UM2022

User Meeting 2022

1st & 2nd December

Australian Synchrotron
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Contents

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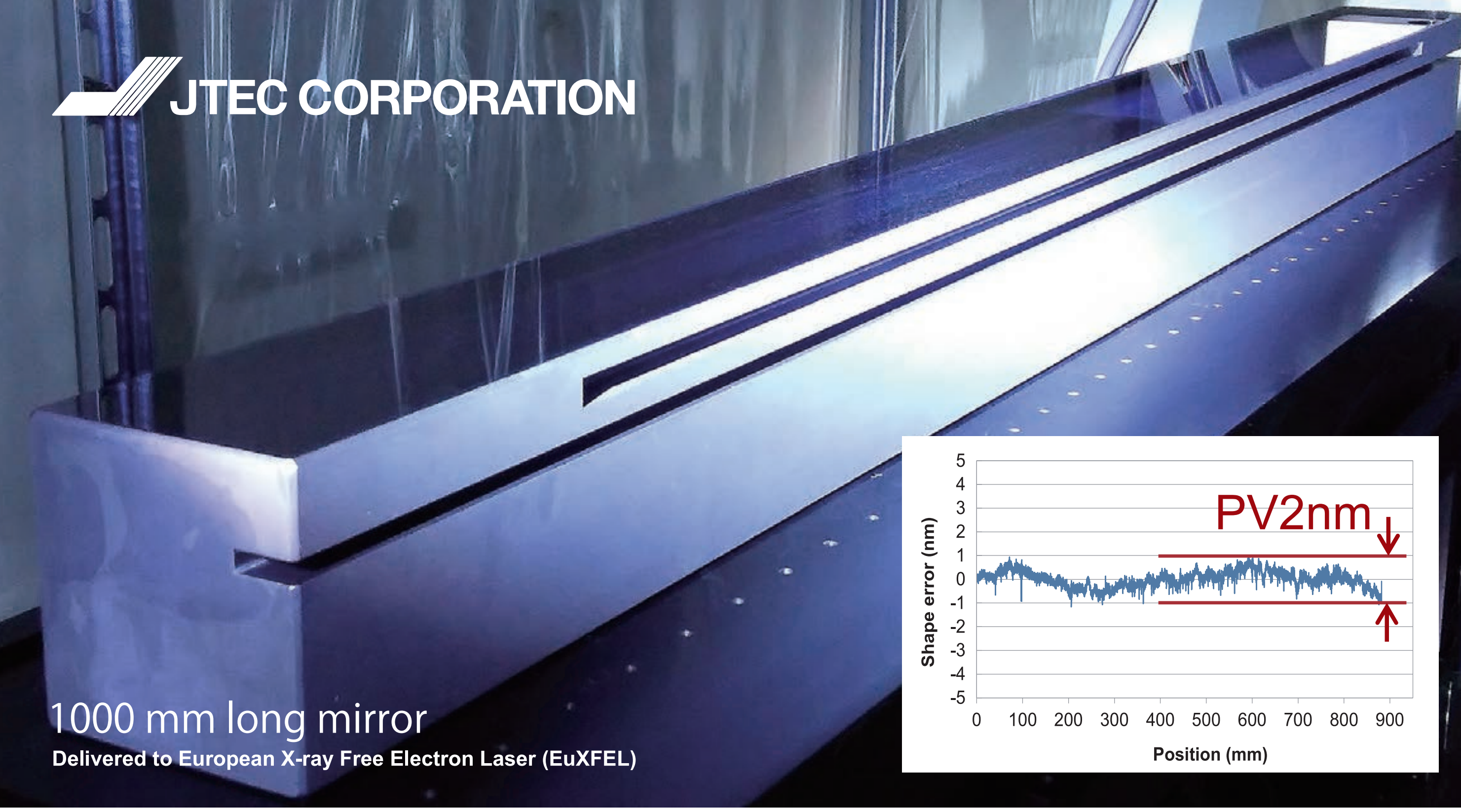

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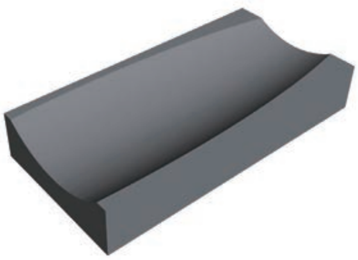

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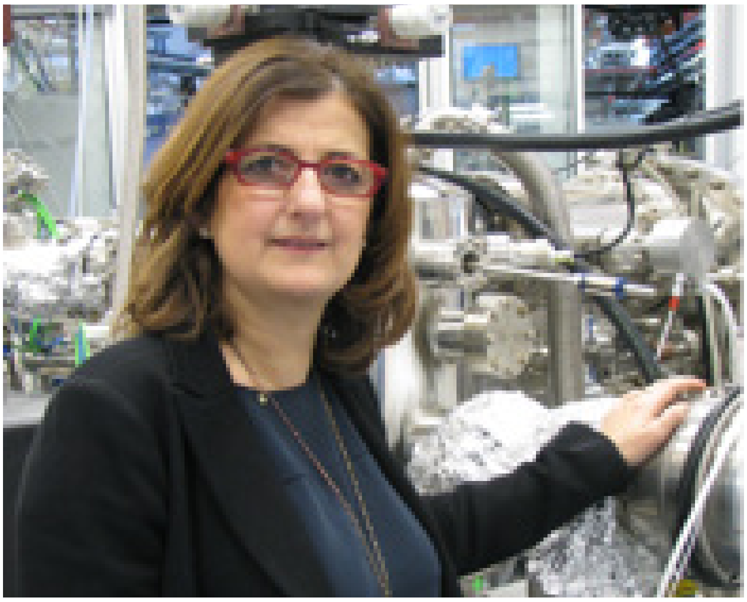
Plenary Speakers

Prof. Carolyn Larabell

Carolyn Larabell is Professor and Vice-Chair of the Department of Anatomy at University of California, San Francisco. She holds a joint appointment with Lawrence Berkeley National Laboratory where she is an Advanced Light Source Professor, Director of the National Center for x-ray Tomography, and Head of the Cellular and Tissue Imaging Department. She received her Ph.D. from Arizona State University and did postdoctoral research at Stanford University and University of California, Davis. She is a Cell Biologist with an extensive background in light and electron microscopy and a long history of developing and implementing new imaging technologies. For the past two decades, she has been developing biological soft x-ray tomography. To image molecules with respect to cell structures, her lab developed cryo fluorescence tomography. This enables localizing specific molecules using cryo fluorescence tomography and placing them in the context of native-state structures in the same cell seen with cryo soft x-ray tomography.

Dr Amina Taleb-Ibrahimi



Amina Taleb-Ibrahimi is a CNRS senior scientist. She joined the CNRS institution as a research fellow (CR1) in 1989 after a «Doctorat d'Etat ès Sciences Physiques» from University Pierre & Marie Curie, Paris VI and 3 years of post-doc at IBM T.J. Watson Research Center, Yorktown Heights, New York. She is now director of research (DRCE2) at CNRS.

Amina has been in charge of 3 beamlines for spectroscopic studies using synchrotron radiation, the IBM- U8 photoemission beamline at NSLS, Brookhaven Lab, the French-Swiss beamline at SUPERACO (LURE), the pionneer synchrotron radiation center in Orsay, France and the high resolution ARPES (Angular Resolved Photoemission) CASSIOPEE beamline at Synchrotron SOLEIL in Saclay, France.

Amina is a condensed matter physicist with strong expertise in low dimensional systems (growth, atomic structure, electronic structure). Her recent interest focussed on multiepitaxial graphene with a reference work (PRL 2010, Nature Physics 2013, Nature 2014, PRL 2015, Nanolletters 2017, nanotechnology 2020) and topological insulators thin films (PRL 2013, Nature Com 2014, PRL 2016, Science Advances 2017).

Amina has been participating to several national contracts (ANR, Labex PALM) and international (PUF- USA; JSPS-Japan). She is a scientific expert in a great number of institutionnal councils (French Universities, CNRS, HCERES,METSA, IRRMN, LNCMI,...) and also international councils of large scale facilities (LLB, ILL, ESS, ESRF, SOLEIL, XFEL, ...) and international scientific panels (ELETTRA, ALBA, Diamond, BESSYII, NSLSII, ANSTO, HMFL-FELIX, Univ.LUND, RAC Stockholm, ARTEMIS, HZB, Swedish council, STFC,...).

From 2012 to 2016 Amina was Deputy Scientific Director in charge of large scale facilities at the Institute of Physics at CNRS.

Amina co-authored >200 publications including (Science, Nature group, PRL, Nanolett, ...) with >11000 citations. She has presented over 50 talks/lectures in international conferences and schools.

Amina is very active regarding gender issues and equal opportunities. She is chair of the European Conference of Surface Science board ECOSS and member of the condensed Matter Department CMD board of the European Physical Society EPS.

Amina Taleb-Ibrahimi was nominated Science Director for Physical sciences at Synchrotron SOLEIL in September 2016.

Dr Qun Shen

As the Deputy Director for Science of the National Synchrotron Light Source II (NSLS-II), and a Senior Physicist at Brookhaven National Laboratory, Qun oversees the development and strategic planning of the scientific programs at NSLS-II, including interactions with the broad scientific user community, development of high-level user access policies and user community partnerships, as well as spearheading the annual NSLS-II strategic plan process.

From 2008 to 2013, Qun served as the NSLS-II Experimental Facilities Director and a member of the executive leadership team during the construction phase of NSLS-II, and was responsible for development of all aspects of experimental programs in the NSLS-II Project.

Before joining BNL, Qun was Head of the X-ray Microscopy and Imaging Group at the Advanced Photon Source in Argonne National Laboratory. He also held Adjunct Professorships in Materials Science & Engineering at Northwestern University and in Physics at Purdue University. Prior to Argonne, he was a Senior Staff Scientist and Head of the X-ray Optics Group at Cornell High Energy Synchrotron Source, and held an Adjunct Associate Professor in Materials Science & Engineering at Cornell University.

Qun was a Scientific Member and Developer during the early stages of the Synchrotron Radiation Instrumentation Collaborative Access Team (SRI-CAT) at the APS, with the particular emphasis on X-ray physics of materials and polarization studies.

