AUSTRALIAN SYNCHROTRON

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NATIONAL RESEARCH PRIORITIES

Australian synchrotron

Scheduled to open in 2007, the Australian Synchrotron will dramatically increase the nation's access to techniques essential for globally competitive science.

Very few Australian facilities have equal potential to contribute across all national research priorities. This national platform for leading edge research will support the enabling sciences and key technologies of the future. The Australian Synchrotron will deliver better results faster, across the spectrum of Australian research. Structural and cellular biology, biosystems, nanotechnology, advanced materials and environmental sciences—and their innovative applications in many areas of national significance—will benefit from this new national asset.

The Australian Synchrotron will improve Australia's ability to benefit from the intellectual property developed by the national research community. Its versatility will promote formation of the multidisciplinary teams that are increasingly important to modern research. It will cater for experienced users, as well as training new users to realise the facility's potential to contribute to their particular research objectives.

Since 1996, Australian access to overseas synchrotrons has been facilitated through the federally funded Australian Synchrotron Research Program. This has made it possible for Australians to conduct valuable research and to enhance their expertise and international standing. But demand is growing, and inherently inefficient suitcase science can no longer satisfy the growing need for synchrotron access. Disadvantages include difficulties with protecting intellectual property, transporting fragile samples, customs barriers and adjusting project requirements to fit in with the long lead times required for access.

The range of techniques to be made available at the Australian Synchrotron will complement many advanced analytical capabilities, such as the neutron beam techniques provided by ANSTO's new research reactor in Sydney.

"With the commissioning of new world-class photon and neutron sources in Melbourne and Sydney respectively, the next few years will be incredibly exciting for Australian scientists. Not previously available at this level, except by travelling overseas, these tools will completely revolutionise the study of materials, including those of biological origin, in the coming decade. They will enable Australia to compete effectively with researchers in the strongest northern hemisphere countries."

Prof. Rob Robinson, Head, Bragg Institute, ANSTO

"It will be a crucial tool, for decades to come, in making the scientific breakthroughs we need to keep Australia's economy growing.

It is a 'must-have' facility, and will greatly assist the Australian research community and industry to deliver on the Federal Government's National Research Priorities"

Geoff Garrett, Chief Executive Officer, CSIRO

Courtesy: Peter Bennett
Photographer

Australia's national research priorities

Announced by the Australian Government in 2002, Australia's multidisciplinary national research priorities reflect the social, economic and environmental values and aspirations of the nation and its people. They address areas of strength, opportunity or need in Australian research and are supported by more specific goals devised by national funding bodies and key research agencies.

The four national research priorities are:

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

The Australian Synchrotron will strengthen the nation's capabilities and achievements across all national research priorities as well as providing an enabling platform for industry-specific research and development of new technologies.

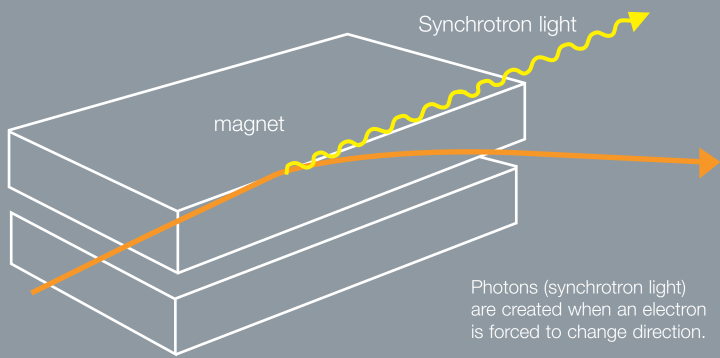
It will also strengthen Australia's international science relationships and opportunities for collaboration, particularly in South East Asia and around the Pacific Rim. The Australian Synchrotron will complement the capabilities of lower-energy synchrotron facilities in Singapore, Thailand, China and Taiwan. The Australian synchrotron community has already established close ties with facilities in the US, Japan, Europe, Taiwan and Canada, and with NZ scientists.

This publication

This publication highlights the many ways in which synchrotron techniques will expand the nation's research horizons and contribute to social, economic and environmental benefits for all Australians. Many of the synchrotron techniques featured in the following sections are relevant to more than one national research priority.

What is a Synchrotron?

In a synchrotron, electrons moving at velocities close to the speed of light are forced to change direction under the action of a magnetic field. This change in momentum causes the electrons to emit electromagnetic radiation (synchrotron light).



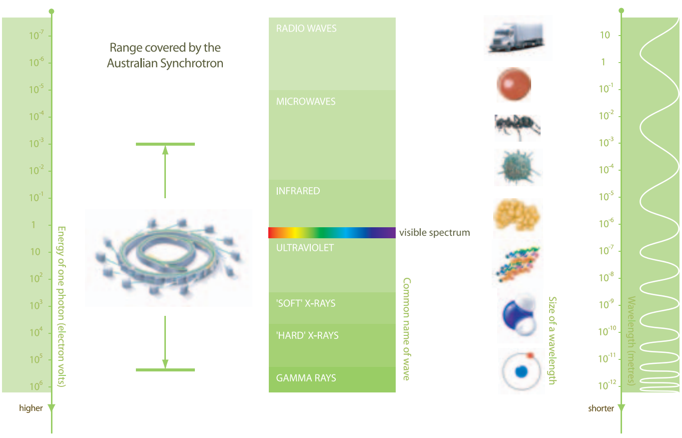
Features of Synchrotron Light

The combined properties of synchrotron light make it a unique and significant enhancement over conventional photon sources.

