

Possible Future Projects

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Australian Synchrotron



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What should we be doing?

- What is the world doing?
 - Who are our contemporaries/competitors?
- What can we do well?
 - What projects are well-suited to the technical specifications of the AS?
 - How might we enable science independently of the technical specifications?
 - In what areas do we have a track-record of excellence to build on?
- Where do we have high demand?
- What are the facility drivers?

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Facility Drivers (1)

- Upgrade and development
 - New plans should be framed around specialising, optimising and upgrading existing beamlines
 - Accelerator development
- Compatibility, complementarity and cohesion with existing capabilities
- Leading-edge capabilities
 - Everything we build must be world-class

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Facility Drivers (2)

- Increased resolution in...
 - Space
 - Time
 - Energy
 - Very small – microscopy across the spectrum
 - Very fast
 - Time-resolved experiments
 - High throughput – maximised efficiency
 - Extended capabilities e.g. Tomographic imaging
 - Extended energy ranges
- Combined capabilities e.g. TXM/IR, micro-XRD/XFM

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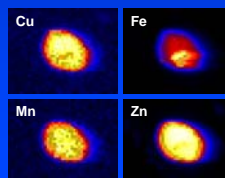
Accelerator Development

- Top Up Mode
 - Required to be world competitive
 - Beneficial to beamlines and ultimately users
 - Greater accelerator stability
- Compact Tera Hertz Source
 - Existing accelerator infrastructure and potential would allow operation
 - Low-emittance electron gun development is a key science driver in accelerator physics
 - Combined with a short superconducting structure could be used as a tera hertz infra red source for users
- IR FEL

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X-ray Microscopy & Imaging

- Upgrade and development of existing beamline
 - Double multilayer monochromator (DMM)
 - Increase flux and throughput particularly with the Maia detector
 - Dedicated optics for more efficient operation
 - Fluorescence Tomography?
- Long Coherent Nanoprobe Beamline



SXRF maps at 550°C of a natural fluid trapped as a 50 µm inclusion in quartz. The maps show that Cu, Mn, and Zn are dissolved in the fluid. – Berry *et al*

Long Coherent Nanoprobe Beamline

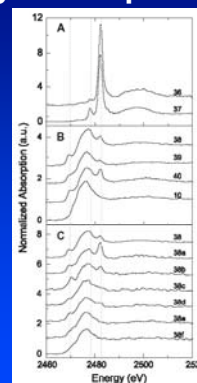
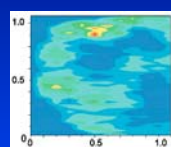
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20 μm

- Long beamline (~150m)
- Undulator
- In vacuum cryo-cooled nanoprobe sampling
- Optimised for biosciences
- Coherent Diffraction Imaging
- Complementary performance and capability to existing XFM-1

Tender X-ray Microspectroscopy



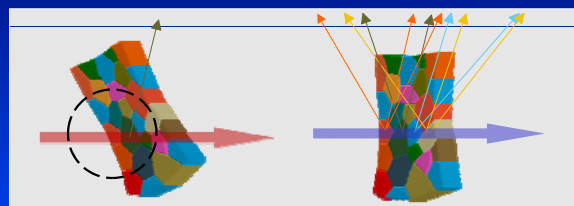
- 1– 4 keV
- Scanning undulator
- Zone Plate and KB optics
- Sub-micron achromatic focussing
- Applications in Materials, Biological, Earth Sciences (Al – Ca K absorption edges)

The distribution of S as S²⁺ in a 1 x 1 mm² sample of glass (above) and S K-edge XANES spectra identifying the presence S²⁺, S⁴⁺, and S⁶⁺ (right) in various glasses – Berry *et al*, ESRF

Microdiffraction Fluorescence Probe

- Sophisticated tool for fundamental and applied applications in materials, earth and biological sciences
- Potential wiggler beamline offering hard X-rays (4-40 keV) in a beam spot size down to 1-2 microns
- Monochromatic, pink and white beam capable
- Simultaneous XRF and XRD imaging
- Phase, strain (3D) and composition (2D) mapping
- Selected area XAS capability
- Contact : Prof. Andrea Gerson
University of South Australia

Polychromatic Microdiffraction



- Sample does not need to be rotated! Therefore no sphere of confusion.
- Single crystal information from each grain.
- 3D nondestructive probe of stress/strain/crystal structure!

