.

Research Applications

SRCD can provide powerful new information in specific areas.

Protein folding

Rapid conformational changes, for example following dilution of a protein or peptide from denaturant are hard to follow by conventional CD due to the absorbance of the denaturant and the poor signal to noise ratio that results from the need to sample rapidly. These problems can be overcome by SRCD. In addition, data can be acquired to low wavelength even in denaturant (e.g. at 190 nm) providing more detailed resolution of the structural transitions occurring. One recent highlight is the demonstration that the formation of helices is a much slower and more complex process than previously thought[1].

Turbid solutions

CD spectra on highly turbid solutions can be obtained by SRCD, opening the door to studies of membrane proteins, protein aggregates and large protein complexes. One highlight includes CD data on highly turbid solutions of the self-assembly system of clathrin coat protein. This is the first time CD data have been collected on this type of system[2].

Membrane proteins

Membrane proteins are notoriously difficult to study using high resolution structural methods. Nevertheless, detailed information about membrane protein structure has been obtained on a number of membrane proteins[3]. This information has been used as part of the project to construct a CD database for this type of protein, which will allow accurate secondary structural content to be determined and used to aid structure prediction. In addition, conformational changes that occur during membrane protein functions (transporters, receptors and channels) can be determined using SRCD.

Structural genomics

Developing conditions that permit data collection to 158 nm in aqueous solution has extended the secondary structural information content of CD spectra. Accurate data such as this can provide key information to differentiate between alternative models for proteins produced, for example, by structural prediction methods. In addition, SRCD can be used as a rapid screening process for the structural integrity of samples prior to setting up for crystallography[4].

Macromolecular dynamics and function

SRCD can screen for ligands for proteins, and conformational changes occurring upon ligand binding or assembly processes can be assayed in physiologically relevant buffers, and their thermodynamics and kinetics can be determined using SRCD methods. For example,

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[1] D. Clarke et al. Proc. Nat. Acad. Sci. U.S.A., 1999, 96, 7232-7237.

[2] D. Clarke and G. Jones, Biochemistry, 1999, 38, 10457-10462

[3] For a review, see B. A. Wallace, Circular Dichroism Spectroscopy and X-ray Crystallography: A Dynamic Duo. CCP4 Newsletter 37:29-30, (1999)

[4] Rodi et al, J Mol. Biology 285:197-204 (1999)

CD was used to screen a library of phage-displayed peptides to identify the human apoptotic protein Bcl-2 as a taxol-binding protein. This information will probe proteins in action in real time and complement results emerging from high resolution structural methods.

Physical sciences

Some areas of further interest at the lower energy end of the spectrum might include atmospheric chemistry, electronic spectroscopy of free radicals, and optical metrology of insulating materials.

Beamline Design

The beamline is planned to accommodate a range of experiments including:

- the collection of steady-state CD spectra using a conventional scanning monochromator
- the collection of CD spectra in the sub-millisecond time domain using the energy-dispersive method
- time-resolved CD measurements using stopped-flow, continuous-flow, pressure-jump, and temperature-jump techniques
- the possibility of collecting vibrational CD spectra in the amide-1 region.

Because the beamline is complementary to protein crystallography and would require similar sample preparation facilities, it will be sited close to beamlines 1 and 2.

Also, as for the protein crystallography beamlines, it is expected that there will be a requirement for high throughput and for remote operation so it will be equipped with robotic assistance for automated handling and collection of CD spectra.

Figure BL12.1 shows a schematic representation of the beamline. It is based on beamline CD12 at the SRS (Daresbury) with some modifications. The beamline will be sourced from a bending magnet.

The monochromator mechanism must have the capacity for at least four interchangeable optical elements. As optical elements operating in the VUV–UV region are highly susceptible to contamination, vacuum levels of around 10^{-10} mbar must be maintained in the mirror and monochromator chambers.

Control of beam polarisation is an important consideration for the CD beamline. Ideally, 100% horizontally polarised light is required at the photoelastic modulator. Beamline reflections should be in the 'S' plane for optimal reflection of horizontally polarised radiation, and this is the case for the beamline design shown in figure BL12.1. However, because the polarisation of the synchrotron radiation varies through the vertical plane of the beam, there is also a requirement to select specific regions of the beam to ensure that the optimal polarisation is maintained at the modulator position. This can be achieved by the use of independently adjustable baffles situated before and after the monochromator. These baffles will provide full control of the selected radiation, allowing selection of the optimal combination of polarisation and beam intensity. This method is already being employed at SRS, Daresbury, UK.

End Station

The end station will include:

- a CaF_2 photoelectric modulator
- a linear detector (PMT) for wavelength scan
- an array detector for white light measurements plus spectrograph
- an IR detector for VCD measurements
- laser temperature and pressure jump devices
- stopped flow apparatus.

The set up will be capable of simultaneous detection of absorption and CD spectra.

Two possible detector configurations are shown in figure BL12.1 – a detector system for scanning CD measurements and a configuration for the measurement of energy-dispersive CD.

For monochromatic CD, the photoelastic modulator and sample should be behind the exit slit. For dispersive CD, they should be in front of the exit slit.

The sample stage will provide:

- variable and controlled temperature (for 'thermal melting' curves)
- variable sample-to-detector geometry (for membranes and other scattering samples)
- long, short and variable path-length cells.

Estimates of the performance of this beamline are given below. These figures are intended as a guide to the type of performance that might be expected, and will be confirmed when a detailed design has been completed.

