

ABSTRACT BOOK

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THE AUSTRALIAN INSTITUTE OF NUCLEAR SCIENCE AND ENGINEERING

New Zealand Synchrotron Group

ANSTO

Mark John Hackett

DAY 1

ABSTRACT 124

A (Spectroscopic) Picture Paints a Thousand Words: Studying Metal Ion Speciation in Brain Tissue with XANES Spectroscopic Mapping

Memory loss occurs during natural ageing, neurodegenerative disease, or following brain injury, and has limited treatment options. The lack of effective therapies can be attributed in part to an incomplete understanding of how ageing, disease, or injury perturbs brain chemistry, in particular the brain chemistry involving metal ions. Metal ions are known to be essential for healthy brain function, serving as vital structural or catalytic components of numerous enzymes, or even as low molecular weight neuro-signalling species themselves. At the bulk tissue level, altered levels of metal ions have long been associated with disease pathology, with recent research in the field now revealing how metal ion content and distribution changes at the cellular and sub-cellular level. How the chemical form of metal ions (oxidation state, coordination geometry, ligand binding) change in association with altered concentration and distribution remains largely uncharacterised.

Characterising different chemical forms of metal ions that are altered in brain tissue during natural ageing and brain disease has long been an analytical challenge. X-ray fluorescence microscopy (XFM) and X-ray absorption near edge structure (XANES) spectroscopy, however, have well-recognised capability to visualise metal ion distribution (XFM) and speciation (XANES) in situ, within cells and tissues. To this extent, our research team has been developing analytical protocols to visualise the chemical forms Fe, Cu, and Zn within brain tissue sections, i.e., visualising the “neurometallome”. A key consideration of our method development has been to determine how sample preparation can disturb distribution and speciation of metal ions, with the aim to develop sample preparation protocols that best preserve in vivo metal ion homeostasis, and are compatible with multi-modal work flows.

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ORAL

Danielle Martin

DAY 1

ABSTRACT 118

ANSTO: Facility update and new developments

This talk will provide an overview of ANSTO's ANSTO and new developments across the beamlines. The facility has seen many changes and updates, with new BRIGHT beamlines in operations and changes to infrastructure moving forward, including updated beamline capability. I will touch on various projects including: progress with the SXR X-Ray Nanolithography Facility (XRNF) project; the rollout of the MX2 robot and goniometer upgrade; the PD Mythen III detector upgrades; alongside other facility developments that are currently underway.

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ORAL

Andreas Moll

DAY 2

ABSTRACT 3

Data, Beamlines and Everything In Between: A Year of Scientific Computing

The Scientific Computing team at the ANSTO had a busy and productive 2026, with several changes designed to make data handling and beamline operations smoother for users. This presentation will walk through our transition to Globus for data download, sharing what the uptake looks like so far, the most common issues we see in practice, and the best ways to get support when you need it. I will also highlight the upgrade work completed on MX2 and introduce the new interfaces and capabilities now available at MX3, SAXS/WAXS and XAS. These improvements aim to make data collection more intuitive and give users more flexibility during experiments. Alongside this, I will showcase several technical solutions developed for ADS and other beamlines - practical enhancements that quietly remove friction from day-to-day workflows. To wrap up, I will give a forward look at the upcoming ASCI Desktop refresh and outline our priorities for the year ahead, including continued improvements to data workflows, user interfaces and computational tools across the facility.

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DAY 1

ABSTRACT 26

The Infrared Microspectroscopy (IRM) beamline

The Infrared Microspectroscopy (IRM) beamline provides chemical and structural information for a diverse range of samples across the biological, biomedical, materials, forensic, food, cultural heritage, and geoscience fields. Using a bright, tightly focused synchrotron infrared source with a high signal-to-noise ratio, the beamline enables chemical mapping of samples at microscopic spatial resolution. The IRM beamline can be operated in transmission, reflection, and high-resolution Attenuated Total Reflectance (ATR) modes, supporting the analysis of a wide variety of sample types.

This presentation will highlight recent advances in beamline operations, including our new multimodal holder for cross-beamline samples characterisation and piezo-controlled ATR for in-situ battery experiments.

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Andrew Langendam

DAY 1

ABSTRACT 33

Rapid, multimodal X-ray microscopy at the XFM beamline

The X-ray Fluorescence Microscopy (XFM) beamline still retains its place as one of the fastest X-ray Fluorescence (XRF) microprobes in the world. The past two years have seen the continued development of the beamline, with the Dual Multilayer Monochromator (DMM) entering regular service and the continuing development of capabilities to augment XFM's toolkit.

This workshop will give an overview of the beamline, give an update on the DMM commissioning and inform users new and old about complimentary techniques offered by the beamline, including 2D X-ray Absorption Near Edge Spectroscopy (XANES), XRF tomography, diffraction techniques and ptychography.

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Adam Round

DAY 1

ABSTRACT 125

Imaging Beamline Group - Enabling Discovery from Fundamental Research to Clinical Translation

The Imaging Group combines the complementary capabilities of the Imaging and Medical Beamline (IMBL) and the Micro-CT Beamline (MCT) to provide advanced X-ray imaging across a broad range of sample sizes and length scales. Together, the beamlines enable investigation of structure, function and dynamic processes in systems ranging from large biological specimens, geological samples and engineering components to cellular features and material microstructures, creating unique opportunities for multi-scale characterisation.

IMBL provides large-field-of-view synchrotron X-ray methods, including propagation-based phase contrast, dynamic imaging and specialised infrastructure for in vivo, preclinical and translational research. Dedicated infrastructure, including robotic positioning systems, specialised sample environments and clinical workflows, enables efficient and automated studies ranging from large and complex specimens to clinically relevant imaging studies. IMBL also hosts the world's only active Microbeam Radiation Therapy (MRT) research program, supporting radiobiology, dosimetry and next-generation spatially fractionated radiotherapy, while providing advanced dose measurement and verification capabilities that support quantitative studies and clinical translation.

MCT provides high-resolution X-ray microscopy and tomography, enabling non-destructive three-dimensional characterisation of biological tissues, advanced materials, energy devices, fossils, geological samples and engineered components at the micrometre scale. Together with emerging virtual histology, digital pathology and advanced reconstruction methods, MCT enables detailed investigation of microstructure and its relationship to larger-scale behaviour in complex biological and material systems, with future developments extending towards nanometre-scale imaging. Ongoing developments in automation and high-throughput workflows are expanding opportunities for efficient large-scale studies and multi-scale imaging investigations.

Across both beamlines, ongoing developments in instrumentation, data processing, automation and imaging methodologies are expanding the scope of possible experiments and creating new opportunities for research spanning the physical, life and medical sciences.

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Porun Liu

DAY 1

ABSTRACT 20

Probing Sub-Nanoscale Catalytic Active Sites for Water and carbon dioxide Electrolysis

Advancing sustainable energy conversion and storage relies heavily on mastering heterogeneous electrochemical processes at electrode interfaces. However, tracking the real-time evolution of sub-nanoscale active sites in inorganic electrocatalysts under operando conditions remains a core challenge. This work addresses this gap by employing a suite of advanced in-situ techniques—including X-ray Absorption Spectroscopy (XAS), X-ray Diffraction (XRD), and Raman spectroscopy—to monitor transition-metal catalysts (Mn, Fe, Co, Ni, Cu, Ru, Bi, Ag, Ir) in real time. We investigate these systems across the applications in water and CO2 electrolysers.

The resulting data unveils the dynamic transformation of precursors into active sub-nanoscale states and maps the relationships between electronic/structural modulation and performance. Specifically, we attribute enhanced catalytic activity to substrate-induced electronic interactions and the unique coordination environments of sub-nanoscale geometries. This comprehensive mechanistic framework enables the rational engineering of resilient, high-efficiency catalysts for green energy technologies.

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Hongzhe He

DAY 1

ABSTRACT 46

Promotion on the Understanding and Synthesis of High-Loading Single-Atom Catalysts based on Synchrotron Analysis

Single-atom catalysts (SACs) offer maximal atom utilization and tunable electronic structures, yet achieving high metal loading while maintaining structural stability and achieving scalable synthesis remains challenging. In the past years, we synthesized high-loading Pt SACs (up to 36 wt%) on CoNi substrates using vacuum direct current arc discharge (DCAD), and employed synchrotron-based X-ray absorption spectroscopy at the MEX-1 beamline to uncover the atomic structure of the as-synthesized SACs and to establish the respective structure-activity-relationship. Extended X-ray absorption fine structure (EXAFS) analysis reveals that, even at the Pt loadings of 36 wt%, Pt atoms are preferentially anchored by the CoNi substrate as densely dispersed Pt SAs. XANES further identified an electron-rich Pt state, evidencing strong electronic coupling between Pt and the CoNi substrate, which enables effective anchoring interactions and stabilization of Pt during rapid quenching. Additionally, in-situ powder diffraction from room temperature to 900 °C further demonstrated that this anchoring remains effective under high-temperature conditions.