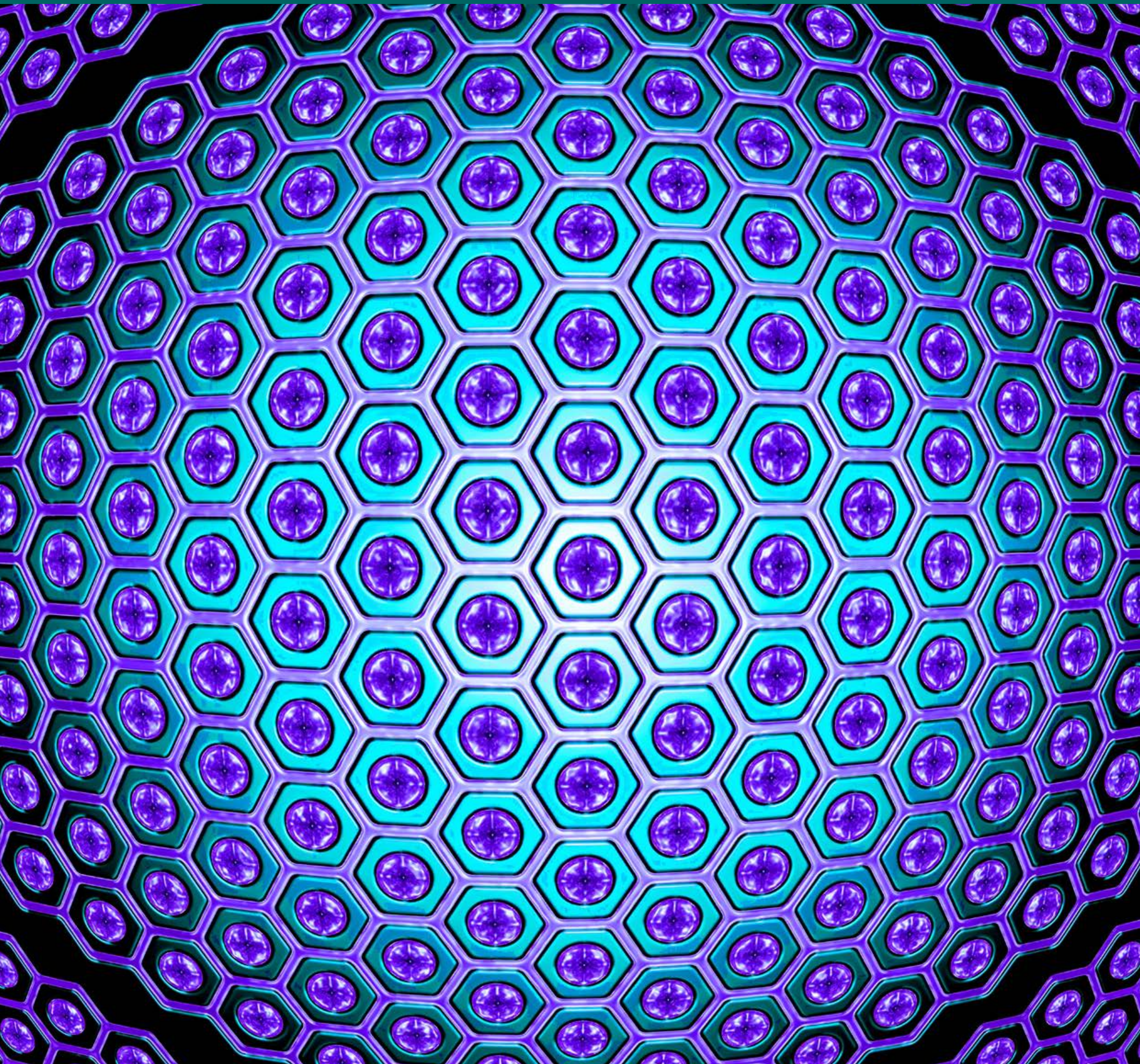
Abstract

The National Synchrotron Light Source II (NSLS-II) is one of the newest synchrotron facilities in the world. It provides extremely stable and bright photon beams from infrared to hard X-rays, with a data infrastructure to enable multiscale, multimodal, high-resolution studies on diverse systems of materials. Since its start of user operations in 2015, NSLS-II has transitioned 28 beamlines into user services and supported wide range of user science projects from clean energy, quantum, and microelectronics, to synthesis & manufacturing, the environment, and human health. In addition to the 28 operating beamlines, 5 other beamlines are under various stages of development and construction. When these are completed in 2027-28 timeframe, NSLS-II will have 33 beamlines in operations, out of its full capacity of ~60 beamlines.

Recognizing the needs to develop additional beamlines, NSLS-II organized a strategic planning workshop entitled “Exploring New Science Frontiers at NSLS-II” in 2019. Based on the interactions with the community at this workshop and follow-up discussion with the SAC, NSLS-II has identified 20+ new beamlines to be developed to complete the beamlines buildout portfolio, providing additional capabilities to meet the research needs of the scientific community. In this presentation, I will provide an update on the current status of our beamline buildout plan, and our considerations of various factors that impact our new beamlines selections and prioritization process.

National Synchrotron Light Source II is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704.

Advanced Materials & Hard Matter



The Nanprobe Beamline at the Australian Synchrotron

Presenter: Martin de Jonge

Abstract ID#: 4

A hard-X-ray Nanoprobe beamline is under construction at the Australian Synchrotron. Taking input from the user community and incorporating recent technological advances we have developed an instrument that can tailor the probe to address a range of investigations, delivering 60 nm focussed-beam sizes with modest sensitivity or 300 nm beam sizes at high intensity. Ptychography will enable imaging at resolutions of the order of 15 nm.

The beamline will optimise sensitivity by using a Double Multilayer Monochromator, transporting 1e12 photons/s into the 300 nm focus. Detectors will be optimized for ppm elemental mapping (Si-U) via fluorescence, but the Nanoprobe will also support a raft of on-axis transmission methods including ptychography, absorption, differential phase, and dark-field contrast, and nano-SAXS and nano-diffraction mapping. Tomographic acquisition will be routinely available. A future stage-2 upgrade will enable spectroscopy via a Double-Crystal Monochromator retrofit.

The Nanoprobe instrument will sit at around 100 m from the storage ring, inside a concrete endstation housed within a satellite building. In order to realise the extreme resolutions that we target, we have considered vibration isolation, relative motions between the endstation and the X-ray source (which occur over multiple years due to water-table fluctuations), and temperature stabilisation of the endstation and surrounds.

In this presentation we outline the design of the Nanoprobe with a focus on applications and the laboratory facilities that will be available to support user science. We welcome input from all potential users with a view to preparing for the first user experiments in 2025.

Swift heavy ion modified materials: applications and characterisation using small angle X-ray scattering

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Presenter: Patrick Kluth

Abstract ID#: 9

When energetic ions pass through a target material, they can generate long, narrow cylindrical damage regions a few nanometres wide and up to tens of micrometres long, termed 'ion tracks'. Ion tracks have many interesting applications in areas such as materials science and engineering, nanotechnology, geology, archaeology, nuclear physics, and interplanetary science. Ion track damage often exhibits preferential chemical etching over the undamaged material. This etch-anisotropy can be used to create high aspect-ratio pores with pore diameters as small as several nanometres, which have been studied for many advanced applications including ultra-filtration, bio- and medical sensing, nano-fluidics, and nano-electronic devices. Detailed characterisation of ion tracks and track-etched nanopores, however, remains challenging. Small angle X-ray scattering (SAXS) provides a powerful tool to study the structure of ion tracks and track-etched nanopores, as it is sensitive to density changes on the nanometre length scale. It is non-destructive and can yield high precision measurements of the track and pore structure in many materials. Short acquisition times associated with the high photon flux at 3rd generation synchrotron facilities enable in situ studies.

The presentation will give an overview of our recent results on using SAXS for the study of ion tracks in minerals, glasses and polymers, as well as nanopore membranes fabricated using ion track etching. This will include fabrication of conical pores in SiO2 and their application in nanofluidic diodes, separation membranes and biosensors, in situ ion track etching in polymers and in situ annealing of ion tracks in minerals in diamond anvil cells to investigate track annealing under high pressure conditions.

Four-Angle Polarisation Synchrotron-FTIR Technique for Materials Orientation Analysis at Australian Synchrotron

Presenter: Jitraporn (Pimm) Vongsvivut

Abstract ID#: 18

Molecular orientation in materials can play a significant role in overall mechanical performance and chemical properties. Infrared (IR) absorption by specific functional groups occurs preferentially when the electric vector of the probing beam is aligned with the dipole oscillation corresponding to the absorbing frequency, and can therefore be used to gain information on the molecular orientation of analysed materials. The team at Tokyo Institute of Technology has developed a mathematical procedure, so-called *"4-angle polarisation"*, to visualise the dipole orientation angle of a certain vibrational mode as *vectors* for each pixel of a hyper-spectral image, using polarised absorbances measured at four different angles [1].

At Infrared Microspectroscopy (IRM) Beamline, we have applied this method for orientation analysis of a range of samples, using synchrotron-IR microspectroscopy. This presentation will demonstrate successful applications, including silk fibres [2], poly-lactic acid (PLA) composites, paracetamol [3,4], and bone sections. Through the successful Australian Academy of Science (AAS) grant, the new *"4+ angle polarisation"* widget has been developed and made available in the open-source Quasar/Orange data analysis platform. We expect that this method will represent a new cutting-edge technology to underpin the molecular orientation analysis at the IRM beamline to benefit wider synchrotron-IR user community.

References:
[1] Hikima et al. *Macromolecules,* **44**, 3950 (2011).
[2] Ryu et al. *Scientific Report,* **7**(*1*), 7419 (2017)
[3] Honda et al. *Applied Surface Science,* **473**, 127 (2019).
[4] Honda et al. *Nanomaterials,* **9**, 732 (2019).

***Acknowledgement:** We acknowledge the financial support from Regional Collaborations Programme COVID-19 digital grant 2021, funded by Australian Academy of Science (AAS), to the project entitled *"Web Platform for Remote Data Analysis and Processing of Synchrotron Data"*.*

Radiography tilt series used for depth determination during radiation testing

Presenter: Chris Hall

Abstract ID#: 34

Synchrotron x-ray beams such as those produced on **IMBL** have unique properties which can be exploited for testing radiation damage effects on integrated circuits. With energies around 40 keV the scatter in low Z materials is of the same order as the penumbra of the beam (~10 microns FWHM for **IMBL**). The consequence is not only an ability to image the device under test, but to limit the dose given to specific areas of the circuit. The effects of this local integrated dose (**LID**) is useful in determining mission risk factors for engineering space flight electronics.

The linear energy transfer of these photons is very close to constant for thin materials. So knowing the depth of the material in the beam is required for accurate dose maps. During testing a relatively simple way of achieving this it generate a series of images with the integrated circuit set at different angles to the beam. Using parallax analysis methods these tilt series yields positions and depths in the direction of the beam in a similar fashion to tomo-synthesis. The tilt series can be captured using only a small fraction of the total dose used for the radiation testing.

Strain measurement, depth-resolved diffraction, and in situ phase mapping of bulky samples - Energy-Dispersive XRD at the Australian Synchrotron

Presenter: Renata Lippi

Abstract ID#: 35

Energy-dispersive diffraction (EDXRD) will be a new technique on offer for Australian Synchrotron users. EDXRD is particularly relevant for large samples that require non-destructive depth-resolved analysis, such as large engineering parts. This technique uses polychromatic X-ray beam (a.k.a. white-beam or pink-beam) to obtain diffraction patterns. The ADS-1 beamline will provide high-energy polychromatic X-rays that will enable probing of bulky samples and will be well-suited for EDXRD experiments. Given the novelty of EDXRD at the Australian Synchrotron, a brief background of this technique will be presented, highlighting similarities and differences with traditional angle-dispersive powder XRD. Furthermore, details on the technical capability for EDXRD experiments at the ADS-1 beamline will be discussed, followed by research case studies using overseas EDXRD facilities. Examples will include depth-resolved characterisation, strain measurements, phase identification, mapping, and others.

NEXAFS Spectroscopy of alkylated benzothienobenzothiophene thin films at the carbon and sulfur K-edges

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Presenter: Paul Chantler

Abstract ID#: 47

Alkylated benzothienobenzothiophenes are an important class of organic semiconductor which exhibit high performance in solution-processed organic field-effect transistors (OFETs). In this presentation the molecular orientation of alkylated benzothienobenzothiophene (BTBT) thin films with angle-resolved near-edge X-ray absorption fine-structure (NEXAFS) spectroscopy at both the carbon and sulfur K-edges will be discussed. Specifically, a focus is placed on BTBT derivative (C10-BTBT-C10) functionalised with two decyl side chains. Interestingly, the dichroism of the dominant, lowest energy peak is opposite at the carbon and sulfur K-edges. First-principles calculations using the density functional theory-based Many-Body X-ray Absorption Spectroscopy (MBXAS) method are presented that enable the assignment of the peaks observed at both absorption edges to specific molecular orbitals. While the lowest energy peak at the carbon K-edge is assigned to carbon 1s ⊠ ⊠ transitions with transition dipole moment (TDM) perpendicular to the planar BTBT core, the lowest energy peak at the sulfur K-edge is assigned to sulfur 1s ⊠ ⊠ transitions with TDM oriented along the long axis of the BTBT core. This work highlights differences in the sulfur and carbon K-edge NEXAFS spectra of sulfur containing organic semiconductors and that care needs to be taken when interpreting sulfur K-edge data. When interpreted properly, the NEXAFS data at both edges support a highly end-on orientation of the BTBT molecule with respect to the substrate.