Beamline 12 – Circular Dichroism	
Source	Bending magnet
Energy range	2–10 eV monochromatic radiation; 5–8 eV in white light operation
Resolution $\Delta E/E$	10^{-4}–10^{-3}
Beam size at sample (horizontal × vertical)	3.5 mm × 0.2 mm
Polarisation	70–90% linear, controllable by vertical aperture
Acceptance angle (horizontal × vertical)	35 × 7 mrad

Beamline 13: Lithography

Potential Research Fields

Life sciences

- Biotechnology and bio-sensors

Physical sciences

- Advanced materials
  - nanomaterials and composites
  - micro-electronic and magnetic materials
- Engineering
- Chemical reactions and catalysts
- Agricultural and food technologies

Advanced manufacturing

- Production of micro-devices

Introduction

Lithography stands alone in synchrotron applications as the only technique that creates artefacts, i.e. parts and devices.

Lithography is the process of making mechanical parts and structures by photographically exposing light-sensitive material (usually a resist) to create patterns that may be used either directly or as shields to allow selective etching of lower layers, or as moulds to fill with metals, ceramics, polymers, glasses or even bio and nano-engineered materials.

Lithography more generally, as opposed to x-ray lithography, is the cornerstone of the semiconductor industry where the world's top ten manufacturers have combined sales in excess of $US400 billion annually. The great competitive advantage of lithography over other machining methods is that the costs of devices are determined by the batch process costs rather than the costs to machine individual parts. Hence we no longer consider buying transistors one at a time, but use transistors in their millions as they are lithographically patterned into integrated circuits. This naturally leads to miniaturisation and integration, since by so doing, only the pattern in the photographic image is made more complex (the batch processing steps are no more complex) and the productivity and profit margins of the manufacturer increase as a result of producing more parts per batch. Hence in lithography making things smaller often makes them cheaper to produce (measured on a per part basis). Now we are able to apply this efficiency to fabricating integrated, three-dimensional mechanical systems.

Advantages of a Synchrotron Source

Lithography using synchrotron radiation sits at the top of the list of other lithography techniques in terms of resolution, aspect ratio and tolerance. The other techniques include excimer laser micromachining, UV lithography, electrodischarge machining and electrochemical machining. Collectively these techniques are applied to the creation of high aspect ratio micro systems (HARMST). In comparison to other techniques LIGA provides the following unique features:

- aspect ratios (depth : width) >100, essential for power transfer in micro devices
- optically smooth side walls, vital for telecommunication applications
- almost perpendicular walls, a consequence of the collimation of the synchrotron x-rays.

User Community

At the recent HARMST 2003 conference held in Monterey, USA, more than 300 researchers gathered from more than 16 countries to discuss the science, technology and commercialisation of HARMST, and in particular LIGA.

It is intended to set up this beamline so that it is capable of high volume production. It will incorporate an advanced design of scanner and will work in tandem with the nearby MiniFAB facility. As such, it is expected to attract substantial international user interest.

Already there are several industrial users interested in exploring the product development potential of LIGA. These include Masterfoods, Varian, Micromachines Ltd and AMCOR. All of these are pursuing their interests through MiniFAB Pty Ltd, a private venture that has expressed early support for the industrial application of

LIGA, and which operates supporting infrastructure, for example clean rooms, mask aligner, laser ablation, deposition and moulding.

The CRC for MicroTechnology has been developing an industrial capability in LIGA, assisted by the ASRP. Industrial users require that the LIGA process be specification driven, that is that it is able to provide a reliable, guaranteed service. Such a service can only be provided if it is underpinned by a sound understanding of the fundamentals of LIGA, and can only remain globally competitive if supported by a strong scientific R&D program.

International partnering

Preliminary discussions with the LIGA representatives of the new Canadian Light Source and the UK Diamond facility indicate that they would partner in this development, with the aim of building three scanners for installation at each of the new synchrotrons.

Research Applications

This beamline will provide opportunities to support basic research in nanoscience as well as manufacture of complex, deeply structured micro-devices. In basic science, it will be useful for the preparation of substrates for nano devices, photonic crystals, and fuel cell studies.

New applications in the production of micro-devices being researched internationally include:

- fuel cell development
- deposition nozzles
- cochlear implant moulds
- accelerometer sensors
- micro-relays
- x-ray lens fabrication
- micro gas bearings
- ink jet printers
- micro spectrometer development
- micro-optic fabrication
- micro medical devices (forceps, tweezers, micro-needle arrays, etc)
- direct synchrotron machining of polytetrafluoroethylene resin (Teflon®)
- variable reluctance stepping motors.

There is substantial effort and debate in the local and international LIGA community concerning developments in modelling of the full process (including electroforming and moulding), metrology, characterisation, resist development, and the development of infrastructure. Theoretical models for the exposure have only been developed for polymethylmethacrylate, and the complexities of secondary electron emission, scattering processes, top-to-bottom dose ratios, thermal effects and others remain important in gaining a fundamental understanding of the x-ray interaction with resists.