The resulting high-loading Pt SACs exhibit superior performance to commercial Pt/C at a comparable Pt mass loading for the hydrogen evolution reaction, demonstrating the enhanced intrinsic activity enabled by atomic dispersion compared with Pt clusters. Meanwhile, the atomic-level structural insights provided by synchrotron X-ray techniques further guide the rational selection of substrates and SA sites, enabling the DCAD strategy to be extended to other high-loading SACs, including Ir (16 wt%).

These findings highlight the pivotal role of synchrotron techniques in uncovering the atomic-scale stabilization mechanism of high-loading SACs and translating this understanding into rational synthesis strategies.

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DAY 1

ABSTRACT 127

Transforming ultramafic mine waste into artificial laterites for critical metal recovery and CO_2 capture

Ultramafic mine wastes represent a significant opportunity for both critical metal recovery and carbon dioxide sequestration. Through engineered weathering, these materials can be transformed into artificial laterites enriched in trace metals while capturing atmospheric CO_2 in stable mineral phases. Understanding the mineralogical and geochemical processes controlling these transformations is essential for developing effective mine waste valorisation strategies.

This study uses synchrotron-based techniques to investigate metal mobility and mineral transformation reactions during artificial laterite formation. X-ray absorption spectroscopy (XAS) provides insights into the speciation of critical metals, while X-ray fluorescence microscopy (XFM) reveals mineral-metal associations and the distribution of reaction products at micron scales. These measurements are integrated with conventional geochemical and mineralogical data to track the evolution of metal-bearing and carbon-bearing phases.

The results provide new insights into the coupled processes of metal concentration and CO_2 capture in engineered weathering systems. This work demonstrates how synchrotron techniques can accelerate the development of sustainable approaches for transforming mine waste into a resource for critical metals and permanent carbon storage.

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Christopher McNeill

DAY 1

ABSTRACT 90

Resonant Grazing Incidence Wide-Angle X-ray Scattering of Semiconducting Polymers

The performance of semiconducting polymers is intimately linked to their molecular packing and microstructure. However, the paracrystalline nature of these materials often yields only a small number of diffraction peaks in conventional grazing-incidence wide-angle X-ray scattering (GIWAXS) experiments, limiting the structural information that can be extracted. Resonant X-ray scattering provides a powerful route to overcome this challenge by exploiting changes in atomic scattering factors near elemental absorption edges, adding sensitivity to the arrangement and orientation of specific atoms within the unit cell. This talk will explore the challenges and opportunities of performing resonant scattering measurements of semiconducting polymer films in grazing incidence geometry at the sulfur K-edge. Near an absorption edge, refraction, absorption, and waveguiding effects are all strongly energy dependent, requiring new approaches to data analysis and simulation in order to decouple these effects.

Progress toward analytical tools that incorporate these effects within a distorted-wave framework will be discussed, along with data acquired on thin films of the semiconducting polymer poly(3-hexylthiophene) of varying thickness, and with varied X-ray polarization.

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Adam Round

DAY 1

ABSTRACT 57

Progress Towards the World's First Live-Human Synchrotron Breast CT: From Research Platform to Clinical Trial Readiness

Breast cancer screening relies on low-dose X-ray imaging, but the resulting reduction in image quality can limit the detection of subtle early-stage disease, particularly in women with dense breast tissue. The IMPACT project (IMplementation of x-ray PhAse-Contrast Tomography to transform cancer diagnosis), funded by an NHMRC Synergy Grant, is translating synchrotron phase-contrast breast CT from research into a clinically deployable imaging modality.

Developed on the Imaging and Medical Beamline (IMBL) at the ANSTO, the system combines synchrotron X-rays with phase-contrast imaging to generate three-dimensional breast images with enhanced soft-tissue contrast at radiation doses comparable to, or below, those used in conventional breast screening. Studies of resected breast tissue have demonstrated substantially improved visualisation of tumour architecture and other clinically relevant features compared with conventional imaging approaches.

A major focus of the project has been overcoming the technical and regulatory barriers to first-in-human imaging. Through extensive engineering development, commissioning and validation, the team has resolved the key challenges associated with system stability, image quality, patient safety and operational reliability. In addition, approval has been granted by the Australian Radiation Protection and Nuclear Safety Agency (ARPANSA) to proceed with clinical trials. This presentation will provide an update on the IMPACT Breast CT program and the progress towards what is anticipated to be the world's first three-dimensional synchrotron breast CT imaging of a living human, representing a major milestone in the clinical translation of synchrotron imaging and a significant step towards a new gold standard for breast cancer detection and diagnosis.

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DAY 1

ABSTRACT 12

Using small-angle X-ray scattering to characterise binding of DNA aptamers to small-molecule targets

In the field of biosensors, antibody-based immunoassays are the gold standard in new sensor development, but with the rise of high-yield chemical DNA synthesis, short, high affinity DNA sequences (aptamers) have become an appealing alternative due to their enhanced thermal stability and ease of production. However, applications of high-affinity aptamers on biosensing platforms (aptasensors) have repeatedly resulted in significant decreases in affinity, specificity and selectivity.[1,2] Further aptasensor optimisation is limited by the lack of structural information required to explain this underperformance and the relative difficulty in obtaining this information.

Addressing this issue requires a more streamlined approach to aptamer structural characterisation. Traditional characterisation routes, such as full 3-D nuclear magnetic resonance (NMR) characterisation or X-ray diffraction, can be informative but are time-consuming and do not always produce useful data. As an alternative, we combine medium resolution data collected on the ANSTO's biological small-angle X-ray scattering beamline with high-resolution 1-D NMR, molecular dynamics and docking, along with AI structural predictions to produce accurate 3-D models of aptamer shape before and after target binding. This information supports evidence-based rationalisation of aptamer sequence modifications and/or changes to sensing methodology. Current data have already provided explanations for the performance of aptasensors of aminoglycoside antibiotics, cocaine and Δ9-tetrahydrocannabinol (psychoactive present in cannabis) with ongoing work focused on implementing proposed changes and expanding the strategy to new target molecules.

1. Y. Liu, R. Pandey, M. J. McCarthy, O. Raymond, Anal Chem 2025, 97 (2), 1097-1106.
2. Y. Liu, R. Pandey, M. J. McCarthy, O. Raymond, Anal Chem 2025, 97 (9), 5234-5243.

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Marie-Christine Zdora

DAY 1

ABSTRACT 4

Dual-sample multimodal X-ray imaging for high-throughput acquisition

Multimodal X-ray imaging methods provide complementary attenuation, phase-contrast, and dark-field information beyond conventional absorption imaging[1]. However, existing modulation-based multimodal approaches are limited to a single sample and cannot separate multiple objects overlapping in projection without additional image views.

Here, we introduce dual-sample multimodal imaging (DSI), an approach that enables the simultaneous retrieval of multimodal images from two overlapping samples in a single scan[2]. Rather than using a dedicated optic to generate intensity modulations for multimodal signal retrieval, DSI exploits the relative motion between the two samples such that each acts as a modulator for the other. Using the Unified Modulated Pattern Analysis (UMPA)[3], attenuation, phase, and dark-field signals are independently extracted for both samples from the same dataset.

We demonstrate DSI on biological samples and microelectronic devices measured at the ANSTO's MCT beamline and at SPring-8. Quantitative comparison with conventional X-ray speckle-based imaging shows comparable spatial resolution, angular sensitivity, and contrast-to-noise ratio while recovering information from both samples. Robust performance is demonstrated even for challenging cases with nearly identical samples with sparse, strongly absorbing features. By enabling both multimodal and spatial separation of two overlapping samples without additional optics or angular views, DSI doubles imaging throughput while maintaining image quality, providing a pathway towards faster and lower-dose multimodal imaging. We further discuss ongoing work to better understand and improve dark-field retrieval in the presence of noise, particularly for highly absorbing specimens, extending DSI towards dose-limited and high-throughput applications.