- **Continuous, wide spectrum—**from deep infrared to hard x-rays, enabling a wide range of experimental techniques.
- **Tuneable—**a single wavelength or narrow wavelength range can be selected using monochromators. By tuning the wavelength, particular elements can be detected or ignored, and energies can be scanned to obtain information about the chemical state of a particular element.
- **Extremely intense—**Synchrotron light is hundreds of thousands of times brighter than EMR from conventional sources, enabling rapid acquisition of data from small samples. Measurements can be collected over a wide wavelength range in short times (milliseconds) enabling time-resolved studies of processes and reactions.
- **Highly collimated—**the rays are almost parallel and can be collimated or focussed, resulting in a small spot size (ranging from less than a micron to several mm) and high signal to noise ratio. This feature is particularly important for crystallography applications, where structures from biological macromolecules and complex advanced materials can be analysed with high resolution.
- **Polarised—**can be linear, circular or elliptical, revealing the shape of complex molecules, especially proteins and the properties of magnetic materials.
- **Pulsed—**the light is emitted in very short pulses (typically less than a nano-second), enabling the measurement of very fast molecular processes.
- **Non-destructive—**synchrotron analysis does not necessarily alter or destroy a sample, making it particularly useful for analysis of forensic and other high value samples.

Synchrotron measurements enable characterisation across scales, ranging from life-size imaging down to nano-, molecular and atomic structures.

The key advantage of a synchrotron is that it delivers much better results much faster than conventional facilities.



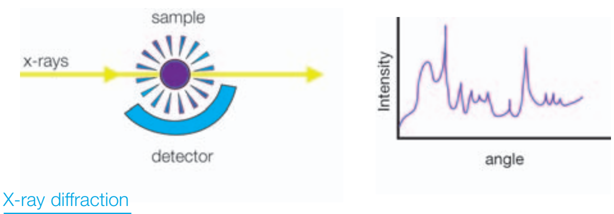
Electromagnetic spectrum

Diffraction/scattering

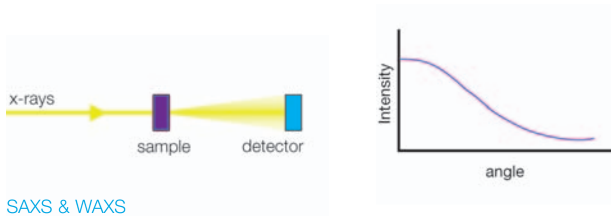
X-ray diffraction (XRD) is the most widely used method for 'imaging' substances at atomic resolution and determining their structures with a high degree of resolution. The technique uses the patterns produced when x-rays are scattered from regular crystal structures. **Powder diffraction (PD)** techniques are used when diffraction-quality single crystals cannot be obtained.

The brightness and tunability of synchrotron radiation enables high-throughput structure determination, which is essential for molecular biology research. For example, structural proteomics uses protein crystallography to systematically determine the 3D structures of large numbers of proteins. Other synchrotron techniques (circular dichroism and infrared spectrographic imaging) can then be used to study molecular mechanisms and ligand-binding properties at atomic resolution.

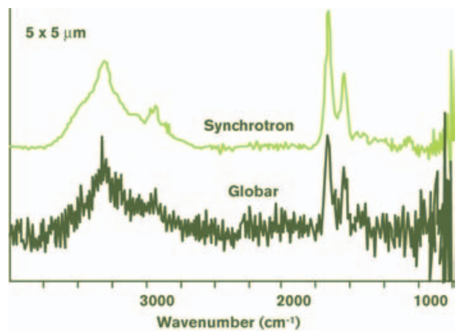
Small angle x-ray scattering (SAXS) detects x-rays that are elastically scattered from a sample at a small angle relative to the original direction of the x-ray beam. It provides information on the size and shape of relatively large structures such as polymers, proteins, colloids, emulsions and living organisms. **Wide angle x-ray scattering (WAXS)** yields structural information on a scale comparable to standard XRD techniques. The information obtained from SAXS and WAXS complements data from x-ray crystallography, NMR and microscopy techniques.



X-ray diffraction



SAXS & WAXS



IR spectra

Comparison of IR spectra obtained from the same sample using a conventional globar-based instrument (black) and a synchrotron IR beamline (green). The signal to noise ratio is substantially improved due to the greater stability of the synchrotron source.

Spectroscopy

X-ray absorption spectroscopy (XAS) techniques collect information about energy emissions and electron excitations initiated by the absorption of x-ray energy.

A well-established quantitative analytical technique used in research and industry applications, XAS provides atomic-scale information about a wide range of liquid and solid systems. Because it probes short and medium-range order and can measure disordered samples, it is complementary to XRD.

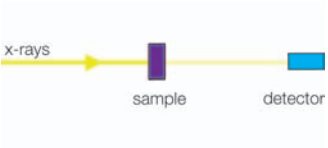
XANES provides information about the oxidation state (speciation) and coordination chemistry of a particular element, while **EXAFS** provides information on nearest neighbour distances and ligating atoms.

X-ray photoelectron spectroscopy (XPS) is an important and versatile technique for the chemical characterisation of surfaces. Synchrotron XPS offers the additional ability to vary the analysis depth from as little as two atomic layers, making it possible to obtain a non-destructive chemical depth profile.

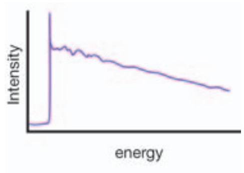
Synchrotron-based **infrared (IR) spectroscopy** and **microscopy** offer significant advantages over measurements using a conventional source in terms of data quality and spatial resolution, including the ability to resolve spatial details down to the diffraction limit of 5-10 microns.

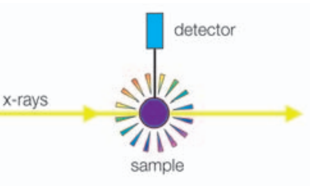
Synchrotron techniques such as **x-ray fluorescence (XRF)** are particularly useful for forensic analysis of tiny samples because they are non-destructive and the small beam size makes it possible to determine the distribution of metals within a small sample

For trace element analysis, **XRF** or **x-ray emission spectroscopy (XES)** offer better detection limits than conventional techniques. The technique also offers simultaneous determination of multiple elements.

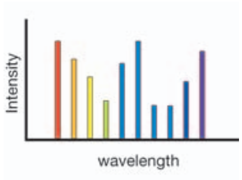


X-ray Absorption Spectroscopy





Fluorescence

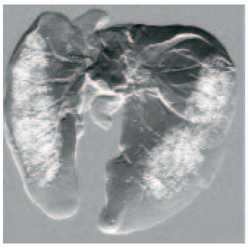


Imaging techniques

Conventional x-ray images rely on the fact that different substances absorb x-rays to different degrees depending on composition, thickness or density.