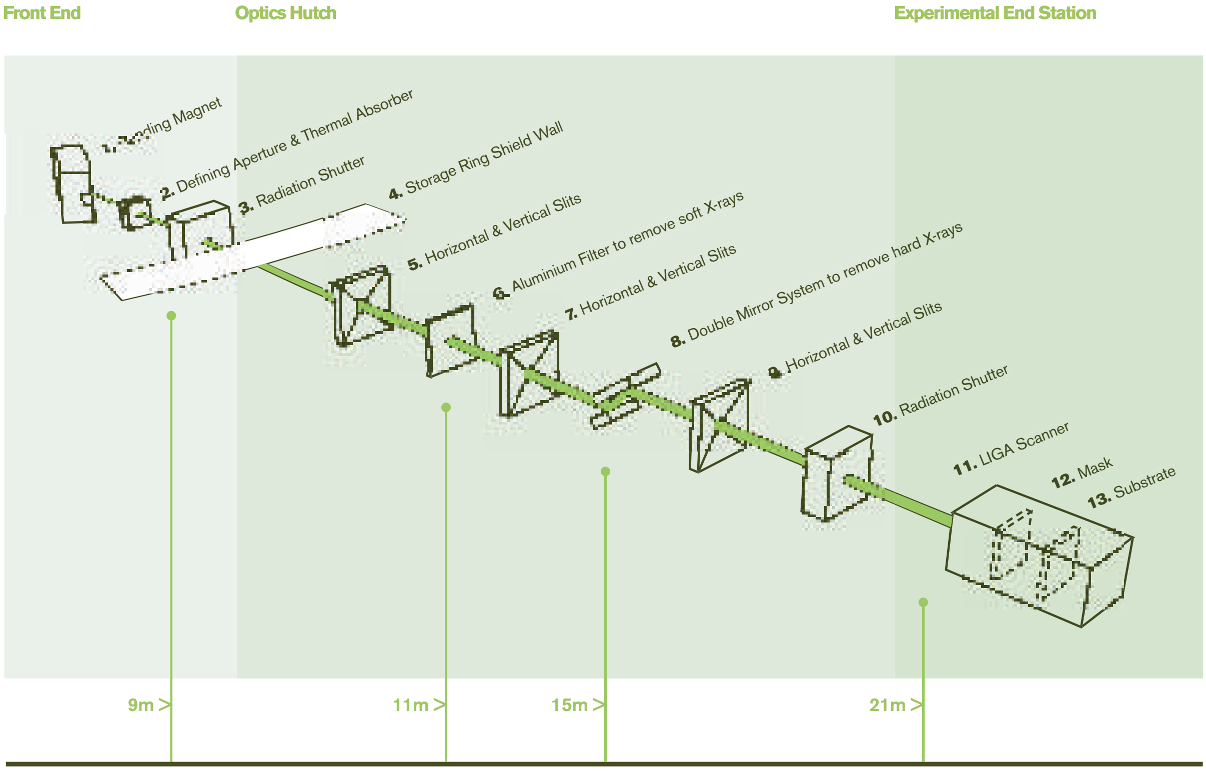


Figure BL 13.1. *Schematic for the lithography beamline.*

Beamline Design

Two LIGA beamlines will be designed to operate from a bending magnet beam and will supply the LIGA scanner with a range of x-ray energies (2–30 keV) to suit the application.

The beamlines will have appropriate mirrors and filters to remove unwanted high energy and low energy x-rays, respectively. The first beamline will be suitable for deep x-ray lithography (DXRL) with resist thicknesses up to 500 microns The second beamline (not budgeted for in this proposal) is planned for ultra deep x-ray lithography (UDXRL) on resist thicknesses up to 2000 microns.

The mirror systems will have the ability to be driven out of the beam to allow the beamline to 'switch' between harder and softer x-ray photon applications.

An advanced technology LIGA scanner will be designed to provide multiple degrees of freedom and hence different exposure strategies. It will be capable of accommodating wafer sizes in the range 100–200 mm, exposed with a range of x-ray energies to suit the application.

It is proposed that two beamlines be installed with the following specifications:

LIGA Line DXRL

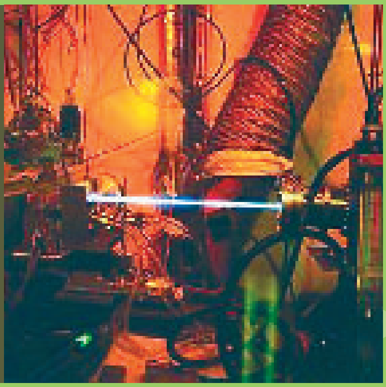
Mirror	7500 eV cut-off Ni mirror (single or double)
Windows	500 micron Beryllium
Absorber	15 microns Aluminium
Energy	2–8 keV

LIGA Line UXRL

Mirror	None
Windows	500 micron Beryllium
Absorber	80 microns Aluminium
Energy	5–40 keV

Beamline 13 – Lithography	
Source	Bending magnet
Energy range	2–8 keV (DXRL); 5–40 keV (UXRL)
Resolution $\Delta E/E$	10^{-4}
Beam size at sample (horizontal × vertical)	200 × 200 mm
Resist thickness	500 microns (DXRL); 2,000 microns (UXRL)

Appendices



Appendices

IMAGE: Gas ionised by an x-ray beam from the X25 wiggler at the National Synchrotron Light Source, Brookhaven, USA

Appendices

APPENDIX 1: BEAMLINE COSTINGS

It is proposed that the Australian Synchrotron should commence with a core suite of between nine and thirteen world class beamlines. Details of the proposal are given in chapter 4.

The following cost estimates for the design, construction and commissioning of each of the thirteen beamlines were prepared by the beamline proponents with support from the National Scientific Advisory Committee, the International Scientific Advisory Committee, the International Machine Advisory Committee and a number of individual Australian and overseas experts.

Work is continuing on the specifications for each beamline, and as details are finalised these cost estimates will be refined. In the meantime, every effort has been made to ensure that the beamline costing estimates are based on the most reliable and reasonable figures currently available in 2003.