[1] Zdora, *X-ray Phase-Contrast Imaging Using Near-Field Speckles* (Springer, 2021).
[2] Zdora et al., *Optica*, in press (2026).
[3] Zdora et al., *Phys. Rev. Lett.* 118, 203903 (2017).

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Natinael Koyra

DAY 1

ABSTRACT 13

Modelling the Curvature Tuning Strategy of Monoolein-Based Lipid Nanoparticles by Tricosene Doping: Insights from High-Throughput Synchrotron SAXS

Lipid nanocarriers (LNCs) have become a cornerstone in modern drug delivery, particularly in mRNA vaccines, where ionizable lipids facilitate endosomal escape and the release of fragile nucleic acids (Yonezawa et al., 2020). Elucidating the structural and interfacial thermodynamic parameters governing LNCs is fundamental to predicting and controlling their nanostructural organization, interactions with biological membranes, and ultimately their ability to overcome biological barriers.

However, the independent contribution of LNC nanostructure to membrane interactions remains poorly understood because conventional formulation strategies simultaneously alter both the polar headgroup and non-polar hydrophobic interfaces, making it difficult to identify the origin of the observed effects. Here, we overcome this challenge by selectively tuning the non-polar region while maintaining comparable lipid-water headgroup chemistry, enabling precise control over LNC nanostructure. We introduced tricosene to a pH-responsive monoolein-based LNC system targeted to tune the curvature of the hydrophobic lipid membrane. Tricosene induced a progressive phase transition within LNC from low curvature inverted cubosomes (QII) to high curvature hexagonal (HII) phases. We built a predictive phase-lattice library by analysing ~400 synchrotron SAXS datasets, enabling the quantitative determination of key structural descriptors of LNC mesophases, including the effective chain volume, lattice parameter, phase structure, lipid volume fraction, and headgroup area. We further detected the structural organization and stability of these LNCs in the solid surface using advanced interface-sensitive synchrotron techniques. These analyses underscore the indispensable power of synchrotron SAXS, coupled with theoretical modelling, as a predictive platform for engineering LNCs with tailored structural and functional properties for advanced nanomedicines.

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Amir Entezam

DAY 1

ABSTRACT 100

Enabling Real-Time Patient-Specific Dosimetry for Synchrotron Breast CT: 23-Fold Faster Mean Glandular Dose Estimation

Accurate mean glandular dose estimation in breast computed tomography (BCT) requires realistic patient anatomy. We previously developed and validated an EGSnrc-based Monte Carlo (MC) framework using patient-specific voxelated phantoms generated from synchrotron propagation-based phase-contrast BCT (PB-PCT) images of mastectomy samples acquired at the Imaging and Medical Beamline (IMBL), in preparation for the first-in-human PB-PCT study at the ANSTO. With live participant imaging commencing at IMBL, increasing number of patient-specific datasets will impose substantial computational demands on dosimetry workflows and computing infrastructure. This study therefore aimed to determine the extent to which patient-specific phantom resolution could be reduced to improve MC efficiency while maintaining MGD accuracy, thereby enabling scalable and real-time patient-specific dosimetry for the IMBL PB-PCT program.

Five patient-specific phantoms were systematically downsampled using combinations of in-plane voxel size and slice thickness. MGD was recalculated and compared with high-resolution references. Primary MC photon histories were progressively reduced for downsampled phantoms while maintaining comparable statistical uncertainty. Across all samples, a 0.3 × 0.3 × 3 mm^3 voxel size maintained MGD within 5% of reference values, significantly reducing memory requirements and enabling a 15-fold reduction in photon histories while maintaining comparable statistical precision in the MC calculations. Together, these improvements produced an approximately 23-fold reduction in MGD computation time. Reducing phantom spatial resolution can substantially reduce the computational burden at IMBL. This approach also enables real-time patient-specific dosimetry, using a very-low-dose pre-scan to generate a reduced-resolution phantom for rapid MGD estimation before diagnostic imaging, enabling individualised dose and imaging setup optimisation.

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Brendan Dyett

DAY 1

ABSTRACT 63

First Contact: Lipid Nanoparticles Orient and Restructure at Interfaces

Lipid nanoparticles (LNPs) enable the delivery of nucleic acids, and often incorporate inverse non-lamellar mesophases linked to membrane fusion, yet their structural evolution at biological interfaces remains unresolved. Using in-situ grazing-incidence small-angle X-ray scattering (GISAXS), we directly resolve the interfacial cross-sections of LNPs prior to and during membrane interactions. Inverse cubic nanoparticles adopt preferred orientations such that water channels run parallel and normal to the substrate, while inverse hexagonal nanoparticles lie flat with channels aligned along the surface. Notably, upon contact with membrane mimics, structurally distinct LNPs, including cubosomes, hexosomes, and clinical COVID-19 vaccine LNPs, undergo interfacial mesophase restructuring toward common inverse mesophase intermediates associated with membrane fusion, regardless of their initial internal organization. These findings reveal dynamic nanostructural adaptation during membrane interactions and establish GISAXS as a platform to resolve in situ dynamic interfacial states inaccessible to other methods including conventional bulk solution scattering approaches.

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Caitlyn Smith

DAY 1

ABSTRACT 110

Extracting Microstructure Properties by Quantifying the Scattering in X-Ray Dark-Field Images

The first demonstrations of X-ray imaging were based on the attenuation of X-rays by thick or dense materials. This allowed for bones to be distinguished from the surrounding tissue, however could not distinguish between objects with similar density, such as skin and organs. In recent years, novel imaging techniques have been developed that utilise the scattering of X-rays to collect the “dark-field signal”, and hence visualise microstructures too small to be seen using traditional X-ray techniques. One such method is grid-based X-ray imaging, which introduces a grid between the source and the sample. By analysing how the sample blurs the reference grid pattern, dark-field images can be extracted.

In 2024, this technique was applied to lung health at the IMBL, with dark-field CT scans taken of mouse models. The mice had either healthy lungs or lungs affected by lung cancer or emphysema, and scans revealed a correlation between the alveoli size and the dark-field signal detected. This project aims to determine a numeric relationship between the measured dark field and the microstructure of samples. In 2026, dark-field images will be taken of various porous materials at the ANSTO’s IMBL, which will be compared to the dark-field signal found from microspheres. This numeric relationship will then be utilised to quantify the size of alveoli.

The ability to quantitatively map and measure the microstructure of the entire lung would enable earlier diagnosis of lung disease and more precise tracking of disease progression and treatment effectiveness.

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Hank Qi Han

DAY 1

ABSTRACT 10

Decoding protein crystallisation and aggregation in ionic liquids with high-throughput SAXS, GISAXS and machine learning

Ionic liquids (ILs) provide tunable solvent and additive environments for proteins and peptides. This presentation summarizes three related studies, with the main focus on SAXS and machine-learning analysis of protein crystallization, followed by a crystallization benchmark and oral insulin delivery. The main part examines lysozyme crystallization in aqueous ethylammonium nitrate (EAN) using small-angle X-ray scattering (SAXS). High-throughput 96-well screening, in situ heating and time-resolved measurements were used to follow structural changes before crystal formation. SAXS profiles were converted into descriptors including pseudo-Rg, crystallinity index and oligomeric-state information. The results support a two-step pathway, where EAN first promotes dense protein intermediates and ordered crystals then form within a limited composition window. Machine-learning models captured this non-linear crystallization region better than linear models, suggesting a practical route for screening prioritization.

The second part briefly introduces a solvent- and ion-aware crystallization benchmark that links condition chemistry, retained non-polymer species in deposited structures and structural readouts such as solvent content and resolution. This benchmark separates condition-side additives from species actually observed in structures, providing a more interpretable basis for data-guided crystallization screening.

The final part discusses choline-based IL/salt formulations for oral insulin delivery. Solution and protein SAXS, pH and critical micelle concentration measurements connected pH-dependent self-assembly, buffering and insulin oligomeric state, while grazing-incidence SAXS (GISAXS) on supported lipid bilayers resolved how ILs reorganise the epithelial membrane. Selected formulations enhanced insulin permeability, but gastric mucosal injury depended strongly on formulation. Overall, these studies show that IL-based systems should be designed by considering ion chemistry, nanostructure and biological response together.

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James Pollock

DAY 1

ABSTRACT 102

Understanding diaphragmatic hernias using phase-contrast CT and neural network airway segmentation.