Pioneering work at the University of Melbourne, CSIRO, Monash University and several synchrotron laboratories has led to the development of **phase-contrast x-ray imaging** techniques that dramatically improve the contrast and detail obtainable for tissue samples (eg. lung, heart, breast).

Imaging

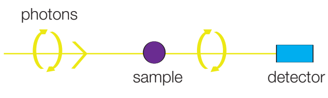


Micromachining

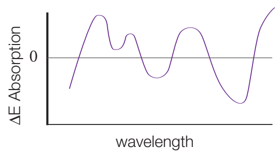
Synchrotron **lithography** is used for manufacturing nano- and micro-devices with very high depth to width ratio and excellent surface finish.

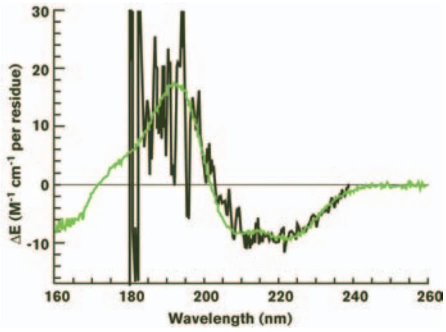
Polarimetry

Circular Dichroism (CD) is a widely used technique for measuring the secondary structure (shape and chain folding) of complex molecules. Thin films, bulk materials and the interfaces between thin films can be analysed. Structural, functional and dynamics information about protein folding and conformation from synchrotron polarimetry complements data from protein crystallography, NMR and small angle x-ray scattering.



Polarimetry





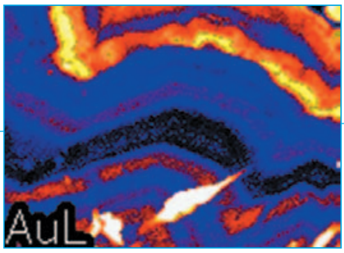
CD spectra

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: GR Jones and DT Clarke, SRS, Daresbury, UK.

National research priority goals in this area are:

1. water – a critical resource
2. transforming existing industries
3. overcoming soil loss, salinity and acidity
4. reducing and capturing emissions in transport and energy generation
5. sustainable use of Australia's biodiversity
6. developing deep earth resources
7. responding to climate change and variability.

Synchrotron-enhanced capability	Recent research
X-ray imaging of solid and liquid phase interactions, animal tissues, geostructures **Goals:** 1, 2, 4, 6	- water movement through the root zone of plants to develop more water efficient crops - bone density and animal health - characterisation of CO_2 sequestration performance - oil release rates from reservoirs
XRD and XAS of hydrated mineral phases, metal sulfides, gas–liquid reactions and catalytic processes **Goals:** 1, 2, 4	- transformations by bacteria to inhibit acid mine drainage - performance of potential CO_2 sequestration systems in saline solutions - potential improvements in automotive emission control catalysts and catalytic converters - interactions of wastewater in clays
SAXS of flocculation processes **Goal:** 1	- dewatering of mine slurries - oil release rates from reservoirs
XAS of heavy metals, hetero-atoms and trace elements **Goals:** 1, 2, 4, 7	- speciation of toxic minerals in groundwater and soils - uptake of minerals from fertiliser formats - investigation of coal combustion
PX of proteins from insects and plants **Goals:** 2, 3	- proteins critical to insect physiology to develop new or improved insecticides - transport proteins in plant roots for salt resistance
IR microscopy of plant cell wall components **Goal:** 2	- lignin, cellulose and lipid distribution to improve animal feeds
Microprobe analysis of elemental distribution and local chemistry **Goals:** 2, 3, 5, 6, 7	- origins of airborne pollutants - bio-accumulation by plants of high value or waste metals - mineral sands processing - uptake of toxic metals by plants, and identify tolerant plant species - localised elemental distributions of contaminants in turtle shells - localised phases of otoliths in fish[1] - fluid inclusions in rocks to improve minerals exploration success rates - phase changes in corals over time associated with temperature variations



Gold AuL

XRF mapping of gold using L-edge x-ray emission

Stackhousia tryonii Bailey

Synchrotron XRF map of a floret of a native Australian nickel hyperaccumulating herb. Red = calcium, blue = nickel green = manganese distributions within the specimen.

Courtesy: Dr Naveen Bhatia (ASRP Fellow, ANSTO) (2005)

"Synchrotrons provide new tools with great potential for in vivo investigations of elements in biological materials and their likely chemical form (speciation). The Australian Synchrotron will be of great importance in helping us to find ways of using plants to remediate environmental damage caused by past mining activities—and to enhance the biological extraction of metals from low-grade ores uneconomical to process by chemical means."

Prof Alan J Baker, School of Botany, University of Melbourne

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

Australia's natural resource-based industries are major contributors to the economy, but must be managed on a sustainable basis. The synchrotron will contribute to the evolution of an environmentally sustainable Australia by enabling:

- research into the fundamental chemical, physical, biological and geological characteristics of the nation's agricultural and mining systems and natural environments;
- better understanding for management of major issues such as water usage, air pollution, climate change, land degradation, industrial site remediation, waste management, and utilisation of deep earth resources;
- improved energy technologies and advanced fuels;
- advances in knowledge to inform the management of natural resources and native biodiversity.

OUTCOMES

Examples of synchrotron capabilities for Australian research

Soil–root interactions

Synchrotron imaging techniques will provide major insights into the soil–root interactions that occur in Australia's complex and often fragile agricultural soils. A research team led by Dr Peter Fisher from the Victorian Department of Primary Industries is conducting a series of innovative proof-of-concept experiments to test the value of synchrotron techniques in this area. If successful, the work could be extended to investigate the different root mechanisms employed by agricultural crops and native plants in hostile conditions. Synchrotrons could also assist the development of crop models that can more accurately predict water and nutrient use efficiency and the design of better subsurface irrigation techniques.