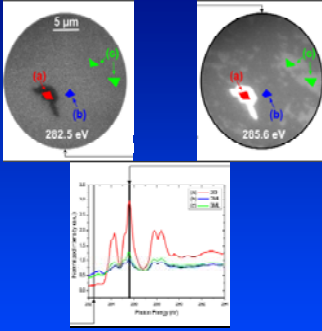
Extended Soft X-ray Capabilities

- “Dirty” sampling (non-UHV-compatible experiments)
- Low-energy Angle-resolved Photoemission
 - 3rd Generation Toroidal Analyser (LaTrobe University)
- Photoelectron Emission Spectroscopy (PEEM)
- Resonant Inelastic Scattering
- Scanning Transmission X-ray Microscopy (STXM)
- Coherent Diffraction Imaging (CDI)

Soft X-ray Beamline Cluster

- Branchline buildout and (temporary) installation of STXM/CDI endstation
 - Optimisation of existing SXR for UHV-compatible XPS/NEXAFS
- Dedicated Extended-range STXM/CDI Undulator Beamline
 - Existing SXR optics not well-suited to STXM/CDI zone plates
 - Strong demand and existing track record of excellence
 - Extended energy range (200 - >2800 eV) – unique multilayer/grating optics
- General Purpose Soft X-ray Bending Magnet Beamline
 - Two branch lines
 - Dedicated UHV line to host the High-speed Angle-resolved Photoemission (Toroidal Analyser)
 - General-purpose NEXAFS branch with vacuum window for high-throughput, non-UHV-compatible sampling

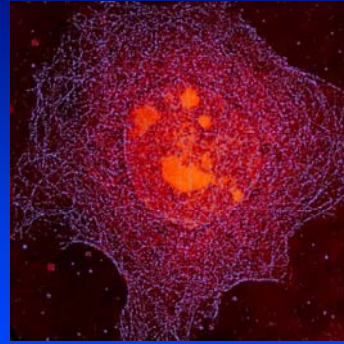
Soft X-ray – PEEM/RIXS



Laterally resolved NEXAFS: both XPEEM images show a nominal 5 ML thick PTCDA film. The left image is taken at a photon energy of $h\nu = 282.5$ eV, the right at $h\nu = 285.6$ eV. Both XPEEM images, are rescaled for contrast enhancement. – Bruce Cowie *et al*

- Apple II undulator
- Horizontal and vertical focussing
- Spatial resolution derives from electron optics
- 10 – 1500 eV energy range
- Surface science applications
- Well suited to a time-sharing beamline with RIXS due to sample preparation requirements and beam optics
- RIXS is well suited to bulk materials for fundamental science

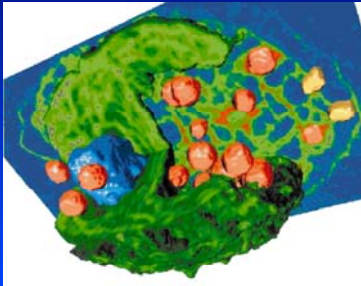
Full Field Soft X-ray Microscopy



TXM Image X-ray Microscope image of the labelled microtubule network (blue) in a whole, hydrated mouse mammary epithelial cell. The cell nucleus containing several nucleoli (orange) is in the centre of the cell

- Bending Magnet (not suited to undulator)
- Beam size – 10s of microns for full-field cell image
- Spatial resolution to 10s of nanometres for intracellular organelle imaging
- Relies on transmission contrast using zone-plate or condenser optics
- Well suited to tomography

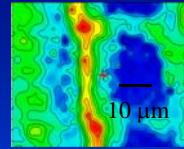
Correlative IR-TXM Beamline



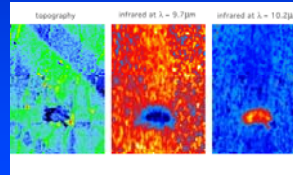
3D image of microalgal cell, *Chlamydomonas reinhardtii*. The single chloroplast is shown in green, the pyrenoid body is in blue and the lipid containing vesicles in red. Collected at U41 Bessy II.