Congenital diaphragmatic hernia (CDH) - where abdominal organs protrude through structural defects in the diaphragm in utero - is known to affect up to 1 in 10,000 births in the US alone, with mortalities reaching up to 38% due to the resultantly inhibited lung development (hypoplasia). As such, there is a significant need for improved early diagnosis and prognosis. Biological modelling in large animal models (lambs) provides an analogous physiological environment for study; however, visualisation of small airway development at high branch generations (up to branch number 40 and beyond) requires high-resolution phase-contrast imaging to resolve. Using propagation-based phase-contrast Computed Tomography (CT) at the ANSTO, alongside surgically implanted lung obstructions to emulate various hernia cases, our team was able to observe the effects of different hernia severities on lung development. However, analysis of the smallest airways has been limited by partial volume effects and severe motion artefacts impacting the required segmentation. Herein, we describe a neural network-based approach for circumventing these issues, trained on a minimal number of labelled slices using a 2.5D bidirectional convLSTM architecture.

Preliminary results show clear learning trends and significantly superior segmentations compared to conventional thresholding-based approaches, even in minimally affected cases. These results are presented alongside the developed neural network package, before finally touching on the underlying lung development trends across the range of obstruction severities.

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Cameron Kewish

DAY 1

ABSTRACT 16

The Nanoprobe beamline at the ANSTO

The Australian Nuclear Science and Technology Organisation (ANSTO) has commenced the construction of a 100 m-long Nanoprobe beamline at the ANSTO, as part of the BRIGHT project delivering 8 new beamlines. A cryogenic permanent magnet undulator source provides hard X-rays for fluorescence mapping and ptychography imaging. The optical layout of the beamline includes a secondary source aperture, used to define the beam coherence and render the endstation insensitive to subtle variations in angle and position of the source. A double-multilayer monochromator will maximize the intensity at the sample.

To achieve the spatial resolution target of 60 nm for fluorescence mapping, with a reasonable working distance of 80 mm between the focusing mirror vessel and the sample, the endstation is located far from the source in a dedicated satellite building. The building was designed to minimize the effect of thermal variations, drift, and vibration at the sample location, as well as providing convenient laboratory space for the users. The sample scanner provides 3 mm scan range in all directions with <10 nm positioning precision, with a rotation stage enabling tomographic extension of all imaging modalities. The status of the ANSTO Nanoprobe construction project will be presented.

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Caite Setter; Helen Brand

DAY 1

ABSTRACT 49

Diffraction Group Update Session

This session will provide an overview of the capabilities of the PD and ADS beamlines. The first call for proposals for the ADS beamlines will be open during the User meeting and so there will be an opportunity for the User community to ask questions and engage directly with the beamline teams.

PD The PD beamline was one of the original suite of beamlines at the facility, with User operations commencing in mid – 2007. The primary end station can accommodate a wide variety of experiments, particularly those utilising in situ sample stages and cells. The beamline team are upgrading the Mythen detector ready for R1 2027, and this contribution will discuss that upgrade and the new capabilities it will enable.

ADS-1 will offer white and monochromatic X-ray diffraction and imaging capabilities with a monochromatic energy range of 50 – 150 keV. A multipurpose array of detectors with a highly flexible positioning system will facilitate a wide range of experiments, including those combining multiple data types. The ADS-1 sample stage assembly will support loads of up to 300 kg and offer fast rotation speeds suitable for tomography.

ADS-2 will be capable of monochromatic diffraction experiments at three fixed X-ray energies (45, 74 or 87 keV). These higher energies will be well suited for powder and single crystal diffraction from highly X-ray absorbing samples, as well as total scattering (Pair-Distribution Function), and high-throughput applications with a range of standard sample environments.

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Nick Phillips

DAY 1

ABSTRACT 47

A new spin on quantitative 3D elemental imaging with laminographic XRF

Obtaining quantitative 3D elemental distributions from X-ray fluorescence measurements of extended samples is challenging using traditional tomographic methods. However, laminography is a relatively recent volumetric imaging implementation that can be used to determine 3D distributions across extended specimens such as integrated circuits, leaves, and other planar specimens. We build upon our development of laminography at the ANSTO XFM beamline with a new measurement geometry that enables not only the benefits of the method, but which also simplifies the (largely intractable) self-absorption problem. In this presentation we report our experiences with the measurement and describe the new measurement geometry and its benefits. This approach is applied to the study of crop pathogens, mineral enrichment processes in modern hydrothermal vents and the search for life of Mars.

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Ani Baker

DAY 1

ABSTRACT 15

Synchrotron-based X-ray techniques for studies of arsenic distribution and speciation in the novel extremophile nematode Tokorhabditis tufae

Arsenic exposure through groundwater contamination is a global issue which impacts over 200 million people worldwide. *Tokorhabditis tufae* (*T. tufae*) is a novel species of extremophile nematode which thrives in the highly saline, alkaline, and arsenic-rich environment of Mono Lake, California, providing a tractable model for mechanistic studies of adaptation to mineral-extreme environments. Synchrotron-based X-ray techniques, including X-ray fluorescence microscopy (XFM) and X-ray absorption spectroscopy (XAS), have been utilised to interrogate arsenic distribution and spatially resolved speciation in *T. tufae* exposed to inorganic arsenic.

Further investigation of arsenic speciation in bulk nematodes has been achieved using high energy resolution fluorescence detected XAS (HERFD-XAS), offering enhanced spectroscopic resolution relative to conventional XAS. Elemental distribution maps and microprobe As K-edge XANES spectra have revealed differences in arsenic uptake and speciation in *T. tufae* treated with arsenite, As(III), and arsenate, As(V), albeit with substantial biological variation between individual nematodes. Survival assays indicate that both *T. tufae* and *Caenorhabditis elegans* (*C. elegans*) show similar sensitivity to treatment with 1.5 mM As(III). In contrast, *T. tufae* exhibits nearly 100% survival during exposure to 30 mM As(V) for 7 h, accumulating markedly lower concentrations of arsenic than *C. elegans* treated under analogous conditions. In addition, As Kα1 HERFD-XAS spectra on bulk nematodes demonstrates that *T. tufae* exposed to 30 mM As(V) (1 h) contains a mixture of both reduced and oxidised arsenic, whereas As(V) undergoes complete reduction in *C. elegans*. Our results suggest that *T. tufae* may be capable of excluding and/or rapidly detoxifying arsenic via a unique and speciation-dependent mechanism, however, further interrogation of arsenic metabolites is necessary to elucidate potential biochemical pathways.

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Peter Kappen

DAY 1

ABSTRACT 43

Updates from the Spectroscopy Group

In this session, we will provide an overview over the capabilities of the beamlines in the Spectroscopy Group, with emphasis on recent developments and science opportunities across X-ray Absorption Spectroscopy (XAS), Medium-Energy XAS 1 & 2 (MEX1 & 2), and Soft X-ray Spectroscopy (SXR). This will include updates on the micro-probe endstation at MEX1, opportunities to measure liquids at MEX2, sample cooling at SXR, and high energy-resolution spectrometry at XAS.

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James Puli

DAY 1

ABSTRACT 78

X-ray Fluorescence Diagnostics for Flashing Channel Flows

The analysis of multiphase flows with traditional optical techniques faces challenges that make it poorly suited for determining phase concentration fields: many fluid species are optically indistinguishable, and heavy refraction across multiple liquid-gas boundaries limits the use of visible and near-visible fluorescence techniques. X-ray fluorescence imaging overcomes these limitations as X-rays are only weakly affected by refraction, while fluorescent tracer species can be added to mark different fluid phases.

In this work, undertaken during our July 2026 beamtime, we apply X-ray fluorescence to observe water undergoing rapid phase change driven by a sudden pressure drop, often termed 'flash-evaporation', in the presence of a dissolved gas species. Understanding this process has implications for modelling gaseous flashing flows, relevant to industrial applications including medical metered dose inhalers and dissolved gas separation.

We dissolve a known concentration of RbCl tracer into the liquid phase and use Kr as the gas phase. As RbCl has a very low vapour pressure, it remains in the liquid, acting as a marker for the liquid water. By observing the change in Rb fluorescence, we determine the time-averaged distribution of the liquid phase; by mapping Kr fluorescence, we determine the distribution of the gas phase. The water vapour distribution is then inferred from regions where both signals are absent. From these measurements, the vaporisation timescale and the impact of dissolved gas on the phase-change process can be determined and new thermodynamic models developed.

This presentation will focus primarily on the experimental methods and on processing the raw X-ray fluorescence data into quantitative phase distribution maps.