Soil contamination from groundwater

Dr Peter Kappen and colleagues from La Trobe University and Environmental Resources Management Australia are using XAS to study chromium species in contaminated soils. Cr contamination problems can arise as a result of previous industrial practices.[2] The problem is usually addressed by adding a reductant to the soil to transform highly toxic and soluble Cr(VI) into relatively insoluble and non-toxic Cr(III).

Results show how soil takes up Cr from contaminated water. The next step will be to monitor the Cr speciation during remediation treatment. The work will assist the development of more efficient remediation strategies.

Effects of climate change on corals

The Australian Institute for Marine Sciences, Townsville, wants to assess the proxy climate and environmental information that is stored in coral skeletons as growth characteristics (e.g. skeletal extension, density and calcification), through synchrotron microprobe analysis of the geochemical tracers that become incorporated into the skeleton during growth. From such data, sea-surface temperatures, river flow, rainfall, upwelling, salinity and anthropogenic influences can be inferred.

Fertiliser uptake in soils

Australian farmers spend more than $1.6 billion on phosphorus fertilisers a year, but soils that are highly alkaline or acidic can rapidly change fertiliser phosphorus into forms that are not readily accessible by plants. More efficient use of phosphorus fertilisers would save farmers money as well as reducing the potential for phosphorus runoff to affect rivers and lakes adversely.

Dr Enzo Lombi, CSIRO, the South Australian Research and Development Institute, and Dr Roger Armstrong of the Victorian Department of Primary Industries are using synchrotron micro-XRF and micro-XANES to conduct in-situ studies of the fundamental processes that control the availability of fertiliser phosphorus. Results so far have confirmed the team's assumptions and provided additional mechanistic insights. The findings will help to determine whether granular or fluid fertilisers are the best option for particular soil conditions.[3]

Bio-remediation

Plants that can survive and thrive in metal-contaminated soils could contribute to simple and sustainable new technologies for cleaning up polluted environments.

Since the mid-1990s, Prof Alan Baker and University of Melbourne botanists have used EXAFS and micro-PIXE techniques to improve their understanding of the physiological mechanisms plants use to take up, accumulate and localise heavy metals from contaminated soils.

By using synchrotron techniques, researchers can investigate living materials and avoid complex preparative procedures that can disrupt the integrity of in vivo systems and change the ionic form and environment of elements in plant cells.[4]

Air pollution particulate characterisation

ANSTO researcher Dr David Cohen and colleagues are using microbe XRF to characterise particles contributing to air pollution in the Sydney basin and accurately identify the sources from nature or industry. Once the sources are identified, steps can be taken to reduce the problem.[5]

Towards sustainability with hydrogen fuels

We stand at the threshold of a technological revolution driven by hydrogen as an energy carrier and the need for a truly sustainable chemicals and fuel industry. Success will depend on developing novel processes for catalysis and for hydrogen generation/reversible storage, based on a molecular understanding of materials, reactions, catalysts and processes. Federation Fellow Prof Thomas Maschmeyer, Sydney University, uses a range of sychrotron techniques to perform real time, *in-situ* studies of these reactions.[6]

Gold exploration research

Synchrotron studies by Dr Andrew Wilde and his colleagues at the CRC for Predictive Mineral Discovery, CSIRO and Monash University are contributing to a better understanding of the high-temperature, high-pressure geological processes that led to the formation of valuable metal ores. Their research is focused on fluid inclusions trapped during crystallisation of minerals such as quartz, often associated with gold.[7,8]

National research priority goals in this area are:

1. a healthy start to life
2. ageing well, ageing productively
3. preventive healthcare
4. strengthening Australia's social and economic fabric.

Synchrotron-enhanced capability	Recent research
PX of enzymes, diseases and immune responses **Goals:** 1, 2	- Investigating dysfunctional enzymes to understand molecular mechanisms and design new drugs - Malarial proteins involved in red blood cell ingress to develop drugs that block activity - Macrophage proteins in mice to understand inflammation processes - Growth factors in cancer growth to develop strategies to block activity - Characterisation of "immunological synapse"
High resolution x-ray imaging of biological samples and physiological processes in real time **Goals:** 1, 2	- Lung function during treatment to achieve improved asthma treatments - Fluid movement in neonatal lungs to improve clinical practice options for neonatal care - Lung development in wallabies to identify milk proteins associated with development - Porosity of bone to quantify levels of osteoporosis - Tumours with low contrast for enhanced mammography - Angiography methods using contrast agents to improve diagnosis - Low dose images in longitudinal studies of animal models to improve diagnosis
IR of tissue samples **Goal:** 2	- Abnormal tissues to improve screening techniques for cervical cancer
Microprobe analysis of heavy metals and metal containing moities **Goals:** 1, 2	- Arsenic uptake into hair and nails of children to monitor deportment of environmental contaminants - Platinum- and cobalt-containing anti-cancer drugs to provide improved drug products through selective activation
Radiotherapy of tumours **Goal:** 2	- Novel cancer treatment methods (such as microbeam radiotherapy and photon activation therapy)
SAXS of biological reactions in-vitro **Goal:** 2	- Protein kinase reactions to understand regulation of many cellular processes, including in disease states - Proteins in solution and their interactions with other biological components, e.g. lipids
XAS of metal containing moieties **Goal:** 2	- Copper-containing anti-inflammatory drugs to verify stability of formulations
XRD of pathology specimens, bio-ceramic materials, drug formulations and molecular conformational changes **Goal:** 2	- Calcification of heart valves to identify failure modes - Materials for durable and bio-compatible prosthetics and implants - Pharmaco-kinetics in real time to characterise solubility and bio-availability - demonstration of purity and quality of drug formulations
X-ray imaging and mapping of cell growth and dynamics **Goal:** 2	- Scaffolds for burns treatment to improve healing - Nerve cell regrowth using biopolymers to treat spinal injuries
CD of secondary structure of proteins in biological systems **Goal:** 2	- Prion diseases (eg: Alzheimers) to characterise progress of disease pathology
CD and SAXS of biologically active molecules **Goal:** 2	- Investigating molecular conformation and shape to provide comparisons to standards

"Without good ongoing access to synchrotrons, Australian pharmacologists may get left behind in the field of rational drug design."