Swift Heavy Ion Tracks in Polypropylene

Presenter: Shankar Dutt

Abstract ID#: 49

Polypropylene (PP) is the second-most extensively manufactured plastic and has the biggest market share in terms of foil products [1]. Still little is known about the formation of ion tracks (narrow damaged regions created along the path of swift heavy ion irradiation due to intense electronic excitations), including how they are affected by the ion energy, type, and energy loss. Additionally, the influence of antioxidant content on the ion track damage also has not yet been studied. Small-angle X-ray scattering (SAXS) has been established as a powerful technique for characterizing ion tracks in a variety of organic and inorganic materials [2]. The present study examined ion tracks in two distinct kinds of PP foils with different antioxidant concentrations using synchrotron-based SAXS. To fabricate the ion tracks in these foils, Xe, Au, and Pb ions with energies of 2.2 GeV, 710 MeV, and 160 MeV respectively were used. We discovered that in the case of PP foils with high antioxidant content, the ion tracks have a severely damaged core with a gradual transition of the density to the undamaged material, and the relative density of the ion tracks was found to be lower than the bulk due to outgassing of volatile compounds. On the other hand, ion tracks in PP foils with lower antioxidant content absorbed oxygen from the atmosphere leading to the formation of core-shell structure of the ion tracks and a greater overall density than the bulk due to the chain branching processes that induce oxidative deterioration.

References:
1. H. A. Maddah. Am. J. Polym. Sci. 11(2016)
2. P. Kluth, C. S. Schnohr, et al. Phys. Rev. Lett. 101,175503(2008)

Using high-energy x-ray transmission imaging to unlock the complex relationship between spatial and chemical changes in a lead-acid battery.

Presenter: Chad Stone

Abstract ID#: 54

Despite the age of lead-acid battery technology, it still forms a crucial part of the global electrochemical energy storage market. Part of the reason for its continued success is due to its well understood chemistry. However, in recent years it has become clear that complications resulting due to modern battery applications need to consider the spatial dimension of lead-acid batteries, in addition to the chemical composition. One important application is the so-called high-rate partial-state of charge (HRPSoC) cycling, where the exterior of the Pb electrode becomes so heavily utilized that it is thought that the porosity of this region becomes so low that it impedes the movement of electrolyte into the electrode. The problem that researchers often face is how to determine the effects of spatial changes in porous electrodes while relying on imaging techniques which are typically ex-situ, and often cannot observe features below the surface of a sample. Our research shows that using high-energy transmission x-ray imaging via the IMBL, it is possible to monitor spatial and chemical changes in a lead-acid battery in real time. Using a custom-made lead-acid battery, we were able to observe the rapid morphological changes which occur under a HRPSoC duty in-operando. The results suggest that these changes are not solely due to the heavy utilization of active material, as previously thought, but involves the restructuring of the porous material. On a broader level, it shows that synchrotron x-ray imaging could be a useful tool for investigations into the spatial dimension in battery research.

The XAS Beamline in 2023: Efficiency and Reliability

Presenter: Bernt Johannessen

Abstract ID#: 58

The XAS beamline is entering its 15th year of user operations and carries a registered and regular user base exceeding 1000. Outputs have increased steadily with an accumulated total of well over 400 journal publications and over 170 of those in the past three years. Whilst the compounded annual growth rate (3-yearly) still exceeds a healthy 10% one could expect further tapering in the absence of beamline and/or community developments. From this base the beamline scientist team is now ready to expand capabilities and, arguably, our most significant renewal is just around the corner with new fluorescence detectors, new cryogenic (and room temperature) sample stage, new user interface, and energy slew scanning coming online in 2023.

This presentation will give an overview of the current and imminent future state of the XAS beamline. We will touch on general capabilities, discuss the major new pieces of kit, touch on the beamtime proposal process and have a look at beamline (*user community!*) productivity. We will conclude with (*attempt*) a live beamline demo."

High-energy X-ray crystallography at the Australian Synchrotron: New capabilities for challenging single-crystal diffraction experiments

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Presenter: Josie Auckett

Abstract ID#: 66

The Advanced Diffraction and Scattering beamlines (ADS-1 and ADS-2) are two of eight new beamlines currently under construction or commissioning as part of Project BRIGHT. Within the Australian Synchrotron's suite of crystallography-targeted beamlines, ADS-1 and ADS-2 are unique in offering very hard X-rays (45–150 keV; ⊠ = 0.08–0.27 Å) for both monochromatic and white-beam diffraction experiments. The nature of high-energy radiation makes the ADS beamlines especially suited to experiments involving complex sample environments or strongly-absorbing samples, or where access to high momentum transfer (large Q/short d-spacings) is required.

Single-crystal diffraction experiments at ADS will utilise a two-axis, high-payload sample goniometer capable of supporting user-supplied sample environments weighing up to ~2 kg. The large area detectors available at both ADS endstations can be positioned over a wide range of coordinates in *x*, *y* and *z* in order to optimise data resolution and coverage. Here, we present an overview of the planned hardware and software facilities that ADS will offer for single-crystal diffraction and the anticipated timeline for their implementation. We also discuss complementarity between ADS-1, ADS-2 and the MX beamlines, and give examples of science cases that will benefit from the unique characteristics of high-energy diffraction at ADS."

The Simultaneous Reconstruction and Structural Fitting of the Complex Atomic Fine Structure

Presenter: Paul Di Pasquale

Abstract ID#: 78

X-ray Absorption Spectroscopy is an incredibly powerful tool for probing atomic and molecular structures of materials. While it is a very popular and powerful technique, absorption-based measurements are limited when applied to weakly absorbing samples such as thin films or samples with low concentration. This is expected not to be the case with phase-based measurements, which are generally several orders of magnitude larger than the absorption counterpart. This presentation describes a novel technique for measuring complex atomic fine structure, which involves a simultaneous measurement of both absorption and phase components of x-ray interactions with a sample. Explorations into developing a phase analogue of X-ray Absorption Fine Structure is also explored, in which structural fitting of the real and imaginary components will be presented.

Status of the BRIGHT Advanced Diffraction Beamlines for high energy X-ray diffraction and imaging research

Presenter: Justin Kimpton

Abstract ID#: 80

The Advanced Diffraction and Scattering beamlines (ADS-1 & ADS-2) will be two independently operating high-energy X-ray beamlines powered from a single 4.5T super-conducting multi-pole wiggler. ADS-1 will provide both polychromatic and monochromatic (50 keV – 150 keV) beam for a range of diffraction and imaging experiments. The ADS-1 X-ray optical design requires the sample position to be over 55 m from the source to allow the focussing optics to be effective, therefore the experiment endstation is located in a new external building. ADS-2 will be capable of monochromatic diffraction experiments at 45.3 keV, 74.0 keV or 86.8 keV and the endstation is within the main technical building. The ADS beamlines will offer highly flexible experiment configurations and sample environments to enable a wide variety of research capability for the materials, chemistry, engineering and earth sciences communities. Heavy lift sample stages with a 300 kg load capacity are a feature of the ADS-1 endstation. Both ADS beamlines will have state-of-the-art hybrid pixel detectors for low noise, rapid data collection for time-resolved diffraction experiments. In addition to traditional powder diffraction techniques, new techniques to the Australian Synchrotron such as high-energy single crystal diffraction and energy-dispersive diffraction will be important areas for future development. This presentation describes the ADS beamlines, some of the planned techniques and provides a status update on the considerable progress that has been made on the various beamline projects.

Commissioning and first user operations on MEX

Presenter: Chris Glover

Abstract ID#: 90

The MEX beamlines have seen rapid progress through 2022, with finalization of construction, first light, detailed hot commissioning and user operations underway in November.

In this presentation, we will present the beamlines performance, initial results, path way for development of full capabilities and scientific opportunities.

High-energy x-ray studies of piezoelectric materials

Presenter: John Daniels

Abstract ID#: 91

High-energy x-rays offer unique advantages for the study of bulk materials during in-situ perturbation. The combination of penetration depth, small scattering angles, intense and customisable beam sizes make them ideal for investigating anisotropic material response in real-world loading conditions. These properties make high-energy x-rays ideal for studying the response mechanisms of piezoelectric materials. Piezoelectrics are used in a broad range of industries and applications, from ignition systems to high-quality medical imaging. The field has undergone a significant transition in the past two decades due to the increasing use of high-strain single crystal materials in niche applications and the push towards more environmentally friendly compositions for consumer device usage. This presentation includes an overview of piezoelectric materials development over the past decade and the insights provided by high-energy x-ray scattering studies. The actuation mechanisms of both conventional lead-based and more recent lead-free systems will be discussed.

MX3 - the High Performance Macromolecular Crystallography Beamline

Presenter: Daniel Eriksson

Abstract ID#: 93

The High-Performance Macromolecular Crystallography beamline (MX3) will be capable of providing high-flux, microfocus X-rays for small and weakly diffracting protein crystals. The beamline will provide three modes of operation: goniometer, serial crystallography, and in-tray collection. The proposed optical system will maximise flux at the sample position and the use of a secondary source aperture will allow rapid change in beam size.

A high degree of automation will support unattended data collection of entire projects. Given a set of expected outcomes, all samples attached to an experiment can go through screening and data collection without user interaction. If a primary sequence or molecular replacement models have been provided, automated phasing can take place. In addition, if a fragment library is provided ligands can be fitted in the electron density and scored by goodness of fit. For manual inspection, browser tools will provide a quick view of the site in question with difference maps.

Results are entered in a database for easy comparisons across multiple experiments, and access controlled via attached lab members.

In addition to high-speed standard pin-mounted goniometer experiments, MX3 will enable in-plate screening and data collection. These will be performed at room temperature and may require merging data from multiple crystals for a complete dataset. The obvious benefit is that crystals do not need to be looped out of drops, allowing the collection of room temperature in-tray data to be totally automated.

MCT beamline at ANSTO/Australian Synchrotron: Commissioning & first user operations

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Presenter: Andrew Stevenson

Abstract ID#: 101

The Micro-Computed Tomography (MCT) beamline is one of the first new beamlines to be constructed at the Australian Synchrotron as part of the BRIGHT program. MCT complements the X-ray imaging/ tomography capability provided by the Imaging & Medical Beamline (IMBL), and targets applications requiring higher (sub-micron) spatial resolution and involving commensurately smaller samples. MCT is a bending-magnet beamline, operating in the 8 to 40 keV range, based on a novel double-multilayer monochromator. Filtered white and pink beams are also available, the latter utilising a single-bounce mirror. MCT will benefit from X-ray phase-contrast modalities (such as propagation-based, grating-based and speckle) in addition to conventional absorption contrast, and is equipped with a robotic stage for rapid sample exchange. A higher-resolution CT configuration based on the use of a Fresnel zone plate system will also be available soon.

Anticipated application areas for non-destructive 3D sample characterisation include biomedical/ health science, food, materials science, and palaeontology. This presentation will provide a description of the commissioning activities undertaken thus far, leading to the first user operations taking place in the current cycle (2022/3). Future developments on the beamline will also be discussed"

BioSAXS: High flux SAXS beamline dedicated to solution scattering at the Australian Synchrotron

Presenter: Christina Kamma-Lorger

Abstract ID#: 102

A Small Angle X-ray Scattering (SAXS) beamline is currently being commissioned as part of the BRIGHT program. BioSAXS is due to be available for users from March 2023. The beamline was given a 2 m straight at the storage ring and in order to maximize the photon flux, a superconducting undulator and a double multilayer monochromator were selected in order to monochromatize synchrotron X-Rays between 8-15 keV. The experimental end station consists of an in-vacuum photon counting detector, offering full automation of set up changes and optimised conditions for time-resolved dynamic studies of particles in solution. The BioSAXS beamline will host all types of solution scattering experiments ranging from biological systems to soft matter, chemistry and material sciences. The flux at the sample is expected to be ~5 x 1014 ph/sec and will give the opportunity to users to measure weakly scattering samples and low concentration samples, improving the service and capabilities that are offered to the scattering community in Australia, New Zealand and the Asia-Pacific region.