Cost Estimate Assumptions

Some items have already been included in the budget for the synchrotron machine and as such are not included in beamline costings. These include:

- the ‘front end’ equipment (i.e. vacuum equipment, interlocks, controls and electronic equipment on the inner side of the shielding wall)
- a distributed liquid nitrogen system
- the labour costs of the beamlines manager and corporate technical staff. (However, an allowance has been included for labour for design, construction and commissioning of each beamline.)
- costs for survey and alignments, vacuum and control interfacing with the machine and radiation monitoring.

Currency Conversions

Prices quoted are in current Australian dollars. Conversion rates used are:

$A1 = $US0.65

$A1 = $CAN0.90

$A1 = GBP 0.385

$A1 = Euro 0.58

$A1 = Yen 75

Contingency

No contingency has been made for currency fluctuation or uncertainties of the cost of components. Synchrotron technology is evolving rapidly and it is possible that by 2006 some devices may be of lower cost; however, this is impossible to predict at present.

Summary of beamline cost estimates

BL	Title	Category 1	Category 2	Category 3
		$(A)	$(A)	$(A)
1	High-throughput Protein Crystallography*	5,823,000	1,655,000	
2	Protein Microcrystal & Small Molecule Diffraction	7,983,000		
3	Powder Diffraction**	5,300,000		
4	Small & Wide Angle Scattering	4,785,000		
5	X-ray Absorption Spectroscopy	5,110,000		
6	Soft X-ray	4,939,000		
7	Vacuum Ultraviolet		4,990,000	
8	Infrared Spectroscopy	2,600,000		
9	Microspectroscopy	5,339,000		
10	Imaging & Medical Therapy	7,610,000	5,120,000	
11	Microdiffraction and Fluorescence Probe			3,442,000
12	Circular Dichroism		3,100,000	
13	Lithography			4,240,000
Total		**49,489,000**	**14,865,000**	**7,682,000**

Notes: * bending magnet – then an in-vacuum undulator
** bending magnet – moving to wiggler

Beamlines 1 & 2 – Protein Crystallography & Small Molecule Diffraction

Item	Beamline 1 $(A)	Beamline 2 $(A)	
	Category A	Category A	Category B
In vacuum undulator		1,365,000	1,365,000
Liquid nitrogen cooling		200,000	200,000
Water cooled CVDD filter	23,000	23,000	
Quadrant XBPM	40,000	40,000	
4 blade XPBM	40,000	40,000	
Primary slits	114,000	114,000	
Filter unit (carbon & metal filters)	68,000	68,000	
Optical system	640,000	1,000,000	
Bremsstrahlung stop	23,000	23,000	
Secondary slits	28,000	28,000	
3 pixel XBPM	27,000	27,000	
Beamshutter (monochromatic)	23,000	23,000	
3 HLS sensors	7,000	7,000	
Exposure box	23,000	23,000	
Equipment protection system	34,000	34,000	
Micro-crystal diffractometer	752,000	752,000	
Pixel detector	1,360,000	1,360,000	
Controls & data acquisition	387,000	387,000	
Motor drivers (88)	54,000	54,000	
Graphics workstations	34,000	34,000	
Software	60,000	60,000	
Signal & power cables	28,000	28,000	
Vacuum (ion getter & turbo pumps)	122,000	122,000	
Hutches	280,000	480,000	
LAC	22,000	22,000	
Lab equipment	34,000	34,000	
Miscellaneous equipment	200,000	200,000	
Flat panel detector	800,000	200,000	
Robotics system	200,000	200,000	
4-circle diffractometer		450,000	
Cryogenic/heating specimen chamber		185,000	
Labour (@ $90,000 per FTE year)	400,000	400,000	90,000
Totals	**5,823,000**	**7,983,000**	**1,655,000**

Beamline 3 – Powder Diffraction

	$(A)
Wiggler	1,000,000
Cooling system	150,000
Collimating mirror	228,000
Double-crystal monochromator	700,000
Focussing mirror	227,000
Monochromator exit aperture	50,000
Optics & experimental hutches	242,000
Debye-Scherrer diffractometer	300,000
Conventional diffractometer	200,000
Detectors	600,000
Cryostat	80,000
Furnace	60,000
Optical table	20,000
Beamline components	379,000
Electrical infrastructure and controls	364,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Total	**5,300,000**

Beamline 4 – Small & Wide Angle Scattering

	$(A)
In-vacuum undulator 2.2cm period	1,365,000
Liquid nitrogen cooling	200,000
White beam slits (to handle 91 watts/mm2)	125,000
Monochromator (with water cooled diamond crystals)	577,000
Toroidal (doubly focussing) mirror	526,000
Miscellaneous beamline transport and vacuum components	154,000
Optics enclosure	140,000
Experimental enclosure (including utilities and safety system)	278,000
Collimating optics (motorised slits for mono beam)	46,000
SAXS camera (flight tube and associated mechanisms)	154,000
SAXS detector (CCD based on current technology)	385,000
WAXS detector (CCD)	385,000
Labour (5 FTE years @ $90,000)	450,000
Total	**4,785,000**

Beamline 5 – X-ray Absorption Spectroscopy

	$(A)
Wiggler	1,000,000
Cooling system	150,000
Collimating mirror	228,000
Double-crystal monochromator	700,000
Focussing mirror	227,000
Monochromator exit aperture	50,000
Optics & Experimental hutches	242,000
Cryostat	100,000
Furnace	50,000
Optical table	20,000
Fluorescence detector	800,000
Additional detectors	100,000
Beamline components	379,000
Electrical infrastructure and controls	364,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Total	**5,110,000**

Beamline 6 – Soft X-ray Spectroscopy

	$(A)
Variable polarisation undulator	1,500,000
Liquid nitrogen cooling system	80,000
Collimating mirror	228,000
Double-crystal monochromator	700,000
Focussing mirror	227,000
Switching mirror	250,000
Exit apertures (two)	100,000
Optics and two experimental hutches	400,000
Optical tables (two)	40,000
Beamline components	350,000
Electrical infrastructure and controls	364,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Total	**4,939,000**

Note: The two experimental end stations are not included as they are being built at present for other programs and will be transferred to the Australian Synchrotron at the appropriate time.