Dr Denis Wade AM, former managing director of Johnson & Johnson Research

Promoting good health and well being for all Australians

Most Australians expect to live long and healthy lives, thanks to world-class standards of nutrition, hygiene and medical care. Further improvements in life expectancy, health and productivity will require attention to the needs of children, older Australians and those at risk of particular ailments or injuries as a result of their social, economic, environmental or genetic circumstances. Improving the health of the Australian population will enhance the nation's productive capacity as well as helping families and individuals to live healthy and fulfilling lives.

In the areas of health and medicine, synchrotrons are essential tools for rational drug design, biological research, biotechnology, structural proteomics, food science and medical imaging, as well as showing exciting potential for innovative medical therapy applications.

OUTCOMES

Examples of synchrotron capabilities for Australian research

Natural lung surfactants

A group led by Assoc Prof Dr Ian Gentle, University of Queensland, is studying natural and synthetic protein components of natural lung surfactant, hoping to understand its action at the air/water interface that exists in the alveoli. One component, known as SP-B, is known to be essential to lung function, and this material is the focus of the work. It works in combination with other proteins and lipids, making the system complex. The team has used SAXS and synchrotron x-ray reflectometry to reveal the subtle conformational changes undergone by SP-B at the air/water interface upon compression.

Biological processes—protein kinases

Dr Jill Trewhella, a Federation Fellow based at Sydney University, is studying the global structures of large biological molecules in solution. Her aim is to investigate how these molecules work together to regulate key cellular processes that underpin specific biological responses such as a muscle twitch, particularly focusing on kinases, enzymes that modify the actions of other proteins by attaching or detaching phosphate groups.

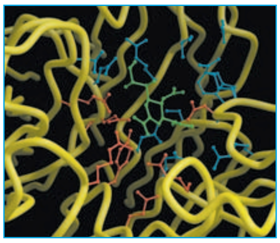
Trewhella's findings will contribute to human health through a better knowledge of the cellular processes that underpin healthy biological functioning or are implicated in disease states.[9,10]

Therapeutics for chronic inflammatory diseases

Chronic inflammatory diseases represent one of the greatest health problems in the developed world, and macrophages play a central role in the inflammation process. Researchers from the University of Queensland are investigating macrophage proteins from mice. They want to develop a better understanding of the inflammation process in arthritis and other chronic inflammatory diseases and to identify targets for the development of new anti-inflammatory therapeutics.

Assoc Prof Jenny Martin and her colleagues have established a bacterial expression system to screen hundreds of proteins to identify those that are suitable for structural studies. Proteins that express well in the small-scale bacterial system are then produced in large scale and evaluated further by structural techniques.[11,12]

Rational drug design—influenza

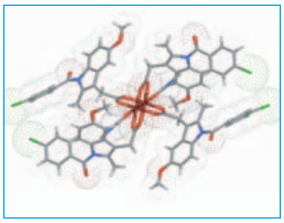


Relenza

The ability of synchrotron x-rays to reveal the detailed structures of biological proteins and their interactions has enabled researchers to develop a new approach to drug discovery. Rational drug design identifies opportunities to block or modify molecular interactions.

The anti-influenza drug Relenza™ is the world's first structure-based anti-viral drug and an early example of rationally based drug design methodologies. Relenza™ was developed in the mid-1990s by a CSIRO team led by Peter Colman and Jose Varghese. Colman and Varghese used synchrotron XRD to create a high resolution picture of the neuraminidase protein on the virus surface.[13,14]

Non-steroidal Cu anti-inflammatories



Copper Indomethacin

Technology from Sydney University with Biochemical Veterinary Research/Nature Vet and the University of Western Sydney involves new non-steroidal anti-inflammatory formulations that use copper complexation to minimise side-effects caused by the active ingredient, indomethacin. The researchers, led by Prof Peter Lay, significantly improved the copper-indomethacin formulations after using synchrotron techniques to determine the core structure and stability in formulations and investigate its transformation in cells. XAS data were collected on Cu Indo complexes. One complex was subsequently used in new formulations although crystals could not be obtained for XRD structure determination. The structure was therefore determined by XAFS analyses, validated against the structure of related Cu complexes for which the XRD structure was known.[15]

Cervical cancer screening techniques

Dr Don McNaughton from Monash University is using IR spectroscopy to investigate abnormal tissue samples to improve screening techniques for cervical cancer. Synchrotrons are a unique source of detailed information about subtle physiological changes that can herald the need for preventive treatment or major medical interventions. This detailed information is assisting the development of more accurate diagnostic tests.

Food safety, quality and nutrition

Dr Raymond Mawson and other researchers from Food Science Australia plan to use synchrotron techniques to advance their understanding of molecular food structure for a range of applications. These include managing nutrient availability, protecting and delivering 'bioactive' components in functional foods, assessing microbiological risks associated with food structures and processing and packaging surfaces, developing models and technologies for improving food texture and flavour release, and ensuring the stability of food materials during processing.

National research priority goals in this area are:

1. breakthrough science
2. frontier technologies
3. advanced materials
4. smart information use
5. promoting an innovation culture and economy.