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Han Wu

DAY 1

ABSTRACT 123

Understanding Aqueous Battery Chemistry through Operando Synchrotron-Based Characterisation

Aqueous batteries are promising for safe, cost-effective, and sustainable energy storage, but their practical development is often limited by complex interfacial reactions and structural changes during operation. This presentation focuses on understanding and regulating these dynamic processes to improve battery reversibility, stability, and practical performance. Synchrotron-based techniques, such as Infrared Microspectroscopy (IRM), Powder Diffraction (PD), Small and Wide Angle X-ray Scattering (SAXS/WAXS), and Micro-Computed Tomography (MCT), are employed to probe structural, chemical, interfacial, and morphological evolution under in situ and operando conditions. These insights, combined with electrode and interface engineering, provide a deeper understanding of electrochemical reaction mechanisms and support the development of high-loading and practical aqueous battery systems.

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Yameng Fan

DAY 2

ABSTRACT 122

Seeing Batteries in Action: Multiscale Mechanistic Insights from Synchrotron Techniques

Understanding how batteries operate requires insights into dynamic processes occurring across multiple length scales, from electronic and local atomic structures to long-range phase evolution and electrode–electrolyte interfacial chemistry. Synchrotron-based characterisation provides powerful and complementary tools to capture these complex processes and establish direct links between material evolution and electrochemical behaviour.

In this talk, I will present our recent efforts to understand reaction mechanisms in advanced rechargeable batteries using a combination of ex situ, in situ, and operando synchrotron techniques. Synchrotron powder diffraction is employed to track structural evolution and phase transitions during electrochemical cycling, while hard X-ray absorption spectroscopy provides element-specific information on redox processes and local coordination environments.

Soft X-ray absorption spectroscopy further enables investigation of transition-metal and oxygen electronic structures, offering insights into both cationic and anionic redox chemistry. These techniques have been applied across lithium-ion, sodium-ion, and aqueous battery chemistries to reveal structure–property relationships that are difficult to resolve using conventional characterisation alone. In addition, synchrotron infrared spectroscopy provides a perspective on electrolyte solvation and dynamic electrode–electrolyte interfacial processes.

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Nunzio Motta

DAY 2

ABSTRACT 29

Conversion of Epitaxial Graphene to 2D diamane on Silicon Carbide by Ultra High Vacuum hydrogenation

Hydrogenation of graphene offers a promising pathway for producing ultrathin diamond-like carbon structures through the conversion of sp^2 to sp^3 bonding. Here we examine the hydrogen-induced structural transformation of bilayer epitaxial graphene on SiC using complementary experimental and theoretical approaches. Quasi-free-standing bilayer graphene grown on 6H-SiC(0001) by Chemical Vapour Deposition at CRHEA-CNRS (Valbonne, France) was degassed at 600˚C in UHV and exposed to hydrogen at the Soft X-ray Beamline of the ANSTO in order to induce an sp^2–sp^3 structural transition. X-ray photoelectron spectroscopy (XPS) demonstrates a pronounced rehybridization, with the sp^3 component reaching approximately 90% after extended atomic-hydrogen exposure. High-resolution scanning tunneling microscopy (STM) provides direct structural evidence of diamond-like surface reconstructions coexisting with graphene already at the initial stages of hydrogenation.

Density functional theory (DFT) calculations reproduce the characteristic STM features and reveal energetically favourable reconstruction geometries, linking the experimentally observed structures to specific sp^3 bonding configurations promoted by interlayer interactions. The progression of the sp^3 fraction with hydrogen exposure displays a characteristic two-stage evolution with a double inflection point. This behaviour is quantitatively described by the superposition of two two-dimensional nucleation-and-growth processes, comprising an initial, rapid defect-mediated formation of reconstructed domains followed by a slower conversion of the remaining graphene terraces. The resulting sp^3-rich material exhibits thermal stability up to 500 °C, further supporting its diamond-like character. These findings provide new insight into the mechanisms governing hydrogen-driven sp^2–sp^3 conversion and establish a framework for controlling the formation of ultrathin diamond-like carbon phases with potential applications in scalable nanoelectronic technologies.

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Rachel Williamson

DAY 2

ABSTRACT 95

MX1, MX2 and MX3: Current Capabilities, New Technologies and Future Opportunities for Crystallography at the ANSTO

The ANSTO's Crystallography Group continues to support a diverse community of researchers from Australia, New Zealand, and beyond. Together, MX1, MX2, and our newest beamline in the group, MX3, provide complementary capabilities spanning routine crystallographic data collection, advanced dynamic crystallography experiments, and cutting-edge microfocus applications. Over the past year, MX3 has entered routine user operations, bringing new opportunities for the study of challengingly small and weakly diffracting crystals through its highly focused X-ray beam, high flux density, and advanced sample-handling infrastructure. The beamline enables new experimental approaches, including X-ray rastering centring, unattended data collection, crystallization tray screening, and serial crystallography. Ongoing developments on MX1 continue to expand experimental flexibility and improve user access to dynamic crystallography experiments, including high-pressure crystallography in diamond anvil cells, photocrystallography, and variable-temperature measurements. Meanwhile, the MX2 beamline has undergone a substantial endstation upgrade.

This presentation will provide an overview of the current capabilities of the ANSTO's MX beamlines, recent instrumentation upgrades, and developments planned for the near future. Highlights include harmonized robotic sample handling and goniometers across MX3 and MX2 (new endstation!), new user interfaces, new automation workflows for crystal mounting and centring, and continued development of dynamic crystallography methods. The talk will also showcase recent scientific applications and discuss future directions for crystallography at the ANSTO, including the expansion of fragment-screening capabilities.

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Sowbarnika Senthilkumar

DAY 2

ABSTRACT 75

Ionic Liquid Precursor Films on Graphite: Formation Mechanisms and Interfacial Properties

Ionic liquids (ILs) are molten salts with low melting points that possess exceptional properties, including high thermal stability, negligible volatility, non-flammability, and high conductivity, making them attractive candidates for high-end lubrication in micro- and nanoelectromechanical devices, wind turbines, and aerospace applications. In this study, we employ synchrotron-based X-ray spectroscopy and scattering techniques to investigate the structure and molecular organisation of imidazolium-based ILs from ultrathin precursor films to the bulk phase. In the first part, we examine the ultra-thin precursor films formed by 1-butyl, 1-hexyl and 1-octyl derivatives of the 3-methylimidazolium -based ILs paired with bis(trifluorosulfonyl)imide, bis(fluorosulfonyl)imide and tricyanomethamide anions on highly oriented pyrolytic graphite.

Synchrotron-based X-ray photoelectron spectroscopy was used to characterise the composition of the precursor film and also confirm the absence of chemical interactions between the ILs and HOPG, while near-edge X-ray absorption fine structure spectroscopy determined the molecular orientation relative to the substrate. Our findings conclusively demonstrate the formation of a two-layer patchy precursor film containing equal proportions of cations and anions, with the imidazolium ring of the cation oriented parallel to the HOPG surface. In the second part, we explore the effect of NMR solvents on the structure of bis(fluorosulfonyl) imide-based ILs using Synchrotron small- and wide- angle X-ray scattering. By systematically investigating the solvent-dependent structural changes, we aim to understand the molecular interactions governing the system.

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Wesley Dose

DAY 2

ABSTRACT 119

Deciphering Depth-Dependent Degradation in Layered Oxides with X-ray Spectroscopy

The performance of next-generation lithium-ion and sodium-ion batteries are limited by the storage capacity and degradation rate of the positive electrode material. Materials based on layered transition metal (TM) oxides traditionally rely on TM centres to compensate the charge when lithium or sodium ions are removed. While structural degradation is known to cause a loss in the redox activity, the rate of degradation often varies at different depths within the particles. In this presentation, I will show how combining complementary X-ray spectroscopy techniques enables us to unravel the depth-dependent redox mechanisms across long-term battery aging.

First, our recent studies of nickel-rich positive electrodes for lithium-ion batteries will be outlined, where we use soft X-ray spectroscopy (XAS) in electron yield mode to interrogate the formation of the reduced surface layer and its structural evolution as cycling progresses. Next, to probe the degradation mechanisms of lithium- and manganese-rich positive electrodes, we utilise soft XAS to obtain a depth-resolved picture of redox processes in the bulk and near-surface. These measurements reveal a divergence in the interfacial structure after cycling in different electrolytes, and how incompatibility with conventional electrolyte causes a densification of the near-surface structure that severely hinders bulk redox reactions. Finally, TM K-edge and L-edge XAS are combined to decipher the changes in oxidation state and metal-ligand covalency for a sustainable sodium-ion positive electrode. Combined, the findings reveal how X-ray spectroscopies deepen our mechanistic understanding of bulk and interfacial redox processes and enable the rational design of improved materials for sustainable batteries.