Beamline 7 – Vacuum Ultraviolet

	$(A)
Variable polarisation undulator	1,500,000
Liquid nitrogen cooling system	80,000
Toroidal focussing mirror	228,000
Plane grating monochromator	650,000
Cylindrical mirror	200,000
Toroidal horizontal refocussing mirror	228,000
Exit apertures	50,000
Optics & experimental hutches	220,000
Optical table	20,000
UHV specimen chamber and detectors	400,000
Beamline components	350,000
Electrical infrastructure and controls	364,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Total	**4,990,000**

Beamline 8 – Infrared Spectroscopy

	$(A)
Ultra high vacuum section	
Vacuum equipment & beam tubing	150,000
Motorised mirrors (3)	90,000
Diamond window	50,000
Medium vacuum section	
Beam switchyard	100,000
Stainless steel beam tubes (3)	75,000
Movable mirrors	90,000
Vacuum equipment	150,000
Experimental enclosures (2)	220,000
Optical tables (3)	90,000
High resolution FTIR	600,000
IR microscope	500,000
Data handling & interpretation	60,000
Ancillary & safety equipment	150,000
Labour (3 FTE years @ $90,000)	275,000
Total	**2,600,000**

Beamline 9 – Microspectroscopy

	$(A)
Undulator 22 mm in vacuum	1,365,000
Liquid nitrogen cooling	200,000
Parabolic collimating mirror	228,000
Double-crystal monochromator	760,000
Toroidal focussing mirror	227,000
Monochromator exit aperture	53,000
Optics & experimental enclosures	200,000
KB micro-focus mirrors	60,000
Zone plates	60,000
Optical table	20,000
Fluorescence detector (2)	350,000
Scanning	50,000
Proportional counters	20,000
CCD detector	303,000
Beamline components	379,000
Electrical infrastructure and controls	364,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Total	**5,339,000**

Beamline 10 – Imaging & Medical Therapy

	Stage 1 $(A)	**Stage 2 $(A)**
Source & delivery of beam		
Wiggler (superconducting, variable field 2 – 6 T)	2,500,000	
Cooling system	250,000	
Beamline components (shutters,etc) & shielding	500,000	
Electrical infrastructure and controls	400,000	
Double-crystal (Laue case) monochromator	760,000	
Vacuum components	250,000	
Beam monitoring components	100,000	
Optical enclosure	200,000	
End stations		
Monochromator exit aperture	60,000	
Experimental Hutch #1, including services	200,000	
Optical bench	20,000	
KB mirrors (including 1 multilayer mirror)	200,000	
Tomography stage	200,000	
Imaging plate detector	250,000	
2-dimensional electronic imaging detector	500,000	
Scanning and positioning stages	100,000	
Controls & control system	200,000	
Safety shutters	100,000	100,000
Long beamline		400,000
Separate building, control room and experimental hutch #2		2,500,000
Vacuum components		100,000
Second hutch controls		100,000
Optical bench		20,000
Secondary large aperture monochromator system		1,000,000
Sample positioning system		400,000
Related infrastructure		
Computers and software for control and data processing	100,000	50,000
Labour (construction and commissioning)		
Salary (8 FTE years @$90,000)	720,000	
Salary (5 FTE years @$90,000)		450,000
Totals	**7,610,000**	**5,120,000**

Beamline 11 Microdiffraction and Fluorescence Probe

	$(A)
Water cooled mask and collimator	26,500
White beam slits	44,100
Pre-focussing mirror	441,000
Double multilayer monochromator	485,000
Multilayers	70,500
Monochromatic beam slits	26,500
Fluorescent screen	28,200
Frame grabber	1,800
Photon shutter	35,300
Pipe	44,000
Optics hutch	167,000
Interlock	56,000
Quadrant beam position monitor	21,000
KB mirrors	212,000
Be window	10,500
Slits	35,000
EDX detector	67,000
CCD	264,500
Computers	89,000
Stage and indexer	111,000
Hardware/software	111,000
Table	44,100
Position monitor	80,000
End station assembly	100,000
Optical microscope	90,000
Experimental hutch	121,000
Electrical & safety system	300,000
Labour (4 man FTE @ 90,000)	360,000
Total	**3,442,000**

Beamline 12 – Circular Dichroism

	$(A)
Water cooled entrance slits	50,000
Double-crystal monochromator	550,000
Focussing mirror	220,000
Monochromator exit aperture	50,000
Optics & Experimental hutches	220,000
Photoelectric modulator	100,000
Linear, array & IR detectors	400,000
Laser temperature & pressure jump device	75,000
Stopped flow apparatus	50,000
Optical table	20,000
Beamline components	300,000
Electrical infrastructure and controls	365,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Total	**3,100,000**