Synchrotron-enhanced capability	Recent research
XRD of polymers, metals, biomaterials and nanomaterials. **Goals:** 2, 3	- polymer crystallisation in injection moulded parts for improvements to polymer fabrication process - magnesium samples under stress and strain for models for finite element analysis - enamel in teeth, to analyse bio-mineralisation - nanoparticles in polymer matrices for durable coatings from new composite materials - self-organisation of fullerene and carbon nano-tubes to develop manufacturing protocols for nanomaterials
High resolution x-ray imaging of metals, soft matter, high value samples and nanomaterials in time-resolved and phase-resolved studies. **Goals:** 1, 3	- cast alloy solidification for optimisation of casting processes - phase contrast techniques for new imaging methods - phase retrieval – for directly solving structures, whilst avoiding the “phase problem” - apparatus for detecting energy and location of excitation events – to develop new detector technology
X-ray lithography of high aspect ratio structures for nanometre scale devices and optical fibres. **Goals:** 1, 2	- Investigating phase contrast techniques for developing focussing techniques applicable in nanofabrications - New photonic device fabrication - Variations in refractive index induced by x-rays to develop optical fibre Bragg gratings
X-ray photoelectron spectroscopy of coatings, electron-spin dependant phenomena, valence band electronic structure and metal oxide films. **Goals:** 1, 2, 3	- Non-wetting surfaces to develop coatings for textiles and building materials - Atoms, clusters, ferromagnetic films and surfaces to develop spin electronics for potential applications in quantum computing - Super-conductors, to develop high temperature materials
XAS of materials, metal oxide films and semiconductor substrates. **Goals:** 2, 3	- Carbon, boron and nitrogen containing materials to improve performance of durable coatings for tools - Magnesium oxide for new longer-lasting batteries - Ion-induced disorder in semiconductor substrates, to understand the fabrication process as it relates to device performance
PX of target proteins. **Goal:** 2	- Antibodies, to identify suitable bio-sensor platforms for cancer
In-situ XAS and XRD of deep-earth chemistry and mineral processing. **Goal:** 1	- Extreme conditions comparable to the deep earth to improve understanding of ore genesis - In-situ measurements of simulated mineral processing operations to optimise conditions

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

Australia's world-class research capabilities put us in a strong position to maintain our place in the international research community and to derive social, economic and environmental benefits from new applications of fundamental knowledge.

Synchrotrons are essential tools in international research and Australia's synchrotron scientists are already undertaking fundamental research in many areas of frontier technology.

These include advances in ultra broadband communications (especially photonics), polymers, composite materials, ceramics, metals and alloys, bio- and nano-materials, organic and inorganic chemistry, thin film technologies and advanced manufacturing, including the production of micro-devices for industrial and medical applications.

OUTCOMES

Examples of synchrotron capabilities for Australian research

Amorphous metal nanocrystals

Dr Mark Ridgway from the ANU and international colleagues are studying the fundamental processes that govern the formation and modification of atomic-scale nanocrystalline structures. Their findings include the identification of subtle structural differences relative to bulk material and the surprising discovery that nanocrystalline metals can be rendered amorphous by ion irradiation, an established technique for modifying bulk-phase materials. The transformation to an amorphous form is impossible with bulk metals and contrary to theoretical predictions.

Amorphous metals lack long-range order and crystalline defects, so they are stronger, harder, tougher and more elastic.[16-25] Applications for such nanocrystalline-form metals include optical switches (photonics) and chemical catalysts.

Surface analysis techniques

Murdoch University's Prof Stephen Thurgate is developing a new generation of Auger photoelectron coincidence spectrometers to improve surface analysis techniques with applications in nanotechnology. As an expert in XPS, Thurgate has previously used synchrotron facilities to pioneer grazing incidence XPS, to measure very thin oxide layers on semi-conductors, in the range 20–100 Angstroms.[26]

New imaging techniques

Prof Keith Nugent, Federation Fellow at the University of Melbourne, is seeking to develop new imaging techniques to study molecules that cannot form crystals.

Nugent's group is currently analysing how x-rays scatter from molecules rather than crystals. Current work focuses on large molecules such as proteins and viruses, because only large molecules can scatter enough x-rays to be detected. Synchrotrons are the only possible source of the very intense x-rays required for the development of non-crystalline diffraction techniques. Parallel approaches are being developed using state-of-the-art electron microscopes.[27]

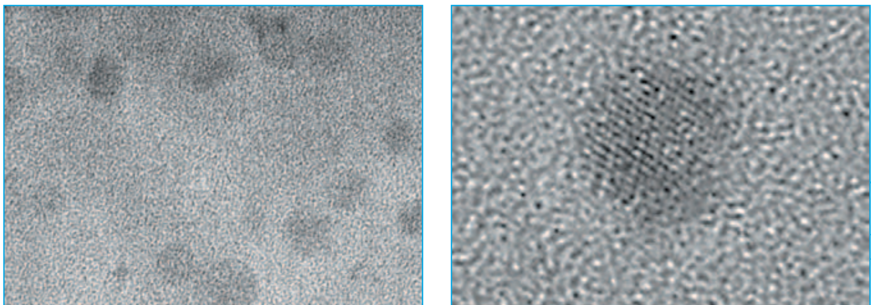
Twenty years of fundamental Australian research into x-ray imaging has led to dramatic improvements in contrast resolution and important spin-offs in medical imaging.

Electron-spin dependent research

Australian researchers are using the unique characteristics of synchrotron radiation to investigate electron-spin dependent phenomena in atoms, clusters, ferromagnetic films and surfaces. Breakthroughs in the field of spin electronics could lead to major developments in quantum computing, new artificially structured magnetic materials and transistors and the next generation of hard disc storage systems.

Structural proteomics

The task of handling and analysing vast amounts of information-rich, high-quality synchrotron data will encourage the development of sophisticated computer systems, particularly in bio-informatics for interpreting the outputs of protein crystallography. This will be essential to support Australia's growing strengths in genomics, proteomics and phenomics.



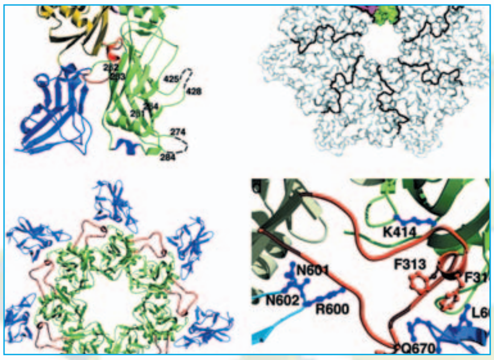
Ge nanocrystals in SiO_2 at low and high magnification, showing lattice planes within an individual nanocrystal (~8nm diameter).