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Andrew Clulow

DAY 2

ABSTRACT 84

Scattering Beamline Group Workshop: New Capabilities, Sample Environments, and User Community Engagement

The Scattering Beamline Group workshop will provide an update on recent developments, sample environments and emerging opportunities across the SAXS/WAXS and BioSAXS beamlines. The session will feature a short overview of current and upcoming capabilities, followed by an interactive discussion where users can engage directly with beamline staff, provide feedback, and explore new opportunities for their research. Selected case studies will highlight the breadth of science enabled across the scattering portfolio.

For the SAXS/WAXS beamline, we will showcase capabilities supporting research across materials science, soft matter, energy, advanced mAustralian National Universityfacturing and nanotechnology. Particular emphasis will be placed on Grazing Incidence Small- and Wide-Angle X-ray Scattering (GI-SAXS/GI-WAXS) for the characterisation of thin films, coatings, interfaces and nanostructured surfaces. The workshop will also highlight the beamline's diverse sample environments, including tensile testing, temperature-controlled measurements, automated sample handling, and a range of in situ and operando experimental approaches.

For the BioSAXS beamline, we will highlight the broad application of solution small-angle scattering to biological, colloidal and dispersed systems. Alongside highly utilised Coflow Batch- and SEC-SAXS workflows, we will showcase capabilities including ambient and temperature-controlled capillary measurements, flowthrough experiments for dynamic and evolving systems, user-supplied fluid mixers and reaction vessels, and other sample environments currently under commissioning. These capabilities support studies of biological structure, molecular self-assembly, stability, interactions and solution behaviour across a diverse range of samples and experimental conditions. Case studies will demonstrate how these approaches can be used to provide nanoscale structural insights beyond those attainable using other analytical techniques for solutions. The workshop aims to foster engagement with the user community, identify emerging scientific needs, and help guide future capability development.

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Annette Dowd

DAY 2

ABSTRACT 109

Collective dynamics in biological membranes: lessons from a decade of low frequency vibrational spectroscopy

Biological membranes are dynamic molecular assemblies whose properties are governed by lipid packing, hydration and collective molecular motions. Low frequency (terahertz) vibrational spectroscopy provides access to intermolecular and collective modes that are not readily accessible through conventional mid-infrared measurements. We developed methods for studying hydrated phospholipid bilayers using the THz beamline at the ANSTO, and investigated how membrane organisation influences low frequency vibrational behaviour.

Reproducible spectral features were observed across multiple phospholipid systems, and comparisons between amorphous lipid films and self-assembled bilayers revealed measurable changes in modes associated with collective lipid dynamics. Molecular dynamics simulations assisted in assigning several prominent vibrational features and their physical origins.

Interpreting the spectra proved more difficult than collecting them. The measurements were sensitive not only to membrane organisation, but also to hydration, film thickness and details of the experimental geometry. As a result, relating spectral changes directly to membrane structure and phase behaviour was often less straightforward than expected. This presentation reflects on both the opportunities and limitations of low frequency vibrational spectroscopy and discusses lessons learned from a decade of efforts to connect spectral signatures with membrane structure, dynamics and phase behaviour.

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Jun Wang

DAY 2

ABSTRACT 81

Watching hundreds of grains at once: energy-resolved Laue diffraction turns a single exposure into a grain-resolved map of a polycrystal

Resolving many grains inside a polycrystal conventionally requires serial sectioning, sample rotation, or point-by-point beam scanning, all awkward while a microstructure evolves. White-beam Laue diffraction offers an escape, since one stationary exposure contains overlapping patterns of many grains, but its indexing relies on the directions of the diffracted beams alone. Every reflection then fixes a scattering vector whose length is unknown, and assigning Miller indices becomes a

combinatorial search that collapses once more than a few grains illuminate the detector together. We lift that restriction by measuring every reflection's photon energy. Sweeping the threshold of a cadmium telluride photon-counting detector at the Micro-Computed Tomography beamline gives each Laue spot an energy. This enables indexation of more than 100 grains from one exposure carrying 1500 reflections. The method turns an existing imaging beamline and a standard detector into a grain-resolved diffraction instrument, with no added hardware, monochromator scan or sample rotation. It offers the materials community a way to follow hundreds of individual grains through heating and deformation and extends the ANSTO toward time-resolved polycrystal crystallography at unprecedented time scales.

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Chris Hall

DAY 2

ABSTRACT 56

Neural network based 4D CT reconstruction at the synchrotron

Advances in deep learning have led to new ways to reconstruct 3D and 4D computed tomography (CT) data from a set of x-ray projection images. In cinematographic computer graphics a technique is used where a neural network can encode a 3D scene completely within its weights and biases. The network is then be used to create a novel view of the scene from any specified camera angle. The technique is called Implicit Neural Representation (INR). Crucially, INR networks do not require training data but refine their parameters based on a small number of real images.

Recent papers by a group at the Norwegian University of Science and Technology (NTNU), and Ruyi Zha at Australian National University, have shown how INRs might be used to speed up data collection in X-ray CT. The potential would be for static CT scans to be collected with significantly fewer projections and therefore lower radiation doses. Alternatively, to reduce CT scan duration so that more rapid time resolved (4D) CT collection can be made. This would open research opportunities on dynamic phenomena that have been inaccessible to synchrotron CT in the past.

This presentation outlines the concept and shows the preliminary work of our teams at the AS and the Australian National University to develop such a capability on the AS Imaging Group beamlines.

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Ryan Hogg

DAY 2

ABSTRACT 36

Absorption effects on Fluctuation X-ray Scattering

The structures of nanoscale disordered materials, such as plastics and liquid crystals, have been hard to study due to their inherent disorder and lack of periodicity. To overcome this, correlation-based analysis of X-ray and electron diffraction data can be used to probe the angular structure. Typically, diffraction analysis involves the pair-distribution function (PDF), which works well for distinguishing the first few neighbor distances but becomes noisy at larger distances.

Current interest in amorphous materials is studying the local 3d-atomic structures associated with medium-range order (MRO), as both short-range structures and MRO are responsible for the macroscopic properties of these materials. To gain this insight, angular cross-correlations can be used to look at more than just 2-body pair correlations (like in the PDF), but also three- and four-body pairs. By taking an ensemble of diffraction patterns using a coherent scanning microfocus beam, the cross-correlation function can be formed in q-space and transformed into a real-space function, the pair-angle distribution function (PADF).

The PADF extends the PDF by incorporating angular information, providing greater sensitivity to the three-dimensional local structure of the material. These extra dimensions improve the visibility of features corresponding to larger real-space structures. Synchrotrons also provide the ability to exploit resonant absorption processes. Resonant diffraction techniques utilize the breaking of Friedel symmetry near absorption edges to gain local structural insight. Combining this with the PADF allows for element-specific sensitivity at distances and angles corresponding to differing elements. This provides a route to understanding chemically specific local structure in disordered systems.

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Shannen Mills

DAY 2

ABSTRACT 65

Exploring pumice textures through Synchrotron Micro-Computed Tomography

Pumice, a product of explosive volcanism, is a porous lightweight material with properties that make it versatile with many modern applications, including horticulture, construction, filtration, and as a natural pozzolana. The Taupō Volcanic Zone (New Zealand) is an active and productive magmatic system, but its abundant pumice deposits are currently underutilized. Pumice-bearing deposits vary greatly in grain size, sorting, volume, and sedimentary features reflecting differences in eruption magnitude, eruptive style, and deposit emplacement mechanisms.

This study focuses on pumice textures from macro- to micro-scale to investigate the magmatic processes that drive explosive eruptions and determine the physical properties most beneficial for different applications. The Micro-Computed Tomography (MCT) beamline at the ANSTO was utilised to obtain three-dimensional quantification of vesicle number densities, shapes, connectivity, and vesicle wall thickness from pumice clasts across twenty-two young eruptive deposits. High-resolution, non-destructive imaging enabled voxel sizes down to 3.6 µm, revealing substantial natural heterogeneity between and within individual clasts.

Preliminary results indicate that pumice textures are dominated by highly interconnected vesicle networks, with thin glass walls (10-40 µm) and vesicle number densities ranging from `10^5-10^6 cm^-3`. Variations in vesicle size, connectivity, and wall thickness indicate different histories of bubble nucleation and growth during ascent. These data highlight the complexity of vesicle connectivity and demonstrate the benefits of using synchrotron imaging to resolve it. The results from this research will provide the foundation for determining the best use for pumice with particular textures, towards creating a potentially viable economic sector for New Zealand.