Beamline 13 – Lithography

	$(A)
Water cooled entrance slits	50,000
Double-crystal monochromator	550,000
Monochromator exit aperture	50,000
Optics hutch	120,000
Lithography scanner – mechanical system	640,000
Lithography scanner – software & control	140,000
Experimental hutch – Class 100 clean room	400,000
Beamline components	300,000
Electrical infrastructure and controls	365,000
Vacuum equipment	250,000
Labour (5 FTE years @ $90,000)	450,000
Separate class 100 clean room for developing samples	675,000
Ancillary equipment	250,000
Total	**4,240,000**

APPENDIX 2

Technical Specifications of the Boomerang Storage Ring

The Australian Synchrotron is based on the Boomerang Storage Ring[1,2] which has a double bend achromat structure (Figure 1) with fourteen cells or superperiods. Each cell comprises two dipoles (D), six quadrupoles (Q) and seven sextupoles (S) separated by appropriate drift spaces. The dipoles have modest gradient fields to provide set horizontal defocussing. There are also small defocussing quadrupoles within the achromat. Each cell includes seven sextupoles that have been carefully position to maximise the dynamic aperture. The main parameters are listed in Table 1 for two operational modes of the lattice. The storage ring will be fed by a full energy booster synchrotron that in turn will be fed by a 100 MeV linac. The contract for the building has been let to Thiess and tenders for the entire injection system are being evaluated.

Table 1 Basic properties of the lattice

	$\eta = 0$	$\eta = 0.24$ m
Energy	3.0 GeV	3.0 GeV
Circumference	216 m	216 m
Harmonic Number	360	360
Number of Available Straights	12	12
Revolution Time	720.5 nsec	720.5 nsec
Revolution Frequency	1.3879 MHz	1.3879 MHz
Current	200 mA	200 mA
Betatron Tune – H	13.30	13.30
Betatron Tune – V	5.20	5.20
Momentum Compaction	1.969×10^{-3}	2.091×10^{-3}
Natural Chromaticity – H	-30.77	-28.33
Natural Chromaticity – V	-23.87	-24.47
Synchrotron Integral – 1	0.425	0.451
Synchrotron Integral – 2	0.817	0.817
Synchrotron Integral – 3	0.106	0.106
Synchrotron Integral – 4	-0.289	-0.306
Synchrotron Integral – 5	0.00132	0.000593
Damping Partition – H	1.354	1.375
Damping Partition – V	1.000	1.000
Damping Partition – E	1.646	1.625
Radiation Loss	932.2 keV	932.2 keV
Natural Energy Spread	1.021×10^{-3}	1.028×10^{-3}
Natural Emittance	15.81 nm rad	6.98 nm rad
Radiation Damping – H	3.428 msec	3.373 msec
Radiation Damping – V	4.641 msec	4.637 msec
Radiation Damping – E	2.819 msec	2.853 msec
Rms Hor. Beam Size – Straights	389 microns	340 microns
Rms Vert. Beam Size – Straight	19.7 microns	13 microns
Rms Hor Divergence	40.8 μrads	20.5 μrads
Rms Vert Divergence	8.0 μrads	5.3 μrads

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[1] J. W. Boldeman, The Australian Synchrotron Light Source, 8th European Particle Accelerator Conference, EPAC 2002, Paris, June 2002, page 650.

[2] J. W. Boldeman and D. Einfeld, The Physics Design of the Australian Synchrotron Storage Ring – Boomerang, NIM, (2003) in press.

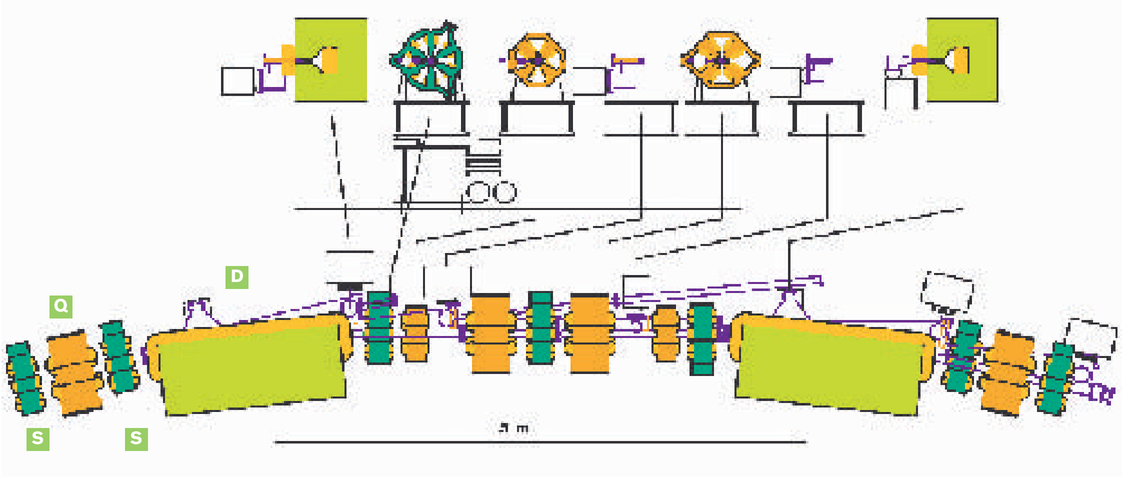

Figure 1. One superperiod of the Boomerang lattice, D – light background dipoles, Q – dark background quadrupoles and S – semi-dark background sextupoles.