Biomedicine & Health

Quantifying Lung Aeration in Neonatal Lambs at Birth using Lung Ultrasound

Presenter: Emily Pryor

Abstract ID#: 23

Background: Lung ultrasound (LUS) is a safe and non-invasive tool that can potentially assess regional lung aeration in newborn infants and reduce the need for X-ray imaging. LUS produces images with characteristic artifacts caused by the presence of air in the lung, but it is unknown if LUS can accurately detect changes in lung air volumes after birth. This study compared LUS images with lung volume measurements from high-resolution computed tomography (CT) scans to determine if LUS can accurately measure lung aeration. Methods: Deceased near-term newborn lambs (139 days gestation, term ~148 days) were intubated and teh chest imaged using LUS (bilaterally) and phase contrast CT scans (Imaging and Medical Beamline, Australian Synchrotron) at increasing static airway pressures (0 cmH2O to 50 cmH2O). CT scans were analysed to calculate regional air volumes and correlated with measures from LUS images. These measures included (i) LUS grade; (ii) brightness (mean and coefficient of variation); and (iii) area under the Fourier power spectra within defined frequency ranges.

Results: All LUS image analysis techniques correlated strongly with air volumes measured by CT ($p<0.01$). When imaging statistics were combined in a multivariate linear regression model, LUS predicted the proportion of air in the underlying lung with moderate accuracy (95% prediction interval ±22.15%, $r2=0.71$).

Conclusion: LUS can provide relative measures of lung aeration after birth in neonatal lambs. Future studies are needed to determine if LUS can provide a simple means to assess air volumes and individualise aeration strategies for critically ill newborns in real time.

Metastatic Surveillance Post Microbeam Radiotherapy

Presenter: Elette Engels

Abstract ID#: 42

Despite recent advances for breast cancer treatment, metastatic disease is still the major cause of terminal treatment failure. Developments in immunotherapy show promising links between radiotherapy and the immune response to metastases. Ultra-high dose-rate radiotherapy (FLASH) and synchrotron microbeam radiotherapy (MRT) show remarkable normal tissue sparing with exceptional cancer control. Furthermore, an observed anti-tumour immune response with MRT could inhibit distant metastases. Here, we associated MRT regimens with local control and metastasis in a 4T1.2 metastatic mouse mammary tumour model.

Tumour cells were implanted into the mammary fat pad of 105 BALB/c mice. Ten days later, tumours were treated with either ultra-high dose rate 285Gy peak-/5Gy valley-dose MRT or 8Gy broad-beam (BB), delivered in a fractionated schedule (one fraction per day for three days for 3xMRT, 3xBB or MRT/BB combinations). Primary tumours, locoregional lymph nodes, lungs, brains and spinal cords were collected in 15 mice per group to determine metastatic burden and quantify immune cell prevalence. Six mice per group were employed for a parallel survival study.

Tumour volume measurements and histology indicated that the long-term local control and survival were superior with the combined MRT/BB treatment. While the metastatic burden was not significantly different between treatment groups, combination of MRT and BB triggered a unique immune response in irradiated tumours that included increased infiltration of macrophages and B-cells. The combined treatment, therefore, can be recommended to further enhance the efficacy of MRT, especially in combination with immunotherapy, that would boost both local control and abscopal responses in non-immunogenic tumours.

Quantifying sample microstructure using x-ray single-grid dark-field imaging

Presenter: Ying Ying How

Abstract ID#: 45

The size of the smallest resolvable sample feature in an imaging system is usually restricted by the pixel size and spatial resolution of the system. This limitation can now be overcome by dark-field imaging, where the dark-field signals are generated by the ultra-small-angle x-ray scattering from unresolved sample features, such as fibres, powders or bubbles. A quantitative dark-field signal is useful since it can provide information about the size or material of sample microstructure, information that is inaccessible from the conventional or phase-contrast x-ray images.

Single-grid imaging is an emerging x-ray imaging technique that has a relatively simple set-up, which only requires one optical element to provide as a reference pattern - typically a grid, but alternatively a piece of sandpaper, in which case the technique is known as speckle-based imaging. The attenuation, phase shift and dark-field signals can be extracted simultaneously from a single sample exposure using this technique, which makes it feasible for dynamic imaging. We have previously derived a new method to extract quantitative dark-field signals using this technique and related them to the number of microstructures.

Here, we extend our previous work by relating the quantitative dark-field signals to the sample microstructure size and investigate the feasibility of performing quantitative dark-field imaging using a single sample exposure. We have applied our algorithm to images of polystyrene microspheres of 5 different diameters captured at the Australian Synchrotron's Imaging and Medical Beamline to evaluate how our measurements align with theoretical predictions. Future directions include performing quantitative dark-field tomography.

Imaging the motion of the lung in 3D to assess the effectiveness of a bacteriophage therapy for lung infection

Presenter: Stephanie Harker

Abstract ID#: 46

X-ray imaging is a useful investigative and diagnostic technique. Recent technological advancements in x-ray imaging have led to the development of Phase Contrast X-ray Imaging (PCXI) techniques which can revolutionise current medical research as well as have future use in clinical imaging. Paired with 4D X-ray Velocimetry (4DXV) it allows for non-invasive assessment of regional lung function, not currently possible with other forms of medical imaging and can be used to non-invasively assess the efficacy of emerging therapeutics. Bacteriophage therapy is a novel antimicrobial treatment which is clinically important due to increasing rate of multi-drug resistant bacterial infections. Bacteriophages are a promising alternative therapy, however current assessment of efficacy is highly invasive and, in many cases, requires the infected animals to be terminally anaesthetised. Our aim is to use 4DXV techniques as a viable, non-invasive alternative to demonstrate the efficacy of bacteriophage therapy in treating Pseudomonas aeruginosa pneumonia by measuring changes in lung function following treatment. Here we present the velocimetry analysis on the time resolved CT images we acquired at the Imaging and Medical Beamline (IMBL) in December 2021. This process will measure lung expansion throughout the breath cycle generating a vector field and measuring the difference in lung expansion between sick, treated, and healthy mice.

Current and future capabilities of the IRM beamline at the Australian Synchrotron, and guidance on applying for use of the facility

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Presenter: Mark Tobin

Abstract ID#: 50

Infrared (IR) spectroscopy provides information on the chemical composition of materials, based on the absorption of infrared light by the vibrating bonds within molecular groups. IR microspectroscopy, using synchrotron light as the infrared source, enables this analysis to be performed on samples as small as 1 – 2 μm in size, with a sensitivity not possible in the laboratory. ANSTO's synchrotron Infrared Microspectroscopy (IRM) beamline is equipped with a suite of accessories to enable the study of a diverse range of materials, including a sample heating and cooling stage, micro-compression cells for improved IR light transmission of dense materials, a liquid flow cell for the study of living organisms in a natural environment, and grazing angle optics for the analysis of thin films on surfaces. The IRM beamline also has several attenuated total internal reflection (ATR) accessories that can be used for the study of challenging materials such biofilms, carbon fibre, leaf surfaces and battery materials, where a thin section of the sample cannot be prepared. More recent developments on the IRM beamline include the use of polarisation optics to determine molecular orientation in materials and operation with a far-IR detector to extend the spectral range to 260 cm⁻¹. Future plans for the IRM beamline include the addition of a second branchline to assist the development of new sample environments, the motorisation of additional functions to improve the ease of use of the beamline, and in the longer term, the additional of nano-IR capability to the beamline. Scientists interested in accessing the IRM beamline are encouraged to contact the IRM beamline team to discuss their research proposals.

Presenter: Elette Engels

Abstract ID#: 53

The spinal cord is a sensitive organ at risk that can limit curative radiation doses in radiotherapy of cancers in the thoracic cavity. Microbeam radiation therapy (MRT) uses an array of microscopic beams for cancer treatment and has remarkable normal tissue sparing capabilities. At the Imaging and Medical Beam Line (IMBL) of the Australian Synchrotron, we previously showed that the spinal cord of rats could tolerate microbeams with doses of up to 400 Gy without acute neurologic adverse effects. However, long-term effects of on the spinal cord and surrounding tissues must also be considered for complete understanding of MRT dose tolerance.

This work will present long-term outcomes of the previous study on acute effects of MRT on the spinal cord. Prior to, and following thoracic spine MRT, adult female Wistar rats underwent neurological testing including gait and balance analysis, motor and sensory tests and electrophysiology measurements. Control rats (n=9) and rats irradiated with 400 Gy MRT (n=8) were followed up to 480 days post-MRT. Survival, body condition, and outcomes of gait and sensory tests were recorded.

MRT survival was not significantly different to controls (p=0.2), and both groups developed spontaneous tumours during the observation period (4/9 controls and 5/8 MRT rats). However, over 75% of MRT rats had mild gait challenges by day 483 post-MRT. These results indicate that 400 Gy MRT may cause late effects on spinal cord function, but does not significantly impact survival or cancer incidence.

Elucidating the antimicrobial mechanism of silver ions using synchrotron macro ATR-FTIR microspectroscopy

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Presenter: Ngoc Huu Nguyen

Abstract ID#: 57

Infection is known to be one of the major risks associated with implanted medical devices. Silver has been widely used in biomedical applications for antimicrobial activity and a few studies reported the concern of silver-resistant bacteria. However, the knowledge on how silver ions can influence the biochemical characteristics of bacteria remains unclear. In this study, we utilised high-resolution synchrotron macro-ATR-FTIR microspectroscopy to investigate biochemical changes, as a result of antimicrobial effect, in Gram-positive *Staphylococcus aureus* and Gram-negative *Pseudomonas aeruginosa*. The results revealed significant changes in polysaccharides, nucleic acids, protein, and lipid compositions in silver-treated bacterial cells. In particular, the absorption peaks characteristic of nucleic acids (1200–1075 cm-1), and polysaccharides (1150–900 cm-1) were observed to be significantly shifted in silver-treated bacteria cells. These alterations may be caused by the formation of reactive oxygen species when silver ions interacted with the bacterial cells. Importantly, this study will elucidate for the first time the molecular mechanism of silver ions on microbial cells, which is critical for underpinning the development of next-generation antimicrobial biomedical devices.

Terahertz spectroscopy of skin biomarkers, a step closer to melanoma detection

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Presenter: Xiaoqiong Qi

Abstract ID#: 68

With global incidence of melanoma on the rise and its prevalence among the most common cancers diagnosed in Australia, new and smarter detection strategies are needed more than ever. While early diagnosis remains the principal determinant of improving survivability (97-99% 5-year survival), the negative consequences of the over- and misdiagnosis of melanoma are less obvious and nevertheless impactful.

A plethora of cancer chemical signal carriers, such as amino acids, proteins and DNA mutations, exhibit unique characteristic spectral responses at THz frequencies, therefore holding great potential to be employed as biomarkers in cancer detection. The nonionizing nature of THz radiation, imparted by its low photon energy (meV), makes it ideally suited for probing biological samples and renders it non-destructive and safe. Thus, THz waves could be the key to providing solid evidence in triage and early diagnosis of melanoma.

Here we report results pointing to a suite of candidates to qualify as skin cancer biomarkers with abundant fingerprints at THz band. One such potential biomarker, the oncogene BRAF is commonly mutated at codon 600 in melanoma with targeted therapies designed to treat late-stage disease. Our recent synchrotron experiment results show that the BRAF (wild-type) and BRAF V600E proteins have clearly different absorbance spectra. We believe these findings will provide an important step towards the use of THz waves as a useful tool for the early detection and discrimination of melanoma.

The Mask of Zorro: Delivering Conformal Radiotherapy Fields with Synchrotron Radiation

Presenter: Micah Barnes

Abstract ID#: 73

Research utilizing synchrotron radiation for radiotherapy applications is becoming increasingly complex as it pushes towards human clinical trials. To date, multiple solutions exist for treatment planning and image guidance for synchrotron radiotherapy. However, treatment fields are still limited to simple geometric shapes based on a selection of prefabricated tungsten masks. Conformal fields are possible; however, they are subject to the time-consuming process of fabricating single-use Cerrobend masks. For this reason, conformal fields are often impractical and are not easily accessible. We present a design and proof-of-concept experiment for a new dynamic collimator design that provides conformal fields for synchrotron radiotherapy.