Such materials can be analysed by Synchrotron measurements. Courtesy M.Ridgeway, ANU

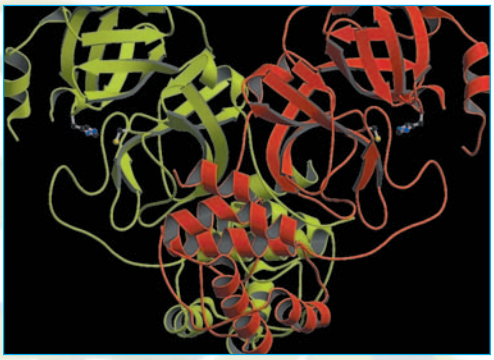
National research priority goals in this area are:

1. critical infrastructure
2. understanding our region and the world
3. protecting Australia from invasive diseases and pests
4. protecting Australia from terrorism and crime
5. transformational defence technologies.

Synchrotron-enhanced capability	Recent and proposed research
PX of target proteins **Goal:** 3	- Control of insect physiology to develop new insecticides with low spillover impact
IR, XAS and microprobe analysis of trace elements **Goal:** 4	- Better methods of analysis of small samples such as gunshot residues and explosives residues to enable convictions
X-ray imaging of bone **Goal:** 4	- Identification of bone micro-structure to discriminate species - Determination of age from image analysis
Microprobe and microscope investigation of fingerprints **Goal:** 4	- Resolution of fingerprints on difficult surfaces such as blood - Determination of layering to define sequence of events
Analysis of paints and inks **Goal:** 4	- Enhanced sensitivity to complement conventional laboratory measurements
Spatial analysis of hairs and fibres **Goal:** 4	- Longitudinal studies to follow uptake of drugs and toxins
Trace element analysis of gemstones **Goal:** 4	- Determination of provenance
XRD and XAS of new materials **Goal:** 5	- Durability of doped metal oxides in ceramic coatings to determine stability under thermal stress
X-ray lithography of micro-components **Goal:** 5	- Fabrication of in-situ condition sensors to monitor status and integrity of operational equipment



Anthrax



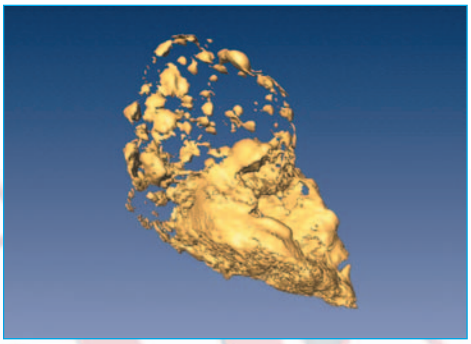
SARS

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

Recent developments such as the increased incidence of major international terrorist attacks, and the ease with which goods, services and individuals can now move from one country to another, could potentially threaten the personal safety of Australians and the security of our industries. The intensity and narrow focus of synchrotron light enables precise characterisation of tiny samples of paint, hair, skin and other substances from crime scenes and crash sites. Synchrotron methods are widely used for forensic investigations in the US, Japan and Europe.

Defence technology

The Australian Defence Science and Technology Organisation (DSTO) uses synchrotron techniques in several key areas including the development of sensor technologies and the characterisation and development of improved ceramic coating materials for aircraft engine components. DSTO has said that the new capabilities embodied in the initial suite of Australian beamlines will be of great value in their ongoing programs for monitoring the health of aircraft, ships and land vehicles and their propulsion systems, and for sensor development.



Synchrotron micro-tomography of gunshot residues

Courtesy: I. Kempson, Ian Wark Research Institute

Biological terrorism

In the international battle against biological terrorism, synchrotron techniques can quickly provide high resolution structures of the proteins involved in the biological processes of infection and proliferation of disease-causing bacteria and viruses. The detailed information contained in high resolution structures is fundamental to understanding how a particular disease organism spreads and kills, and makes an important contribution to the development of successful therapeutic treatments and vaccines. Synchrotron crystallographic techniques were used recently to solve the structure of the anthrax lethal factor, making it possible to pursue the development of anti-toxins.

Biological pandemic controls

Rational drug design is particularly important in developing effective treatments and vaccines for new infectious diseases such as SARS (severe acute respiratory syndrome) and avian influenza that can have devastating consequences if control measures are not quickly made available. Synchrotron techniques were used by Australian researchers Prof Peter Colman and colleagues, to develop the first influenza anti-viral still in use as an effective agent against avian flu.[13,14]

Forensic analysis of crime scenes

To forensic scientists, synchrotron sources are particularly useful when conventional techniques cannot offer the required sensitivity. Synchrotron techniques offer greater spatial resolution, more rapid analysis and higher sensitivity (enhanced signal to noise ratio) than is possible using conventional methods, as well as the opportunity to gather completely new information. They are also generally non-destructive, a considerable advantage when dealing with minute fragments or samples that may need to undergo other forms of analysis.

Around the world, synchrotron techniques have been used for a wide range of forensic examination tasks, including investigating drug incorporation in human hair and longitudinal analysis to reflect exposure to toxins; analysis of single ink dots on paper to detect forgery; developing fingerprint imaging techniques; trace elemental profiling of microgram quantities of drugs, arsenic compounds and car headlight glasses; and gunshot residues.[28]

Microtomography of gunshot residue particles

Synchrotron micro-tomography was used by Dr Paul Kirkbride from Forensic Science South Australia and A/Prof Bill Skinner, Dr Ian Kempson and Dr John Coumbaros at the Ian Wark Research Institute, University of South Australia, to study the morphology and composition of gunshot residues (GSR). The objective was to improve characterisation of GSR particles to relate fired particles' composition to the original unfired ingredients. This will provide a greater ability to discriminate different GSR particles and to relate them to specific types of ammunition, weapons and manufacturers.

Differences in absorption coefficient either side of the Pb L_{III} absorption edge were studied to deduce lead distributions, and revealed that in certain types of fired ammunition, Pb primarily exists in discrete, typically spheroidal volumes with a low density core, unlike Pb distribution in other ammunitions.

e-Research Centres (Virtual Labs)

The e-Research Centres or Virtual Labs are part of a proposed national access grid that will provide capacity to transfer large quantities of data into and out of national research facilities such as the Australian Synchrotron.