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Yue Wang; Hao Zhang; Hongjian Du

DAY 2

ABSTRACT 22

Using in situ synchrotron powder diffraction to study the hydration of Portland cement with seawater CO2 mineralisation precipitate replacement at very early ages

The utilization of seawater CO2 mineralisation precipitate (SMP), mainly composed of magnesium hydroxide and calcium carbonate, presents a promising avenue for reducing the carbon footprint of cement production. However, the early-stage hydration reactions remain less investigated, with significant data gaps critical for assessing performance. Our primary objective is to investigate the evolution of crystalline phases during the early age hydration of blended cement, shedding light on the filler effect and the mechanisms behind strength development. Therefore, this project employs in situ synchrotron X-ray powder diffraction to understand the hydration reactions occurring within the first 14 hours. HighScore software is used for crystal phase identification, and the diffraction data are analysed by the Rietveld method, with results compared to mass balance calculations.

The results demonstrate that replacing 10 wt% of OPC with SMP accelerates early-age C3S hydration through a filler-induced nucleation effect, and the calcium carbonate component participates in carboaluminate reactions with C3A to form hemicarboaluminate and monocarboaluminate. These findings demonstrate that SMP is a feasible low-carbon cement replacement and represents a promising pathway for the viability of SMP in cementitious systems.

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DAY 2

ABSTRACT 83

Beyond Porosity: Synchrotron Micro-CT Characterisation of Multi-Scale Defect Architecture and Fibre–Matrix Interfacial Discontinuities in 3D-Printed Continuous Fibre Thermoplastic Composites

MAustralian National Universityfacturing defects in fused filament fabrication of continuous fibre-reinforced thermoplastic composites are commonly summarised by bulk porosity, although similar porosity levels can contain markedly different three-dimensional defect architectures. This study uses high-resolution synchrotron micro-computed tomography (3.6 µm voxel size) to characterise micro-, meso- and macro-scale mAustralian National Universityfacturing defects in continuous carbon- and glass-fibre-reinforced thermoplastic composites fabricated under a factorial design varying fibre volume and stacking sequence.

Three-dimensional connected-component analysis classifies micro-, meso- and macro-scale void populations and quantifies equivalent spherical diameter, morphology, Feret dimensions, orientation, spatial localisation and connectivity. Particular attention is given to interface-adjacent voids, elongated interlayer discontinuities and connected macro-scale defect networks. These descriptors are interpreted alongside tensile and flexural responses to examine whether defect topology and location provide additional structural information beyond global porosity. Polymer characterisation and surface electron microscopy provide complementary evidence for interpreting matrix condition and fibre–matrix interfacial characteristics.

The work also highlights practical limits of synchrotron micro-CT for these composites. Features approaching or below the effective spatial resolution are affected by partial-volume effects, and phase discrimination depends strongly on X-ray attenuation contrast. This is particularly challenging in carbon-fibre-reinforced specimens, where fibre and matrix greyscale overlap can constrain reliable phase segmentation. Micro-CT also characterises interfacial geometry rather than directly measuring interfacial adhesion. Glass-fibre-reinforced datasets provide more favourable contrast and are being extended toward deep-learning-based phase segmentation. Future work is planned to combine improved segmentation with digital volume correlation to examine three-dimensional strain localisation relative to measured defect architecture, supporting interface-aware assessment of additively mAustralian National Universityfactured composites for lightweight structural applications.

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Alan Salek

DAY 2

ABSTRACT 73

Fluctuation X-ray scattering as an indexing-free extension of serial crystallography

Serial synchrotron crystallography solves structures by merging tens of thousands of individually indexed microcrystal patterns. When many crystals are illuminated at once, the resulting "spotty powder" patterns cannot be indexed and are discarded. Fluctuation X-ray scattering instead exploits angular correlations between Bragg peaks within each pattern, offering a route to structure factors from data which current pipelines cannot use [1]. This would permit denser crystal loading, smaller crystals well-below previous limits (<100 nm), simpler in-tray collection, and shorter mixing times in time-resolved experiments.

We present the first experimental demonstration of fluctuation scattering from serial crystallography data, benchmarked directly against conventional merging using a single thaumatin dataset collected at room temperature.

Data were collected at MX3 (EIGER2 XE 16M, 13 keV) from room-temperature microcrystals in in-situ plates, using fixed-target scripts we developed at the beamline. Of ~230,000 frames, ~73,000 were hits and ~66,000 indexed (90%), merging in $P4_12_12$ to 100% completeness at 1.65 Å with exceptional multiplicity. These data refine to R/R-free 0.164/0.189, a rigorous reference against which correlation-based recovery can be validated.

We computed angular correlations from Bragg peaks in both indexable and non-indexable multi-crystal patterns and assessed the recoverable signal against simulated thaumatin data. We report the practical requirements such as peak statistics, angular sampling, correlation convergence, and describe the 3D-printed fixed-target holder and microfluidic flow cell [2] we are developing. This establishes a controlled testbed for extending the approach to nanocrystals at synchrotron sources.

1. Adams, P. et al. IUCrJ 11, 2024.
2. Deng, H. et al. Phys. Fluids 37, 2025.

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Zoe Johnson

DAY 2

ABSTRACT 105

Synchrotron microangiography to assess cerebral haemodynamic responses to delivery-room resuscitation in extremely preterm lambs

Extremely preterm infants are vulnerable to cerebrovascular injury during the immediate postnatal transition. Delivery-room practices such as umbilical cord clamping timing and oxygen exposure may contribute by destabilising cerebral haemodynamics. We used synchrotron radiation microangiography in preterm lambs to assess how cord management and initial inspired oxygen fraction (FiO_2) influenced early cerebral microvascular filling.

Preterm lambs at 125 ± 3 days' gestation were randomised to physiological-based cord clamping, where ventilation was initiated with the cord intact, using either 0.3 or 1.0 FiO_2, or to standard care, with immediate cord clamping and ventilation with 0.3 FiO_2. In standard care lambs, the cord was clamped 30 s before ventilation, while in physiological-based cord clamping groups, clamping occurred after 10 min of ventilation. Synchrotron radiation microangiography was performed at defined time points to image microvascular filling of the right cerebral hemisphere following iodinated contrast administration into the right carotid artery. Vessel calibre was measured from corresponding cerebral vessel segments in angiographic frames at fetal baseline and 7 min after ventilation onset.

Preliminary analysis of a subset of animals comparing standard care and PBCC-100 lambs (n = 3/group) showed divergent early changes in cerebral vessel calibre. From fetal baseline to 7 min after ventilation onset, mean vessel calibre decreased in PBCC-100 lambs but increased in standard care lambs. These preliminary findings suggest that cord management and oxygen exposure may influence early cerebral microvascular vessel calibre during neonatal resuscitation. Synchrotron microangiography provides a novel and unique approach for assessing haemodynamic responses relevant to cerebrovascular injury risk.

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Shangcheng Yan

DAY 2

ABSTRACT 101

Probing Atomic Coordination and Chirality Evolution in Hierarchical Metal–Amino Acid Complexes

Chiral metal-amino acid assemblies provide a platform for investigating how molecular chirality is propagated across length scales into larger-scale structures. These self-assemblies show multispectral chiral optical responses from UV-Vis to NIR and THz, arising from hierarchical structures encoded from the Angstrom to micrometre scale. Here, synchrotron small-angle X-ray scattering (SAXS) and high-resolution powder diffraction were used to investigate the formation and crystallographic ordering of chiral microparticles formed from metal-amino acid coordination.

In this study we conducted flow-through SAXS measurements at BioSAXS beamline to follow the chiral micro-particle self-assembly. No distinct scattering peaks emerged during measurements; instead, nucleation and growth were accompanied by changes in the low-q scattering slope across millisecond timescales, consistent with evolving larger-scale structural organization. Furthermore, Powder Diffraction beamline measurements showed identical XRD patterns for the left-handed and right-handed particles, whereas a low-angle reflection in the achiral sample shifted from 3.636° to 3.588° in 2θ, corresponding to an approximately 1.3% increase in d-spacing. Combined synchrotron powder diffraction and three-dimensional electron diffraction revealed a well-defined in-plane periodic ordering in the left- and right-handed samples, with a = 5.07 Å and b = 9.69 Å. Pronounced disorder along c-axis prevented reliable determination of the corresponding lattice parameter and assignment of a complete three-dimensional space group indicating the challenge associated with structure determination of self-assembled system with short to medium range order. These results demonstrate the complementary capabilities of ANSTO synchrotron beamlines and electron diffraction. Together, these measurements link formation dynamics and crystallographic ordering in chiral microparticles.