Following wide scale consultation both nationally and internationally, the design objectives for the Australian Synchrotron were as follows:

- an energy of 3 GeV to provide high performance in the x-ray energy range, 100 eV to approximately 65 keV
- that it should be competitive with other third generation compact facilities under construction
- that it should have adequate beam line and experimental stations to satisfy 95% of the research requirements of an expected Australian community of 1,200 different researchers
- provide internationally competitive performance for essentially all Australian industry requirements.

It is believed that these objectives have been achieved. A key measure of the performance of this lattice is provided by either the brightness curves for undulators or flux curves for wigglers. The brightness for a 22 mm in-vacuum undulator is presented in figure 2.

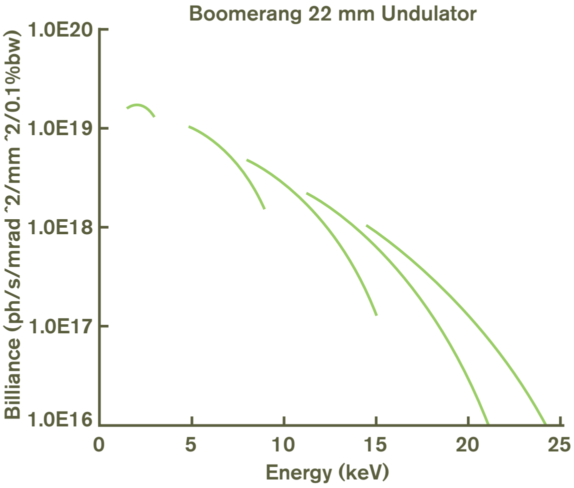

Figure 2. Brightness curves for a 22 mm period undulator in the Boomerang Storage Ring. Distributed dispersion $\eta = 0.24$ *m.*

APPENDIX 3. Recent events providing information on synchrotron applications

Date	Event	Venue
2002		
March	IATICE Italian Australian Technological Innovations Conference & Exhibition	Melbourne
July	Australian Institute of Physics National Conference	Sydney
August	AusBiotech 2002 national conference	Melbourne
September	Joint meeting of Australian Institute of Physics (SA branch) and Australian Institute of Biology	University of Adelaide
October	The Australian Synchrotron: New Opportunities for Soil and Environmental Science	Melbourne
October	Monash Research Cluster for BioMedicine Research Linkage Seminar	
November	ClubBio	Coolum, Queensland
November	Royal Australian Chemical Institute (RACI), Victorian Branch AGM	Melbourne
November	Materials and Packaging Challenges for Micro Nano Technology	Melbourne
November	Commercialise 2002	Melbourne
December	The Small Technology Revolution: Biotechnology meets micro nano technology	Melbourne
2003		
January	Australian Synchrotron: A workshop for potential users	Melbourne
February	Italian–Australian workshop: Future directions in spectroscopy & imaging with SR	Lorne, Victoria
February	RACI Inorganic conference (IC-03)	Melbourne
February	27th Annual Condensed Matter and Materials Meeting	Wagga Wagga, NSW
February	Bioactive Discovery in the New Millennium	Lorne, Victoria
February	Australian Microbeam Analysis Society Symposium	Melbourne
February	Presentation to Alfred Hospital	Melbourne
March	Royal Society of Victoria	Melbourne
March	Biotechnology applications seminar at Monash	Melbourne
April	Victorian Institute of Animal Science seminar	Melbourne
April	Polymer Microfabrication for Bio- and Nano-technology Applications	Melbourne
May	Department of Primary Industries forum	Melbourne
May	Mineralogy Society of Victoria	Melbourne
May	Department of Primary Industries forum	Horsham, Victoria
May	CRCs Connecting Communities: Meeting National Research Priorities	Canberra
June	Department of Primary Industries workshop	Melbourne
June	Deakin University, Department Ecology & Environment	Geelong
June	Department of Primary Industries workshop	Knoxfield, Victoria
June	Bio 2003	USA
June	Department of Primary Industries workshop	Melbourne
June	International Workshop on Non-crystallographic Phase Retrieval	Cairns
July	International Seminar on X-ray Imaging	Melbourne
July	Synchrotron Radiation Beamlines: An Optical Engineering Perspective	Melbourne
July	5th International Congress on Industrial and Applied Mathematics	Sydney
August	International Crystallography Meetings	Broome
August	AusBiotech 2003 national conference	Adelaide
August	4th Revolution: Bio Micro Nano Technology	Melbourne
August	Australian Synchrotron Clinical Applications Workshop	Melbourne
September	New Zealand Users' Workshop	Auckland, NZ
September	Australian Institute of Physics – Vic branch	Melbourne
September	5th Australian Conference on Vibrational Spectroscopy	Melbourne
October	Materials 2003 conference	Sydney
October	Society of Economic Geologists/Monash Ore Deposits Research Exploration Group mini-symposium	Melbourne
October	Forum on the Application of Synchrotron Radiation in Photonics and Related Industries	Melbourne
October	Western Australian seminar for potential users	Perth
November	Australian Nuclear Association conference	Canberra
November	Applications Forum in collaboration with Minerals and Surface Science Group, La Trobe University	Melbourne
November	Workshop for Minerals Sector in collaboration with AMIRA	Adelaide
November	Institution of Engineers Aust (Vic), Electrical Division	Melbourne
November	13th AINSE Conference (Nuclear Techniques of Analysis & 8th Vacuum Society of Australia Congress)	Sydney
2004		
January	Synchrotron Summer School: Photons @ Work	Canberra
February	Australian Conference on Microscopy and Microanalysis 18 (ACMM18)	Geelong
February	Membrane Protein Structure Workshop (associated with Lorne Protein Conference)	Lorne, Victoria
February	Australian Geological Convention	Hobart