National Access Grid

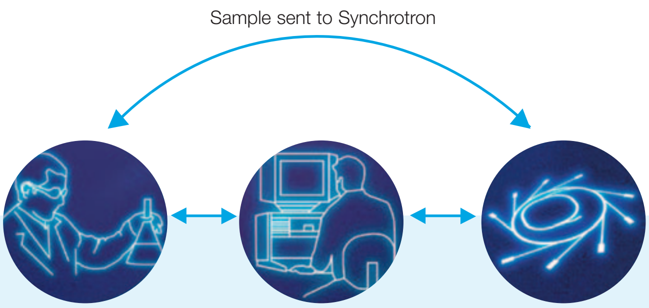
The national access grid would enable interstate researchers to communicate with staff at the Australian Synchrotron, to collect and interpret data remotely, and to collaborate in a secure and flexible manner. It will allow 'many-to-many' interactions and communications simultaneously, so that researchers from multiple sites can share and discuss data and experiments in real time.

Features of e-Research Centres

It is planned that each e-Research Centre linked to the Australian Synchrotron will provide:

- a nexus to connect secondary storage, institutional and personal storage, as part of a private high-speed network for transfer of large amounts of primary data from the Australian Synchrotron, without firewall restrictions;
- tele-presence for collaboration, training and pre-visit preparation;
- remote control of data collected at the Australian Synchrotron;
- advanced visualisation and computing resources;
- a connection point for managing data storage resources;
- data transcription without firewalls on to portable media;
- dedicated IT staff to provide user support and manage the e-Research Centre;
- a focal point for facility activities remote from the Australian Synchrotron.

Australian Synchrotron Virtual Lab



Remote Researchers

Remote researchers prepare sample and send to Synchrotron. Some team members may travel to the Australian Synchrotron to conduct the experiment on site.

External Virtual Lab

Remote researchers interact with synchrotron and participate in experiment remotely.

The Virtual Lab can:

- be assessed by multiple users
- offer future access to other research facilities
- allow "off-line" analysis of data

Australian Synchrotron (Melbourne)

Sample is loaded by operator or other research team members on site.

Access

Scientists seeking access to beam time may put their research proposals forward for peer review by an access committee. Those assessed on merit and deemed likely to advance science in their fields will be allocated beam time. Beamline funding partners will have access to a special pool of beam time (also merit based), reserved for them during the first 5 years of operation. Researchers and companies willing to pay for access will be able to buy beam time to enable rapid access and retention of intellectual property.

Industry Engagement

The Australian Synchrotron has a strong industry mandate, and has done so since the establishment of the project.

Economic Benefits

Several economic studies have provided compelling evidence of the benefits to flow from the Australian Synchrotron. The direct economic benefits come from construction, operation, cluster formation, productivity improvements and increased capture of intellectual property. Intangible economic benefits come from scientist retention and attraction, postgraduate training, international collaboration, national perception and support for Australia's competitive position.

National Industry Advisory Committee

The Australian Synchrotron has set up a National Industry Advisory Committee, chaired by Prof Denis Wade, to provide input to the development of appropriate systems for industry engagement, including intellectual property management, charging protocols, project management (including selection) and marketing strategies. This Committee sits alongside the National and International Scientific Advisory Committees.

Industry Access

Most industry users will access the Australian Synchrotron through public sector researchers. The systems at the Australian Synchrotron will facilitate such access by driving industry collaboration and brokering relationships between synchrotron users and industry participants.

Industrial Research Program

A synchrotron industry engagement program has undertaken awareness raising activities, including demonstration projects. There are many projects under way and in development, demonstrating that a proactive engagement to industry leads to programs with demonstratable value. Key industry sub-projects related to synchrotron science have been brokered, including the CRC for Biomedical Imaging Development supported by the Australian Government.

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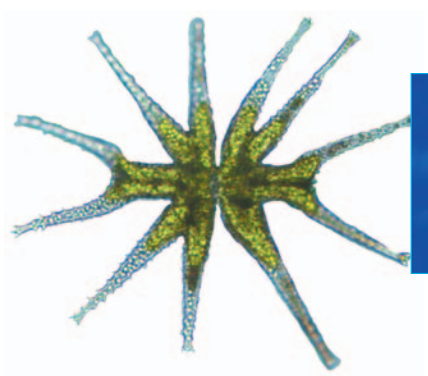
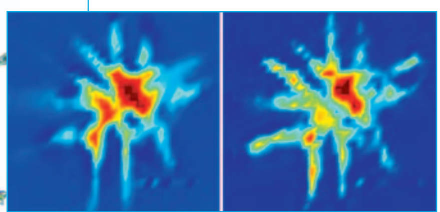
Abbreviations

EMR	electromagnetic radiation ('light')
EXAFS	extended x-ray absorption fine structure
NEXAFS	near edge x-ray absorption fine structure (also known as XANES)
NMR	nuclear magnetic resonance
PD	powder diffraction
PIXE	proton induced x-ray emission
PX	protein crystallography
SAXS	small angle x-ray scattering
SRCD	synchrotron circular dichroism
WAXS	wide angle x-ray scattering
XAFS	x-ray absorption fine structure
XANES	x-ray absorption near edge structure (also known as NEXAFS)
XAS	x-ray absorption spectroscopy
XPEEM	x-ray photoelectron emission spectroscopy
XPS	x-ray photoelectron spectroscopy
XRCD	x-ray circular dichroism
XRD	x-ray diffraction
XRF	x-ray fluorescence





Micrasteria

Micrograph of Micrasterias, a single algal cell, and synchrotron IR maps showing protein (left) and lipid (right) concentrations in a Micrasterias cell.

Courtesy: P. Heraud, Monash University

BEAMLINE CAPABILITIES BEAMLINE CAPABILITIES

Beamline	Techniques	Capabilities
Beamline 1 High through put 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

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