- Correlated measurements using confocal microscopy, IR and TXM simultaneously
- Tomographic imaging down to 20 nm spatial resolution
- Imaging without the use of contrast agents
- Applications: medical and life sciences with cells and tissues; large proteins and membrane pores; nano and material sciences
- Contact: Marian Cholewa Monash Centre for Synchrotron Science

Dispersive IR Microscope



Aleurone cell walls of wheat grain: high spatial resolution *F. Applied Spectroscopy* Volume 62, pp. 895-900(6)



Mid infrared contrast of a polymer blend - Max Planck Institute Martinsried

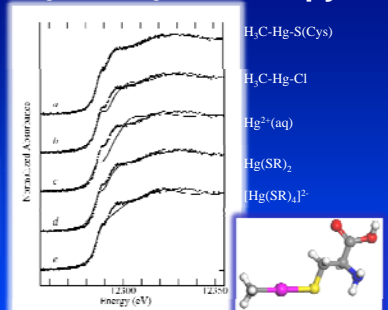
- Bending magnet
- Beyond the far-field diffraction limit
- Dispersive optics and detection for high throughput
- Photo thermal microspectroscopy
- Tip enhanced IR
- Time resolved pump-probe
- IR-ToF SIMS?

X-ray Absorption Spectroscopy

- Advanced X-ray Absorption Spectroscopy Beamline
 - Upgrade & Development of current capabilities
 - Time-resolved XAS (QEXAFS)
 - RIXS/X-ray Raman
 - Ultra-dilute XAS
 - High-energy
 - Extreme environment XAS (e.g. Brugger hydrothermal cell)
- Tender/Hard XAS Beamline

Advanced X-ray Absorption Spectroscopy

XAS of dilute systems – mercury in fish



It is well known that fish contains neurotoxic methylmercury compounds (CH_3Hg-X). But the chemical identity of the methylmercury species in fish is unknown. The levels of Hg are typically μM or less.

Swordfish skeletal muscle
Model compounds _____

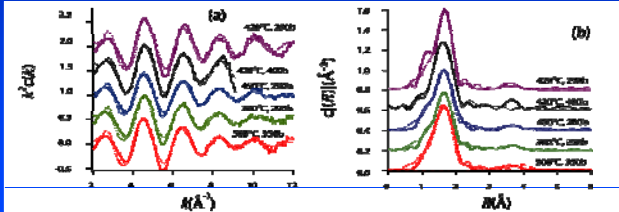
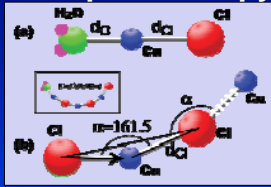
Mercury in Fish is a methylmercury-cysteine species Harris HH, Pickering IJ & George GN. *Science* 2003, 381, 1203.

Advanced X-ray Absorption Spectroscopy

'Extreme Chemistry' Experiments

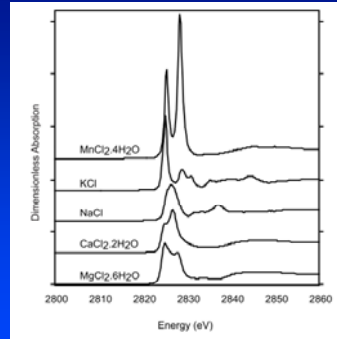
Predictions

- Understanding ore formation
- Reactive transport modelling
- Predictive exploration
- Hydrometallurgical processes



CuCl, first shell does not change with change in temperature/pressure
Weihua et al - data collected at ESRF