Our collimator design consists of six linear motors and two circular collimator leaves. Two motors are used for in-plane alignment of the collimator to the synchrotron beam and two motors are assigned, per-leaf, allowing vertical and horizontal movement of the leaves. As the target is vertically scanned through the beam, the leaves are moved such that they match the curvature of the portion of the target currently in the beam.

We planned a series of simple geometric shapes and real tumour shapes to deliver with our dynamic collimator. Each field was delivered to an imaging detector and DICE scores and Hausdorff Distances were used to measure the accuracy of the delivered fields. We have demonstrated both the limitations and capabilities of the system. Our novel collimator design is on track to be ready to service all radiotherapy experiments on IMBL with conformal treatment fields.

Theory to Reality; curative brain cancer treatment performed at the Australian Synchrotron

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Presenter: Sarah Vogel

Abstract ID#: 107

Whilst modern scientific research has improved the survival outlook for patients with most forms of cancer, the five-year relative survival for brain cancer has remained stagnant since the 1980s. A new, safe, alternative therapy for those suffering from this debilitating disease is long overdue. The Imaging and Medical Beamline (IMBL) at the ANSTO Australian Synchrotron (AS) delivers radiation at exceptionally high dose rates targeted to the tumour site, whilst still sparing surrounding normal tissue; a far safer solution to conventional radiation. This study combined Microbeam Radiation Therapy (MRT) with a novel and stable formulation of Gadolinium Oxide nanoparticles (GdNPs) to deliver a highly successful treatment, showing the potential for curative therapy at AS. 16 Fischer 344 rats were inoculated with 9L gliosarcoma in the right caudate nucleus of the brain. 11 days later, the rats were imaged with Computed Tomography (CT) at Monash Biomedical Imaging to locate the tumour . The following day, GdNPs were injected directly to the tumour of each rat. The rats were then aligned in-beam using the CT scans by comparing the bony anatomy, with a 5 mm bolus positioned over the irradiation site. One radiation fraction was delivered at valley doses of either 8 or 15Gy , with microbeams produced using the 4T magnet and Al/Al filtration. Comparing this GdNP and MRT combination therapy to our previous studies with other nanoparticles, GdNPs provided an exceptional result. Two rodents treated with 15 Gy are beyond 130 days post implantation and are not displaying symptoms. This is a significant improvement over treatment with MRT alone, where survival is approximately 50 days post implantation.

Chemistry, Catalyses & Soft Matter

Following and Controlling the Assembly of Paddlewheel-Based Cages

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Presenter: David Turner

Abstract ID#: 5

Coordination cages constructed around copper-carboxylate paddlewheel nodes are far less studied than their palladium-pyridyl cousins yet offer several advantages. The cages are inherently charge neutral, unless additional charge is embedded in the ligand, and the inclusion of carboxylate-based ligands enables chemistry that is not so readily accessed using N-donor ligands. Although versatile, the mechanisms of assembly and behaviour in terms of stability and ligand exchange is not well understood.
We have developed a series of homochiral lantern-type coordination cages that are based on amino-acid derived ligands arranged in a helical manner around two paddlewheel motifs. The charge neutrality of these cages allows the solution speciation to be followed by HPLC. This method can be elaborated to follow the process of ligand exchange. We have shown that the steric bulk close to the coordinating site is able to control the self-sorting process, even allowing selection of a single heteroleptic product from a mixture of ligands. The side groups control the stability of the complexes and play a determining role in the kinetics of ligand exchange between cages in solution. Ternary and quaternary mixtures of ligands provide more of a challenge, yet judicious choice of ligands dramatically reduces the number of observed species from a purely statistical distribution. Control over forming heteroleptic cages in a rapid, self-assembled system paves the way for these to be utilised with an easy 'mix-and-match' approach to combine an array of functionalities and properties within a cage complex.

Effect of cholesterol on Biomimetic Membrane Curvature and Coronavirus Fusion Peptide Encapsulation.

Presenter: Izabela Milogrodzka

Abstract ID#: 13

Measurements of quaternary systems consisting of monoolein (MO), cholesterol, phospholipids and water were conducted in order to achieve a large library of lipid nanoparticles with a wide range of mesophases. Synchrotron small-angle X-ray scattering (SAXS) was used to screen the phase behaviour of nanoparticles with varying composition of the three lipid components in a high-throughput manner. It has been observed that adding cholesterol and phosphatidylcholines had opposing effects on the spontaneous membrane curvature of the internal mesophase of the final nanoparticles. When in composition is more cholesterol than phospholipid then transition towards negative mean curvature mesophases occurs, but when more phospholipid than cholesterol in the nanoparticulate system then there is transition towards lamellar mesophase with positive mean curvature. Furthermore, encapsulation of the Coronavirus fusion peptide showed that in the presence of cholesterol, the negative mean curvature significantly increases. Cytotoxicity assay showed that by increasing the cholesterol level in the nanoparticles, the toxicity toward HELA cells was dramatically decreased. The addition of the peptide to the nanoparticles even with the lowest concentration of cholesterol resulted in considerable decreased of toxicity toward HELA cells as well. As the results, this work improves the potential for the biomedical end-use applications of the nonlamellar lipid nanoparticles.

Designing new catalysts for energy storage- is the nature of the active site always the right question to ask?

Presenter: Rosalie Hocking

Abstract ID#: 27

One of the greatest challenges of the 21st century will be securing cheap and renewable sources of energy. One of the most promising approaches to this challenge is to design catalysts from earth abundant materials capable of implementing key chemical reactions including splitting water into hydrogen and oxygen ($H2O \rightarrow 2H+ + O2$); and both the oxidation ($H2 \rightarrow 2H+$) and reduction ($2H+ \rightarrow H2$) of hydrogen among many others. In studying catalysts, we often focus on the "nature of the active site" which for classical heterogenous catalysts works well- but not all catalysts work by a surface sorption processes alone! In some systems the redox events between substrate and catalyst and the speed of these processes appear to play a key role in both engineering product selectivity and catalyst stability. In this talk we will explore using some of our observations from both in situ and ex situ X-ray Spectroscopies how understanding redox chemistry between catalyst and substrate maybe key for understanding mechanisms of catalysis. We explore often overlooked phenomena in catalyst systems including "whole of material" stability, structure disorder and thermodynamics (as opposed to kinetic) stability. We examine how the events after catalysis maybe key for understanding the active events of catalysis.

Tuning the nanostructure and surface charge of phytantriol-based cubosomes using choline ionic liquids

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Presenter: Mohamad El Mohamad

Abstract ID#: 37

The structure-function relationship of lyotropic liquid crystalline nanoparticles (LCNPs) is of fundamental interest for their development as sustained release delivery systems. Ionic Liquids (ILs) are tailorable solvents, some of which can be used as designer solvents for LCNPs. We employed synchrotron small angle X ray scattering (SAXS) and zeta potential measurements to investigate the nanostructure and surface charge of phytantriol (PHY)-based LCNPs doped with 12 choline based ionic liquids. Most ILs preserved the diamond cubic (QD2) structure of phytantriol. Cubosomes with a primitive nanostructure (QP2) were also obtained. The ILs mostly increased the lattice paramater of the particles as the IL concentration increased. The phase behaviour of the particles depended on the structure of the anions, and the IL's concentration. Moreover, positively charged cubosomes were obtained in PHY:IL samples prepared in 20 mM citrate and acetate buffers. The charge of the particles depended on the IL's concentration and the pH of the solution. This study validates the efficiency of using biocompatible ILs as tailorable solvents for the preparation of responsive LCNP systems.

Structures and Phase Transition in CaUNb2O8

Presenter: Maria Nicholas

Abstract ID#: 64

$CaUNb_2O_8$ is a rare example of a scheelite-type oxide containing U^{4+} on the 8-coordinate site. Previous low resolution X-ray diffraction studies have revealed that the structure of $CaUNb_2O_8$ at room temperature is lower in symmetry than the archetype scheelite structure. We have prepared $CaUNb_2O_8$ by solid state synthesis and sintering in a reducing environment, and its structure was refined by the Rietveld method using high resolution synchrotron X-ray powder diffraction data. $CaUNb_2O_8$ has a monoclinic structure at room temperature in space group I 2/c, isostructural to fergusonite, with a = 5.3909, b = 11.0987 and c = 5.1069 Å and β = 94.798 °. An in situ variable temperature study, using synchrotron X-ray powder diffraction, also revealed a reversible phase transformation from fergusonite to scheelite, and the transition appeared to be continuous. Heating $CaUNb_2O_8$ above 760 °C resulted in a transition to a tetragonal structure in space group I 41/a, with its lattice parameters at 1000 °C being a = 5.2897 and c = 11.2613 Å. The fergusonite to scheelite phase transition was also observed in a recent neutron diffraction study of NdNbO4, where the transition was considered strictly as first order due to the breaking of the two long Nb-O bonds. With our upcoming in situ neutron powder diffraction measurements, the nature of the fergusonite to scheelite transformation in $CaUNb_2O_8$ will be revisited.

Liquid crystal phase formation of Monoolein in protic ionic liquids

Presenter: Stefan Paporakis

Abstract ID#: 87

Liquid crystal phases (LCPs) formed through the self-assembly of lipids are disordered bulk materials. The ability of lipids to self-assemble into different LCPs is dependent on lipid-solvent interactions, lipid concentration and temperature. Protic Ionic Liquids (PILs) are both tailorable solvents and low melting point liquid salts, where many have been shown to support the self-assembly of lipids. While separately the roles of PILs, lipids and LCPs have proven benefits in biological fields like protein crystallisation, foundational knowledge of LCPs present for lipid: PIL systems is lacking. In this study, the LCP behaviour of the lipid Monoolein (MO) was investigated in a series of 6 PILs known to support amphiphile self-assembly, namely ethylammonium nitrate (EAN), ethanolammonium nitrate (EtAN), ethylammonium formate (EAF), ethanolammonium formate (EtAF), ethtylammonium acetate (EAA), and ethanolammonium acetate (EtAA). The effect on MO self-assembly of systematic changes to the PIL structure was conducted, including increasing alkyl chain length, presence of a hydroxyl group on the cation, and changing the anion. The formed LCPs were studied using synchrotron small and wide angle x-ray scattering (SAXS/WAXS), paired with cross polarized optical microscopy (CPOM). Utilisation of a high throughput LCP identification procedure aided in discovery of hexagonal, bicontinuous cubic, lamellar and multiphase LCPs, leading to the production of intricate phase diagrams for 40-75wt% MO in the temperature range of 25C-75C.

The silver bullet: using silver doped lanthanum manganite to improve preclinical survival of glioma bearing rats

Presenter: Abass Khochaiche

Abstract ID#: 108

Introduction
Successfully treating deadly brain cancer is often limited to adequate targeting strategies. Additionally, sparing surrounding sensitive healthy tissue necessitates more efficient strategies that can selectively target a tumour. This study introduces lanthanum manganite (LAGMO) NPs as promising candidates for a targeted in vivo brain cancer treatment as a selective chemotherapeutic agent and radiation dose enhancer.

Method
Biocompatibility and combinational treatment strategies involve phenotypical cellular analysis, in vitro clonogenic assays, and cancer cell selectivity investigations. In vivo short and long-term survival in Fischer 344 rats bearing brain tumour was investigated using CT imaging analysis at the University of Wollongong and microbeam radiation therapy at the Australian Synchrotron.

Results
Biocompatibility studies of LAGMO NPs revealed that they are cancer cell selective and promote the healthy growth of non-cancerous cells. Clonogenic assays substantiated a significant decrease in the long-term survival of gliosarcoma cells when combining LAGMO NPs with radiation. CT imaging on brain cancer bearing Fischer 344 rats and long-term survival after treatment with and without radiation therapy was investigated.

Conclusion
LAGMO NPS have recently shown significant success in the treatment of brain cancer in vitro. Their unique bio-chemical properties also introduce potential to improve radiation treatment strategies and clinical outcomes. Continuing to push the limits of this NP to improve treatment outcomes in vivo will propel the research of LAGMO NPs and introduce it as a potential candidate for clinical studies.