Abbreviations and acronyms

Å	angstrom
ADFA	Australian Defence Force Academy
AES	Auger electron spectroscopy
AINSE	Australian Institute of Nuclear Science and Engineering (now ANSTO)
ALS	Advanced Light Source, Berkeley, USA
AMD	acid mine drainage
AMIRA	Australian Mineral Industry Research Association
AMRFP	Access to Major Research Facilities Program
ANBF	Australian National Beamline Facility
ANSTO	Australian Nuclear Science and Technology Organisation
APECS	Auger photoemission coincidence spectroscopy
APS	Advanced Photon Source, Chicago, USA
ARC	Australian Research Council
ARUPS	Angular resolved ultraviolet photoelectron spectroscopy
ASRP	Australian Synchrotron Research Program
BESSY	Berliner Elektronenspeicherring-Gesellschaft für Synchrotron Strahlung m. b. H. (Berlin electron storage ring company for synchrotron radiation), Berlin, Germany
CD	circular dichroism
CLS	Canadian Light Source, Saskatoon, Canada
CMR	colossal magneto-resistance
CRC	Cooperative Research Centre
CSES	Centre for Strategic Economic Studies
CSIRO	Commonwealth Scientific and Industrial Research Organisation
CT	computed tomography
CVD	chemical vapour deposition
Diamond	Diamond synchrotron light source, Chilton, UK
DSTO	Defence, Science and Technology Organisation
Elettra	Elettra Sincrotrone, Trieste, Italy
EPR	electron paramagnetic resonance
ESRF	European Synchrotron Radiation Facility, Grenoble, France
eV	electron volt
EXAFS	extended x-ray absorption fine structure
FTIR	Fourier Transform Infrared spectroscopy
GeV	giga electron volts
HARMST	high aspect ratio micro systems
ID	insertion device
IMAC	International Machine Advisory Committee
IP	intellectual property
IR	infrared
ISAC	International Scientific Advisory Committee
KB	Kirkpatrick-Baez (mirror)
keV	kilo electron volts
LICR	Ludwig Institute for Cancer Research
LIGA	x-ray lithography, electroforming (German: Galvanoformung) and moulding (German: Abformung)
LINAC	linear accelerator
MAD	multiple wavelength anomalous dispersion
MEMS	micro-electro-mechanical system/s
µ	micron
MNRF	Major National Research Facilities
MPW	multipole wiggler
mrad	milliradians
MRT	microbeam radiation therapy
MXCD	magnetic x-ray circular dichroism
NEXAFS	near edge x-ray absorption fine structure
NHMRC	National Health and Medical Research Council
nm	nanometre
NMR	nuclear magnetic resonance
nmrad	nanometre radians
NRA	nuclear reaction analysis
NSAC	National Scientific Advisory Committee
NSLS	National Synchrotron Light Source, Brookhaven, USA

NSRRC	National Synchrotron Radiation Research Centre, Hsinchu, Taiwan
PAT	photon activation therapy
PD	powder diffraction
PDF	pair distribution function
PEEM	photoelectron emission microscopy
PIXE	particle induced x-ray emission
PMT	Photomultiplier tubes
PX	protein crystallography
SAXS	small angle x-ray scattering
SLS	Swiss Light Source, Villigen, Switzerland
SPEAR 3	new storage ring under construction at SSRL, a division of Stanford Linear Accelerator Center, Stanford University, Menlo Park, USA
SPring-8	an acronym for ‘Super Photon ring – 8GeV’, Japan, the world’s largest and most powerful synchrotron facility
SR	synchrotron radiation
SRCD	synchrotron radiation circular dichroism
SRIR	synchrotron radiation infrared
SRIXE	synchrotron radiation induced x-ray emission
SRS	Synchrotron Radiation Source, Daresbury, UK
SSRL	Stanford Synchrotron Radiation Laboratory, Menlo Park, USA
Third generation	a synchrotron light source with insertion devices for higher intensity
THz	terahertz
UHV	ultra high vacuum
USAXS	ultra small angle x-ray scattering
UV	ultraviolet
VUV	vacuum ultraviolet light
WAXS	wide angle x-ray scattering
WEHI	Walter and Eliza Hall Institute for Medical Research
XAES	x-ray excited Auger electron spectroscopy
XAFS	x-ray absorption fine structure
XANES	x-ray absorption near edge structure
XAS	x-ray absorption spectroscopy
XES	x-ray emission spectroscopy
XPEEM	x-ray photoelectron emission microscopy
XPS	x-ray photoelectron spectroscopy
XRD	x-ray diffraction
XRF	x-ray fluorescence

Index

Proposed Initial Suite of Beamlines

Beamlines 1 & 2:	Crystallography of macro- and small molecules
Beamline 3:	Powder diffraction
Beamline 4:	Small and wide angle scattering
Beamline 5:	X-ray absorption spectroscopy
Beamline 6:	Soft x-ray spectroscopy
Beamline 7:	Vacuum ultraviolet spectroscopy
Beamline 8:	Infrared spectroscopy
Beamline 9:	Microspectroscopy
Beamline 10:	Imaging and medical therapy
Beamline 11:	Microdiffraction and fluorescence probe
Beamline 12:	Circular dichroism
Beamline 13:	Lithography

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