Tender/Hard X-ray Absorption Spectroscopy

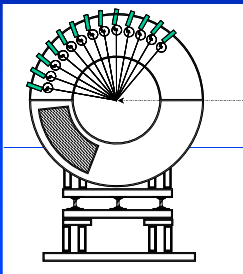


- 1--10 keV (1-4 keV not available at 12ID)
- Bending magnet
- High priority based on both demand and complementary capability
- K-edge elements tin the materials, biological and environmental sciences

XANES of Cl Standards collected at NSRRC, Taiwan
Evans et al

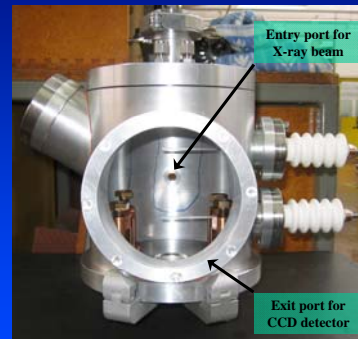
Powder Diffraction

- Completion and optimisation of existing beamline
 - High resolution multi-crystal analyser
 - High throughput optimisation
- Advanced Diffraction and Scattering beamline



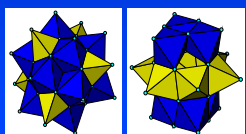
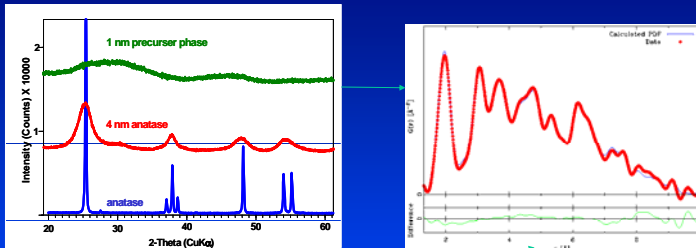
Schematic of the proposed diffractometer at Diamond, Oxfordshire
Multiple analyser crystals/detectors at positive 2θ will record high-resolution data whilst a 60° PSD at negative 2θ will simultaneously record high intensity data.

High Performance Diffraction

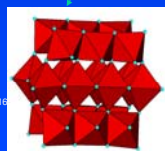


- Wiggler beamline
- Energy range up to 100 keV
- High speed (time-resolved) and high throughput PD
- Polycrystalline protein structure determination
- Pair Distribution Function scattering for quasi-crystalline/amorphous materials
- Tomographic Energy Dispersive Diffraction Imaging (TEDDI)
- Diffraction in in-situ processes Extreme Environments (High P/T)

Pair Distribution Function Analysis



Polyoxotitanate clusters; Left - [Ti₁₆O₄₆]¹⁶⁻, Right - [Ti₁₂O₃₂]¹⁶⁻



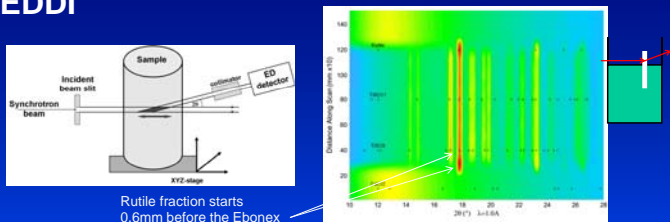
Ti₂₀O₁₅(OH)₅₀ cluster

Structural Models For Sub-Nano TiO₂ In Sol-Gel Photocatalyst Syntheses Ian Grey, Nick Wilson and Pierre Bordet