References

Khochaiche, Abass, et al. "First extensive study of silver-doped lanthanum manganite nanoparticles for inducing selective chemotherapy and radio-toxicity enhancement." Materials Science and Engineering: C 123 (2021): 111970.

Earth & Environment

Using the Australian Synchrotron to characterise low level radioactive by-products from a decommissioned subsea oil and gas pipeline

Presenter: Amy MacIntosh

Abstract ID#: 3

Successful decommissioning of offshore oil and gas infrastructure requires an effective and safe approach to assess and manage chemical and radiological residues. Scale frequently accumulates on the interior surfaces of pipes and other infrastructure and can contain metal contaminants, as well as naturally occurring radioactive materials (NORM). Characterising scale is essential to evaluate the presence of contaminants and inform environmental assessments. This study aims to determine the composition of pipeline scale through high-resolution elemental mapping and speciation analysis by utilising the x-ray fluorescence microscopy beamline at the Australian Synchrotron (XFM). Data will be presented from recent XFM experiments that (i) investigated the homogeneity of metals and radionuclides associated with the scale and (ii) identified any co-location of the barium sulphate with other key elements and radionuclides (Ra-226, Pb-210, Po-210). Nuclear techniques can provide early detection methods to enable petroleum regulators to develop and utilize thresholds at which issues may occur in marine biota. New knowledge and insight into petroleum waste products will enable pipeline scale testing for offshore oil and gas operators on a commercial basis and inform an understanding of the potential risk it may pose to marine ecosystems.

Sequestration of arbuscular mycorrhizal fungal derived carbon in Fe ore tailings

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Presenter: Songlin Wu

Abstract ID#: 6

Organic carbon (OC) generation and sequestration are pre-requisites for aggregate formation and pedogenesis in the Fe ore tailings for sustainable mine site rehabilitation and climate change mitigation. Arbuscuar mycorhrizal fungi play an important role in soil aggregate structure formation and OC stabilization, therefore has great potenital in OC accumulation and sequestration in Fe ore tailings. The present study aimed to characterise the development of AM symbiosis in tailing technosol and their typical role in OC sequestration in the tailings. It was found that that AM fungi formed symbiotic association with Sorghum spp. plant roots in the early eco-engineered tailings amended with plant biomass. AM symbiosis enhanced the formation of micro-aggregates (53~250 um) through the fungal mycelium which entangled mineral particles together as revealed by BSE-SEM analysis. AM symbiosis also enriched the stabilization of organic carbon and nitrogen in the form of organo-mineral association in tailing aggregates. Synchrotron based transmission FTIR analysis revealed that lipids and proteins (or aromatics) derived from AM fungal mycelium associated with tailing mineral particles for aggregation. Synchrotron based C 1s NEXAFS and Fe K edge XAFS analysis further confirmed that organics rich in carboxylic, alkyl, and aromatic groups were intimately associated with Fe rich phyllosilicates and/or amorphous Fe oxyhydroxides (such as ferrihydrite) within aggregates. These findings revealed the critical role of AM fungi in OC sequestration in the Fe ore tailings during eco-engineered pedogenesis for resilient mine site rehabilitation.

Using infrared microspectroscopy to understand the cellular chemistry of alpine mosses for habitat selection

Presenter: Annaleise Klein

Abstract ID#: 60

The Australian Alps are a water-rich landscape with many headwater streams originating from groundwater-fed peatlands. These peatland ecosystems support a range of moss species which subsequently modify the composition of stream waters through exchange and nutrient uptake processes. We have chosen to study and compare two species of moss that are found in the same general location of alpine peatlands however are distinctly spatially separated within the peatland: (1) Sphagnum cristatum, a dominant semi-aquatic moss species located on drier terrain adjacent to groundwater sources, and (2) Blindia robusta, an aquatic moss found exclusively within groundwater source pools. Spatial separation of these two species has been attributed to the different pH of the two environments they inhabit, with the groundwater source pools being more acidic. It is known that Ca2+ can play an important role in cell wall structures, and the uptake of Ca2+ from an external aqueous environment is pH dependent. Therefore, this research focussed on the acid-base chemistry and affinity for Ca2+ of S. cristatum and B. robusta. Using a series of pH and Ca2+ titrations in H2O and D2O medium in conjunction with infrared microspectroscopy (IRM beamline), we determined the pKa and Ca2+ binding constants of S. cristatum and B. robusta. This work has led to better knowledge of the factors controlling metal uptake in these moss species, and the role of water composition in controlling moss distribution in the peatland landscape.

Eat your greens – thallium in cabbages by XFM and XANES

Presenter: Lachlan Casey

Abstract ID#: 71

Cabbages and other *Brassica* varieties, while important and nutritious crops, also have the unusual property of being hyper-accumulators of thallium (Tl), a highly toxic post-transition metal. *Brassicas* have been observed to take up more than 500 µg Tl g-1 when grown in polluted soils, and would pose a significant health-risk if an edible crop were grown in an area of high environmental Tl. Despite this, Tl is not listed as a food contaminant in Australia, and there is little data on its bioavailability in these plants. Secondly, despite its toxicity, Tl is among the most expensive metals due to its limited availability, and the potential for resource recovery via biomagnification is of great additional interest.

To examine the physiology of Tl uptake in these important crops, and therefore the possible consequences of a contamination event, we have grown edible *Brassica* varieties in Tl-enriched media, and imaged these via laboratory XFM, synchrotron XFM and XANES. We observed high concentrations of Tl in the edible leaves, highly enriched at the outer edges of the leaf. We were further able to identify two apparent sequestration types, one in a likely soluble form localised to the minor veins, and a second likely inorganic form localised to micron-scale inclusions throughout the leaf tissue. We performed XANES mapping on a subregion of one area rich in Tl, and found evidence of two distinct oxidation states; Tl(I) in the leaf tissue, and likely Tl(III) in the inclusions. The potential presence of Tl(III) is of particular concern, with these compounds being up to 50,000x more toxic than even Tl(I).

Characterisation of the crystallisable water in precious opal using synchrotron terahertz spectroscopy

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Presenter: Paul Thomas

Abstract ID#: 105

Precious opal is a hydrous silica with the general formula SiO2. nH2O and is predominantly silica (approximately 92% SiO2) with circa 1% alumina (as network former), 0.5% alkali and alkali earths and typically 6 to 7 % water, although the water content can vary significantly and can range up to circa 20%. The water contained in opal is present in both bound and molecular forms. The bound water is present as silanol at internal (pore and voids) and external surfaces, as well as distributed through the silica network. Molecular water is present in pores and voids and is also distributed through the silica network trapped in cages. Circa 20% of the molecular water is contained in pores and voids and is localised in large enough volumes to be crystallisable. Crystallisation of the water in opal has been demonstrated by differential scanning calorimetry and near infrared spectroscopy and is useful in understanding the microstructure of the opal through melt temperature depression in capillaries and voids. This presentation extends this characterisation of the crystallisable water to terahertz region of the spectrum, presenting the outcomes of an investigation carried out at the Australian Synchrotron.

Corals' Metallomic and Crystallographic Signatures: New Methodology for Investigating Coral Resilience

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Presenter: Annette Dowd

Abstract ID#: 112

Coral health is known to suffer as a result of increased water temperature or changes in water quality. The recent discovery that colonies of some open water species of coral can thrive in the warm, muddy environment of mangrove lagoons[1] raises important questions about the unknown strategies used by corals to adapt to extreme environments. Studies of these stress-resistant corals have so far focused on coral soft tissue (metabolomics, physiological diagnostics etc [2]) however the coral skeleton has been relatively neglected. This project aims to answer the question: Is the physiological response of coral to different environments recorded in the skeleton and can it add to our understanding of coral adaptability?

To study the trace elements stored in coral calcium carbonate skeleton, we employed X-ray fluorescence microscopy at the Australian Synchrotron. These high resolution maps were correlated with sensitive laser ablation-inductively coupled plasma mass spectrometry maps to study the anatomical features with altered bioaccumulation of transition metals known to aid stress survival[3]. Temperature resolved powder diffraction was used to study alterations to the microstructure and crystallography of the skeleton, which are related to trace element chemistry and growth rate[4]. We show that the metallomic and crystallographic signatures of coral skeleton has application in studying the fitness of coral to thrive in environmental extremes.

References

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[2] E.F. Camp et al., Marine Ecology Progress Series, 625, 1 (2019).
[3] H. Haraguchi, Metallomics, 9, 1001 (2017).
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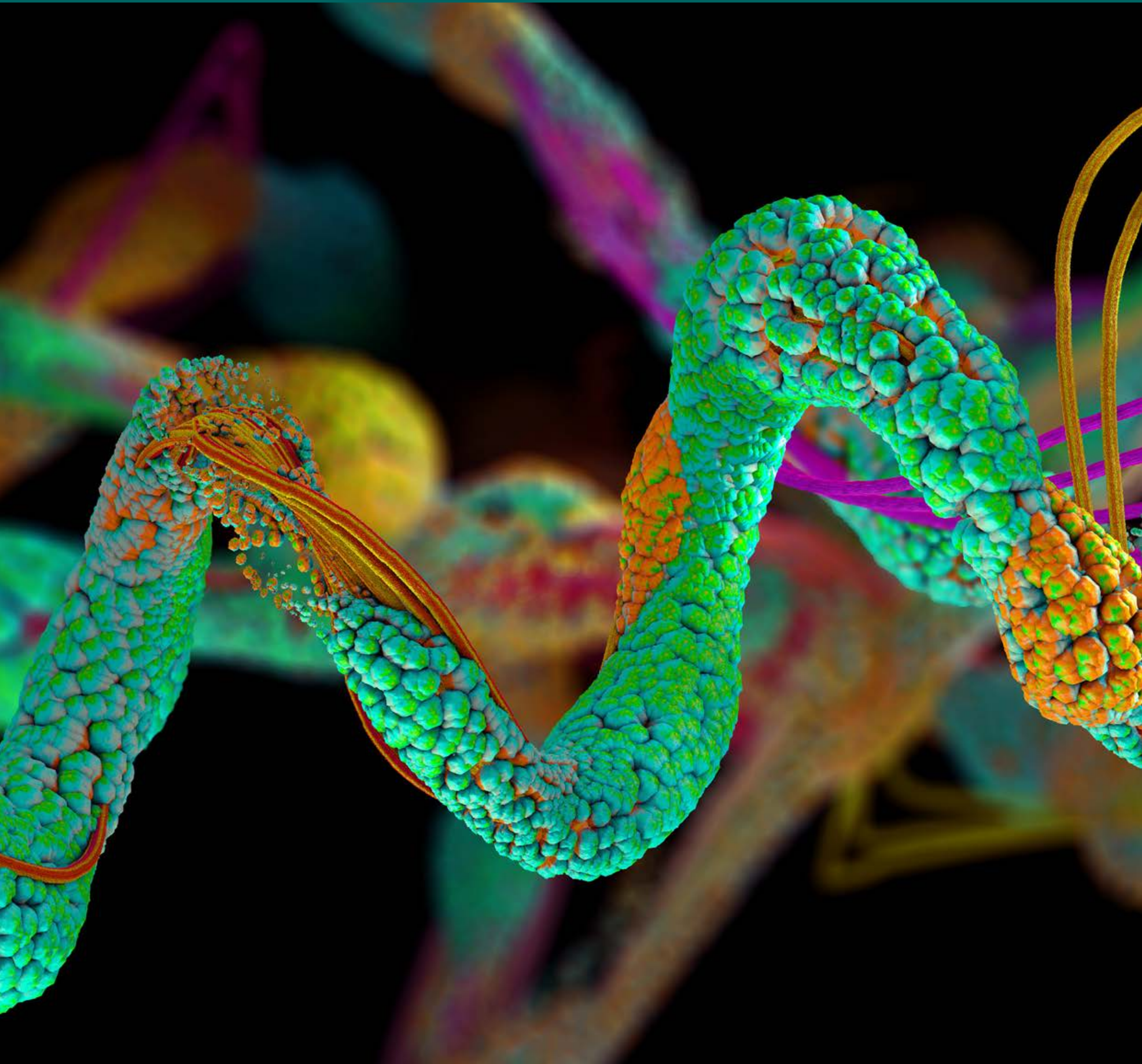
Life Science & Structural Biology



Structure of the metastatic factor P-Rex1 reveals a two-layered autoinhibitory mechanism

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Presenter: Tyler Chang

Abstract ID#: 2

P-Rex (PI(3,4,5)P3-dependent Rac Exchanger) guanine nucleotide exchange factors (GEFs) potently activate Rho GTPases. P-Rex GEFs are autoinhibited, synergistically activated by Gβγ and PI(3,4,5)P3 binding, and dysregulated in cancer. Here we utilise X-ray crystallography, cryo-EM, and cross-linking mass spectrometry to determine the structural basis of human P-Rex1 autoinhibition. P-Rex1 has a bipartite structure of N- and C-terminal modules connected by a C-terminal four-helix bundle (4HB) that binds the N-terminal Pleckstrin homology (PH) domain. In the N-terminal module, the Dbl homology (DH) domain catalytic surface is occluded by the compact arrangement of the DH-PH-DEP1 domains. Structural analysis reveals a remarkable conformational transition to release autoinhibition, requiring a 126° opening of the DH domain hinge helix. The off-axis position of Gβγ and PI(3,4,5)P3 binding sites further suggests a counter-rotation of the P-Rex1 halves by 90° facilitates PH domain uncoupling from the 4HB, releasing the autoinhibited DH domain to drive Rho GTPase signalling.