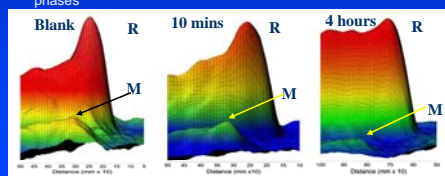
Residual Strain Mapping

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TEDDI



Rutile fraction starts 0.6mm before the Ebonex phases

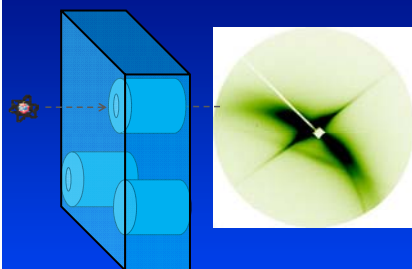


Distance between start of Rutile (R) and Magneli (M) phase peaks at each end of scan represents thickness of the rutile layer

Small Angle X-ray Scattering

- Upgrade and optimise existing beamline
- High-throughput and routine SAXS driven by commercial interest
- New advanced SAXS beamline

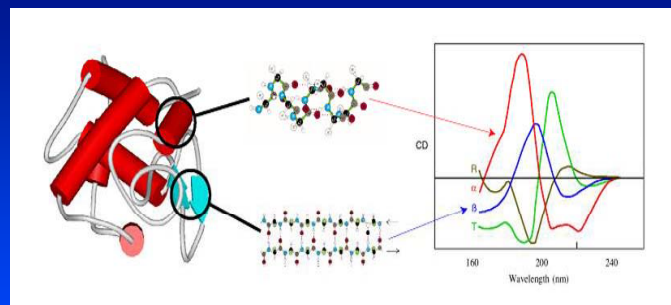
Advanced SAXS Beamline



- Advanced sampling
 - in-situ
 - time-resolved
 - Micro fluidics
 - Protein Folding
- USAXS (Bonse-Hart)
- Flexible geometries
 - Reflectivity
 - GIXD

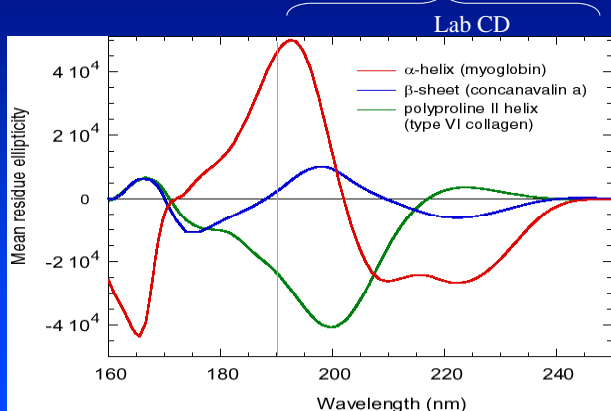
The ion tracks are visible in the (transmission) SAXS image as narrow streaks and yield information about the radial density distribution in the tracks. Shown is an image of ion tracks in CaF_2 irradiated with 1.4 GeV Xe ions
Kluth *et al*, APS

Circular Dichroism



Thanks to Prof. Mibel Aguilar Monash University & Prof. Bonnie Wallace Birkbeck College, University of London

Synchrotron CD Spectra



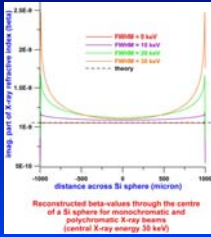
SRCD Advantages

- Lower wavelength data (*higher structural information content*)
- Higher signal-to-noise (*smaller sample requirements*)
- More rapid measurements (*lower requirement for signal averaging*)
- Can analyse samples in high concentration & absorbing buffers (*& membrane samples*)

Micro-CT Beamline

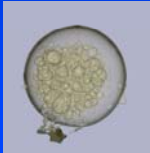


high-speed, e.g. dynamic studies

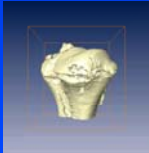


Reconstructed beta-values through the centre of a Si sphere for monochromatic and polychromatic X-ray beams (central X-ray energy 30 keV)

- White/ pink/ monochromatic CT
- Applications
 - Material science
 - Life science
 - Tomosynthesis/Laminography
- Phase- & absorption-contrast mechanisms
- Ability to avoid beam-hardening issues



Silica ceramisphere with enclosed voids



trabecular-bone architecture



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www.synchrotron.org.au