Small-angle X-ray scattering (SAXS) measurements of APO-BEC3G provide structural basis for binding of single-stranded DNA and processivity

Presenter: Elena Harjes

Abstract ID#: 33

APOBEC3 enzymes are polynucleotide deaminases, converting cytosine to uracil on single-stranded DNA (ssDNA) and RNA as part of the innate immune response against viruses and retrotransposons. APOBEC3G is a two-domain protein that restricts HIV. Although X-ray single-crystal structures of individual catalytic domains of APOBEC3G with ssDNA as well as full-length APOBEC3G have been solved recently, there is little structural information available about ssDNA interaction with the full-length APOBEC3G or any other two-domain APOBEC3. Here we investigate the solution-state structures of full-length APOBEC3G with and without a 40-mer modified ssDNA by small-angle X-ray scattering (SAXS), using size-exclusion chromatography (SEC) immediately prior to irradiation to effect partial separation of multi-component mixtures. To prevent cytosine deamination, the target 2′-deoxycytidine embedded in 40-mer ssDNA was replaced by 2′-deoxyzebularine, which is known to inhibit APOBEC3A, APOBEC3B and APOBEC3G when incorporated into short ssDNA oligomers. Full-length APOBEC3G without ssDNA comprised multiple multimeric scattering species, mostly tetrameric. The structure of the tetramer was elucidated. Dimeric interfaces significantly occlude the DNA-binding interface, whereas the tetrameric interface does not. This explains why dimers completely disappeared and monomeric protein species became dominant, when ssDNA was added. Data analysis of the monomeric species reveals a full-length APOBEC3G-ssDNA complex that gives insight into the observed "jumping" behaviour revealed in studies of enzyme processivity. This solution-state SAXS study provides the first structural model of ssDNA binding both domains of APOBEC3G and provides data to guide further structural and enzymatic work on APOBEC3-ssDNA complexes.

High-Resolution Phenotyping for Spatial Localisation and Quantification of Nutrients in Rice Grains

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Presenter: Vito Butardo

Abstract ID#: 81

In a post-genomic era where thousands of rice genomes are already sequenced, the identification of the genetic basis of grain and nutrition traits by genome-wide association is not possible without the availability of high-resolution phenotyping. Current cereal chemistry techniques are rather limited for this purpose because most involve chemically destructive analyses that destroy any spatio-temporal information in the seeds. Here we describe how offline and online synchrotron-based techniques are utilised to characterise the grain ultrastructure and elucidate the spatial mobilisation of nutrients in rice grains. Micro-computed tomography revealed startling details of the grain ultrastructure and identified rice accessions with thick multicellular aleurone layers. Bulk x-ray fluorescence (XRF) spectroscopy followed by validation using XRF imaging showed contrasting rice accessions with elevated Zn and Fe. X-ray fluorescence microscopy and XRF imaging uncovered the mobilisation pattern of micronutrients of germinating rice grains from the aleurone layer to the embryo and the developing roots and shoots. Lastly, bulk mid-infrared (IR) spectroscopy and attenuated total reflectance-Fourier transform infrared spectroscopy estimated the proportion of storage protein, starch, lipid and phenolic compounds in coloured rice grains. Moreover, hyperspectral IR imaging demonstrated that anthocyanins in some coloured rice accessions are present as a distinct layer external to the rice bran. These novel applications of synchrotron radiation pave the way for more rapid grain quality and nutrition screening and for the molecular elucidation of the nutriomic variation of the mobilisation patterns of nutrients in rice and other cereals.

Tiny, Fast and Sweet: IMBL Cyberanatomy of one of the World's Smallest Marsupials

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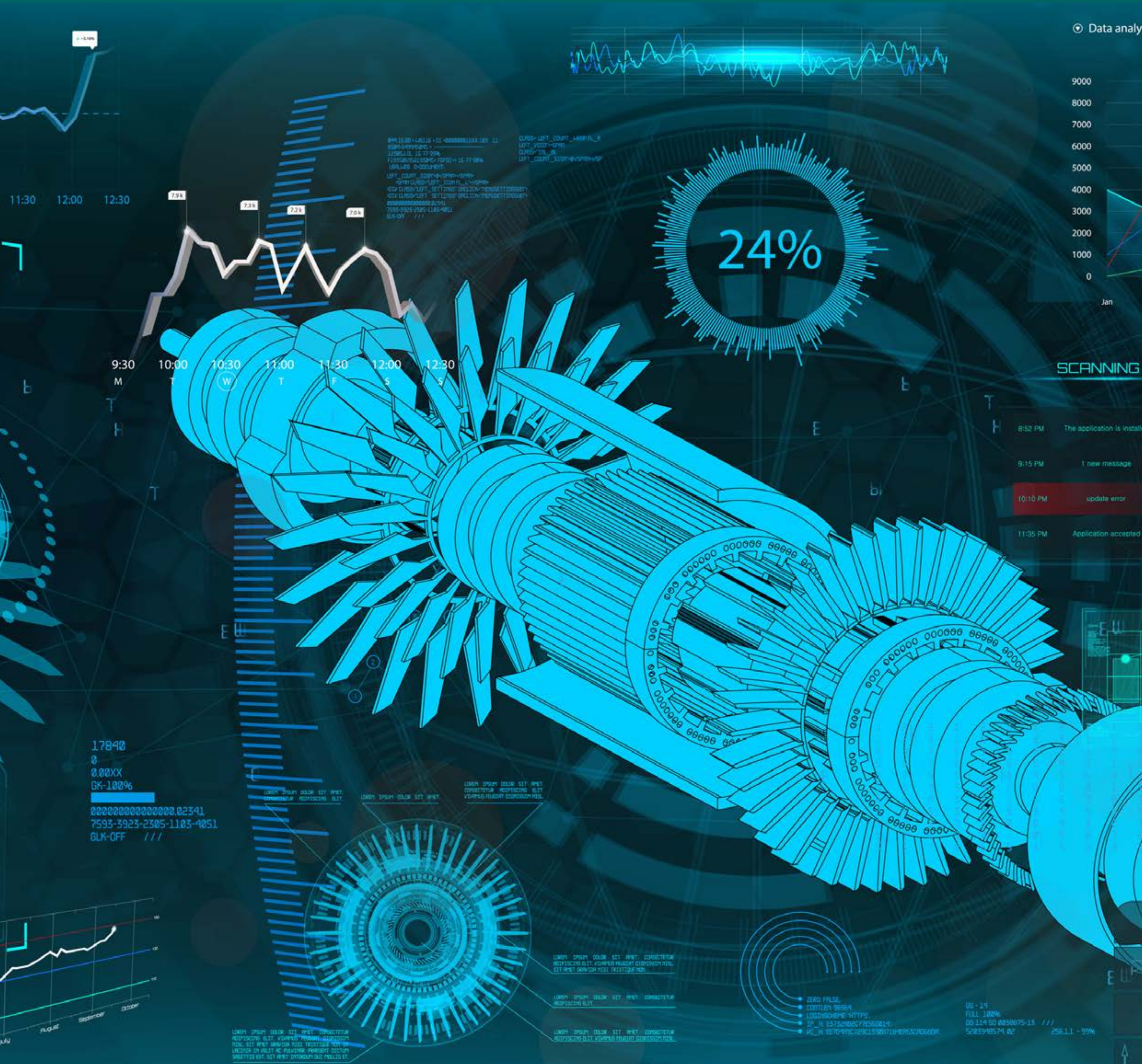
Presenter: Lucy Costello

Abstract ID#: 98

The Australian honey possum (Tarsipes rostratus) is one of the world's smallest living marsupials, measuring less than 10cm and weighing between 5-10g as an adult. They are a keystone species, uniquely adapted to eat nectar and pollen and are also a primary pollinator of banksias across south-east Australian ecosystems. Despite their unique set of adaptive features and physiology, honey possum anatomy remains poorly understood. This lack of basic structural biological data reflects a combination of challenges to traditional anatomical data collection, from their small size to their conservation status. This creates a fundamental gap in our understanding of the biology, behaviour, and evolutionary history of the species. It also presents barriers for designing and deploying biologically grounded conservation approaches for honey possums; a species facing increasing pressure from habitat loss and increasing bushfire risks.

This research presents the outcomes of using the Australian Synchrotron's Imaging and Medical Beamline (IMBL) to investigate honey possum anatomical adaptations using cyberanatomical methods. We present our approach to imaging, digital dissection and volumetric analysis, as well as our exploration of anatomical systems linked to the unique physiology of the honey possum. This includes investigating proportions of major organs and systems impacted by adapting to a specialised diet, from the oral cavity and chewing muscles to cardiac structure and digestive system anatomy supporting their fast-metabolic rate. In doing so, we highlight the power of Synchrotron imaging and cyberanatomy for bypassing the limits of traditional anatomical dissection, exploring novel form-function relationships, and advancing new avenues for non-destructive data collection from museum collections of vulnerable and threatened marsupial species.

Manufacturing, Engineering & Cultural Heritage



Three-Dimensional Phase Imaging with the Near Infrared Synchrotron Beam Using Phase-Retrieval Algorithm

Presenter: Molong Han

Abstract ID#: 11

The infrared synchrotron beam has a unique fork shaped intensity distribution with a spectrum ranging from near infrared (~1 μm) to far infrared (~ 13 μm). All of the spectroscopy and molecular fingerprinting measurements are carried out in the mid to far infrared (NIR) region. Further, the presence of NIR beam reduces the signal to noise ratio by nearly four times. Consequently, a high pass (wavelength) filter is introduced at the entrance of the infrared microspectroscopy unit to block the NIR part. In this study, we have used the usually discarded NIR part of the synchrotron beam for phase imaging. The near infrared synchrotron beam was extracted from microspectroscopy unit. A pinhole with a diameter of 200 μm was inserted in the path of the beam and aligned with one of the lobes of the fork to obtain maximum throughput. The resulting Airy diffraction pattern was incident on different samples such as polystyrene beads, wings of insect and silk samples and the diffracted intensity distribution was captured by an image camera sensitive to NIR wavelengths. A phase-retrieval algorithm with parameters exactly matching the experiment was built with Fresnel propagation between the object plane and sensor plane. At both the object plane and sensor plane, phase is unknown while the intensity is known. The algorithm iteratively estimates the phase of the sample. The algorithm converged rapidly with as low as five iterations and the resulting phase map matched well with the reference images recorded using a microscope.

Rapid Polarization Imaging at the Infrared Beamline of the Australian Synchrotron

Presenter: Soon Hock Ng

Abstract ID#: 12

The infrared microspectroscopy system of the Australian synchrotron has an unconventional fork shaped input beam due to the reflection from a gold-coated mirror with a central slit during the extraction from the storage ring. The infrared synchrotron beam is predominantly polarized with a minor part remaining unpolarized often resulting in peculiar behaviour, while studying birefringent samples. In this study, we observed that the point spread function (PSF) was sensitive to not only spectrum but also the polarization direction of the Thallium Bromoiodide (KRS-5) window installed at the entrance of the microspectroscopy unit. The KRS-5 window was rotated in steps of 15 degrees from 0 to 180 degrees and the polarization PSFs were recorded for the entire spectrum in the first step using the focal point array (FPA) detector. In the next step, a birefringent sample was recorded by a scanning approach using the FPA. The regions of the sample with different polarization orientations were estimated using the recorded PSFs and the relative intensities measured from the different regions of the sample. Preliminary studies on paracetamol sample showed that the polarization map obtained using our method matched significantly with the microscope images of the sample. The time of recording using this approach was significantly smaller than using the single pixel Mercury-Cadmium-Telluride (MCT) detector.

LipSynch Battle: IRM vs XFM for the study of cosmetic traces for forensic purposes

Presenter: Simon Lewis

Abstract ID#: 26

The transferability and variability of cosmetic products makes them an ideal form of trace evidence in criminal investigations (1). Similar cosmetic traces recovered from various people, places or objects may assist in proving contact between them, especially if these traces are chemically distinctive. Although many studies have examined the composition of bulk cosmetics, forensic traces such as lip- or fingermarks are expected to be more complex, due to the impact of exogenous components and environmental factors. Accurate interpretation of cosmetic evidence thus requires an understanding of the trace chemistry and how it changes with time. To date, there has been little fundamental study of cosmetic residues, particularly when deposited onto a substrate via contact transfer.

Building on our previous experience applying synchrotron techniques to study latent fingermarks (2,3), we have recently commenced studies using synchrotron IRM and XFM to colocalise organic and inorganic cosmetic components found in lipmarks and fingermarks as examples of forensic contact transfer. This is expected to generate an understanding of the microscale chemistry affecting cosmetic transfer and persistence for forensic interpretation frameworks. The outcomes will also provide a case study supporting the value of multimodal spectroscopic imaging using synchrotron radiation.

This research was supported by an AINSE Ltd. Early Career Researcher Grant (ECRG) for Georgina Sauzier and an AINSE Ltd Postgraduate Research Award (PGRA) for Rhiannon Boseley.

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2. R.E. Boseley *et al.*, Anal. Chem., 2019, 91:10622-10630
3. R.E. Boseley *et al.*, Analyst, 2022, 147: 799-810.

A comparison of residual stress in straight and curved laser clad light rail components using neutron diffraction

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Presenter: Olivia Kendall

Abstract ID#: 28

To support the increasing passenger demand on public transport networks, new maintenance strategies are required as a substitute to disruptive replacement procedures. As lower steel grades used in light rail systems are susceptible to wear and rolling contact fatigue, laser cladding is one technique which may be used for repairs.

During laser cladding, a high energy laser metallurgically bonds a metallic powder to the rail surface to form a coating that offers improved tribological properties. In comparison to welding techniques, laser cladding requires lower heat inputs which reduces the size of heat affected regions generated below the fusion boundary. Nevertheless, this thermal process results in the generation of residual stresses due to microstructural changes. As the combination of residual and wheel-rail contact stresses governs the fatigue behaviour, accurate measurement of stress is essential to understanding rail performance after cladding repairs.

The manufacturing procedures used to produce curved and straight rails generate regions of tensile and compressive stresses. Understanding how laser cladding influences the stress distribution in different rail geometries is a critical aspect in developing a versatile laser cladding repair strategy. Stellite 6 laser cladding has been carried out on 600 mm sections of straight and curved ex-service tram blades. The Kowari strain scanner was used to record the triaxial stresses across the cladding, heat affected zone and substrate along each blade. The findings show higher stresses at the centre of the rails with a compressive peak in the round blades. The stress measurements will accompany microstructural and mechanical property evaluations to establish the influence of rail curvature on internal stress distribution and by extension, the fatigue lifetime.

XFM beamline capabilities and future directions

Presenter: David Paterson

Abstract ID#: 86

The X-ray fluorescence microscopy beamline (XFM) at the Australian Synchrotron saw first light in 2008 and serves a very diverse user research community. Major upgrades to the X-ray fluorescence detection schemes and scanning microprobe architecture have been made to the original instrument. Improvements have focused on maximizing X-ray fluorescence detection efficiency alongside an in-house designed hyper-efficient raster scan sample stage motion control. Recently, ptychography has been added to the suite of imaging modes, providing complementary nanoscale morphological context to fluorescence data.

Driven by the challenges of the COVID pandemic we have ramped up and improved remote operation and analysis capabilities and consequently have found that many samples are ideal for "mail-in" experiments at XFM.

We describe the XFM beamline's current capabilities and research highlights that employ and demonstrate the outcomes possible from these capabilities. We outline the best practice sample preparation and mounting methods and show the data analysis tools that are available for online (during experiment) and offline (remote and post-experiment) XFM data analysis and synthesis.

Looking forward we describe some short- and longer-term strategic upgrade plans. A major funded upgrade is to "turbo charge" the beamline by incorporating a horizontal-bounce double multilayer monochromator (DMM), increasing flux delivered to the XFM endstation across the 4 to 30 keV energy range [See poster for more details].
In the next 3 years a strategic technique and science goal is to reinvigorate 3 dimensional XFM or X-ray fluorescence tomography with a postdoctoral fellow commencing a project to develop a user-friendly X-ray fluorescence tomography data processing pipeline.

6 Cats, 1 Dog, 3 Chickens - Scientific Computing at the Australian Synchrotron

Presenter: Andreas Moll

Abstract ID#: 96

The Scientific Computing team at the Australian Synchrotron supports our users through the whole experiment lifecyle, from running an experiment to collecting, processing and analysing data. This presentation will provide you with an overview of all the amazing things that we are currently building for our beamlines, including scripting of experiments, automated data processing systems and brand-new user interfaces.

We will also cover the services that we currently offer to our users, together with a few helpful tips and tricks.

Come along to this talk to learn more about Scientific Computing, what we do and what you can expect to see at our beamlines in the upcoming years. Also, there might be pictures of cats, dogs and chickens.

Using in-situ loading methodologies to understand how metals deform

Presenter: Michael Preuss, Agius Dylan

Abstract ID#: 99

Plasticity and failure of engineering alloys remains a topic dominated by empirical rather than mechanistic understanding. The complexity of plasticity in alloys is due to the polycrystalline and often multiphase nature of such materials and their inherent anisotropy at the crystal level. Metals and alloys develop highly localised strain during mechanical loading that leads to stress heterogeneity and eventual failure. As a result of our empirical understanding, life predictions of components are associated with high uncertainties that result in heavy overengineering, i.e. non-efficient use of resources.

High energy synchrotron x-ray diffraction, together with other advanced characterisation tools, has played a major role in providing new insight in plasticity of alloys. This enables us to study materials in-situ during mechanical loading rather than simple post-mortem analysis. The objective here is to monitor the lattice (elastic) strain development in either grain families or individual grains. In addition, detailed line profile analysis can provide information on dislocation densities.

The presentation will provide an overview of these in-situ loading methodologies, give examples, and describe some of the new knowledge generated. In addition, the importance of this integrated experimental approach to the development, verification, and validation of crystal plasticity models will be presented.

Orchestrating a synchrotron ready in-situ experiment in the laboratory environment: Case study on Mg alloy

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Presenter: Sitarama Raju Kada

Abstract ID#: 100

Synchrotron X-ray radiation provides unique opportunities for performing in-situ and in-operando experiments for solving material problems. Critical offline pre-testing can maximise the effective use of limited synchrotron beamtime. Here, we introduce an exciting new in-situ X-ray testing facility for pre-synchrotron screening measurements. Housing a high brightness liquid metal jet X-ray source (max voltage of 70 kVp and a characteristic energy of ~9 keV) the insitX facility has the potential to perform a diverse range of in-situ experiments including, high-energy polychromatic X-ray diffraction, monochromatic small-angle scattering (SAXS) and wide angle x-ray scattering (WAXS) and finally imaging modalities. The facility can provide important independent insight as well as providing for pre-synchrotron testing under 'like' conditions. Here we demonstrate a methodology with a case study on a precipitation strengthened Magnesium-Zinc (Mg-Zn) alloy.

Mg-Zn alloy suffers from strong mechanical asymmetry which is the result of poor strengthening of twinning over slip mechanisms in age-hardened alloy. It is challenging to record the onset of twinning due to its abruptness and this requires high-speed detectors available at Imaging and medical beam line - IMBL at Australian synchrotron. We performed a series of in-situ tensile deformation tests and simultaneously collected in-situ high-energy Laue diffraction data to pre-screen samples and establish best parameters for making an IMBL-ready experiment. The small-angle and high-angle X-ray scattering setups were used to pre-evaluate the precipitate fractions to be used in this study. We also performed a correlative in-situ digital-imaging-correlation and high-energy X-ray imaging investigations to understand the macroscopic strain evolution and crack-growth kinetics in the presence of precipitates in age-hardened Mg-Zn alloy.

Application of Pilatus external trigger mode for real time dynamic materials testing

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Presenter: Peter Lynch

Abstract ID#: 106

Traditional in-situ tensile/compressive diffraction experiments rely on a step-wise incremental loading measurement strategy. Under these conditions the impact of loading strain rate and/or cycle frequency cannot be readily observed. By application of the Pilatus 2D detector triggering capability, dynamic loading experiments are measured in real time. Here we report on the application of the Dectris external trigger mode for real time fatigue testing of Ti6-4 metal alloys. The experiment was setup on the SAXS-WAXS beamline at the Australian synchrotron facility. A transmission diffraction experiment was employed at an energy of 21keV. The sample cross-head positional readout, from an Instron 1kN tensile loading stage, was used to trigger the detector. As the sample was continuously loaded/unloaded diffraction patterns were recorded at the maximum force position of each loading cycle. In total 3 fatigue experiments were performed at a cycling frequency of 10Hz, 25Hz and 50Hz. By monitoring the diffraction data from alpha–phase and beta-phase Ti peaks, the accumulation of the axial and transverse lattice strain and stresses were recorded to the point of sample failure.

Imaging real-time plasticity onset and single twinning events within a bulk polycrystalline magnesium alloy

Presenter: Jun Wang

Abstract ID#: 111

Advanced alloy design and adequate modelling of alloys in service require us to understand the dynamic response of a bulk sample at both individual grain and grain aggregate levels with time resolution down to 10's of milliseconds. However, experimentally observing this has been challenging. We have developed a real-time Synchrotron X-ray Laue diffraction experiment to image the dynamic response of a polycrystalline magnesium alloy (with an average grain size of 20 μm) in one shot, avoiding the time-consuming aspects of diffraction data acquisition based on stage rotation or sample raster scanning. The sample was loaded in tension at a rate of 0.125 N/s and the experiment was conducted at IMBL beamline at the Australian Synchrotron using the polychromatic radiation in a highly columnated beam 200 μm in diameter. We paid close attention to the region near the elastic-plastic transition, which covers 110 s loading and 2500 frames. We tracked the radial position change, peak broadening and integrated intensity evolution of all the registered bright peaks (~100 grains). We then applied step changes analysis which enables us to detect the grain aggregate behaviours in a statistical way. The results show the intermittent nature of the burst of plasticity at the grain scale and the coupling of deformation bursts in nearby grains. In particular, an abrupt intensity drop observed within a time step of 44 milliseconds in some peaks is shown to result from single twinning events. To highlight, the current experiment is able to catch the single twinning onset events that single twins form, propagate and thicken to an endpoint of sorts and then wait for further development.

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