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Lucy Costello

DAY 2

ABSTRACT 111

Enhancing Lung Cancer Diagnostics Through Dynamic Region-of-Interest CT Imaging

Lung cancer is the fourth most common cancer diagnosed and the leading cause of cancer death in Australia. Conventional lung imaging has limited resolution and contrast, which can make it difficult to properly visualise and characterise early-stage lung tumours, with a biopsy typically required. Here, we use Phase Contrast CT (PC-CT) to exploit x-ray refraction and improve lung tissue contrast. We couple PC-CT with the idea of "zooming in" to a suspicious lesion or area of the lungs, utilising a narrow x-ray beam to take a high-resolution region-of-interest (ROI) CT.

Utilising the Imaging and Medical Beamline (IMBL), we imaged large animal lungs in a chest phantom paired with gated ventilator imaging to capture 8 time points throughout a breath cycle. We captured a region-of-interest with a field of view of ~35 mm across with a resolution of around ~0.1 mm, resolving bronchioles and individual alveoli. Comparisons to clinical CT show ROI PC-CT images provide entirely novel information.

Region-of-interest phase-contrast CT could provide advantages for radiomics and the characterisation of early-stage tumours to determine a treatment plan. We examined the diagnostic capabilities of this approach by imaging human lung cancer tissue specimens at the IMBL. Image evaluation included comparisons with virtual histology taken at the Micro-Computed Tomography (MCT) Beamline and conventional haematoxylin and eosin (H&E) stained histology. Our long-term goal is to reduce the need for invasive biopsies and improve lung cancer prognosis via the enhanced soft-tissue sensitivity and spatial resolution provided by ROI-CT imaging.

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Helen Forrester

DAY 2

ABSTRACT 53

Enhancing the treatment efficacy of synchrotron microbeams by adjucant anticancer therapy

The efficacy of Microbeam Radiation Therapy (MRT) with adjuvant systemic anticancer therapy was investigated for a highly aggressive and metastatic 4T1.2 murine mammary carcinoma. MRT, delivered at ultrahigh dose rates (UHDR) at the Imaging and Medical beamline (IMBL) results in high normal tissue tolerance and effective tumour control. Importantly, MRT induces a transient increase in tumour vascular permeability, known as a "permeability window", which was exploited to improve the targeted delivery of anticancer agents.

BALB/c mice were implanted with 4T1.2 triple negative mammary carcinoma cells into the fourth inguinal mammary fat pad. Primary tumour was irradiated with temporal fractionated synchrotron UHDR-MRT with or without FLASH-RT (synchrotron UHDR-broad beam) fractions, combined with three different clinically relevant immunotherapy or chemotherapy agents delivered within the "permeability window". The agents were (1) Antibodies against the immune checkpoint protein PD1, (2) Antibodies against the macrophage cell surface receptor CSF1R, and (3) doxorubicin, a standard-of-care chemotherapy for breast cancer. Changes in primary tumor volume and overall animal survival were compared in treatment and control groups.

Neither antibody therapy alone significantly delayed tumour growth compared to untreated controls, but doxorubicin alone was effective. Radiation was the dominant factor influencing both tumour control and survival outcomes. MRT combined with FLASH-RT was highly effective with or without doxorubicin and was associated with increased survival, and three fractions of MRT, each combined with anti-PD1 therapy significantly improved survival compared to either modality alone. In contrast, CSF1R blockade did not enhance the effects of radiation. The extended survival of tumour-bearing mice indicates that MRT irradiation of the primary tumour produces an anti-metastatic activity.

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Michael Rice

DAY 2

ABSTRACT 42

A γδ T cell receptor recognises the side of the CD1b lipid antigen presenting molecule

T cells comprise the cellular arm of the adaptive immune system and can be categorised into either αβ or γδ T cells. Extensive characterisation of αβ T cells has unearthed their role in the immune response. Comparatively there persists a poor understanding on the functions of γδ T cells that has been hampered by an incomplete ligand repertoire. This is despite γδ T cells playing a vital role in the immune response against viral, bacterial and Plasmodium infections. Therefore, we investigated how γδ T cells recognised a known antigen, lipid antigens, to shed light on this enigmatic T cell population. Here we undertook a multi-faceted biochemical, structural and cellular investigation to uncover how γδ T cells recognised lipid antigens presented by CD1b. Here, we determined to our knowledge the first γδ TCR-CD1b complex structure, that bound CD1b via an unusual side-docking orientation, providing the molecular basis for the observed lipid-agnostic binding. This was in stark contrast to γδTCR-CD1b recognition that contacts the lipid antigen and represented a novel TCR binding mode. We then validated this binding mode via complementary small angle X-ray scattering experiments.

Structurally guided mutagenesis experiments allowed for detailed mapping of key γδTCR contacts that were conserved across CD1 isoforms. Finally, CD1b-tetramer staining of intestinal biopsies then identified Vδ1+ CD1b+ γδ T cells are enriched compared to CD1b- γδ T cells although represent a rarefied T cell population in tissues. Ultimately, we provide the first molecular insights into γδ TCR recognition of CD1b that occurred via an unheralded mechanism.

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Elette Engels

DAY 2

ABSTRACT 82

Unleashing the Potential of Microbeam Radiation Therapy in Spontaneous Canine Sarcoma Treatment

Introduction: Microbeam Radiation Therapy (MRT) is a form of submillimetre spatially fractionated radiotherapy that can be delivered at the Imaging and Medical Beam Line (IMBL) of the ANSTO ANSTO. Preclinical studies demonstrate that high-dose microbeams inhibit tumour growth, disrupt tumour vasculature, and induce anti-tumour immune responses. However, the efficacy and safety of MRT must be evaluated in spontaneous cancers of similar size, growth and microenvironment to those in humans.

Method: Two studies investigated MRT in spontaneous canine sarcomas of the distal limb. Four dogs with osteosarcoma received a partial-field MRT to investigate in-field and out-of-field effects. Eleven dogs with soft tissue sarcoma received full-field irradiation with either MRT (n=6) or FLASH broad-beam (BB) radiotherapy (n=5). An Eclipse-hybrid planning system was used to prescribe doses to the target volumes, 5 Gy for BB and MRT valley doses (150 Gy peak). CT imaging before and after irradiation assessed tumour volumes and bone density, while MRI additionally evaluated osteosarcoma vascular permeability. Tumour tissue and serial blood and urine samples were collected for histopathological, immunological, proteomic and biochemical analyses.

Results: MRT reduced tumour volume in both forms of sarcoma, producing an 80% response compared to 40% with BB in soft tissue sarcomas. Despite receiving only partial irradiation, osteosarcoma regressed in 3 of 4 dogs, accompanied by increased anti-tumour immune responses and vascular disruption. CT, histology, and biochemical analyses showed that the regressing tumour was replaced by new bone via osteogenesis, supporting bone recovery. No skin toxicity or hair loss was observed at six months post-treatment. Conclusion: MRT safely and effectively treated large, spontaneous canine sarcomas, demonstrating promising anti-tumour efficacy and normal-tissue sparing.

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Mohamed Abdelaal

DAY 2

ABSTRACT 6

The antigen presenting molecule MR1 binds host-generated riboflavin catabolites

Major histocompatibility-complex (MHC) class I-related (MR1) protein presents vitamin B-related metabolites to Mucosal-Associated Invariant T (MAIT) cells. Microbial riboflavin precursors are well known MR1 ligands; however, it remains unclear whether host-generated riboflavin degradation metabolites influence MR1-mediated immunity. Here, we report that riboflavin catabolites, including 10-formylmethylflavin (FMF), lumichrome, lumiflavin and alloxazine bind to MR1 with moderate affinity, while riboflavin itself binds weakly.

While the microbial riboflavin ligands are known to increase MR1 cell surface presentation, the riboflavin catabolites were found to moderately reduce cell surface levels of MR1 by stabilizing and retaining MR1 in the endoplasmic reticulum (ER). Our data showed that these riboflavin catabolites bind to the intracellular MR1 and inhibit MR1 release from the ER. They also weakly competed with Vit B-based Ags for MR1 binding, thereby inhibited MAIT cell activation. The crystal structures of MR1 complexed with riboflavin, FMF, lumichrome and lumiflavin, show binding of these three-ringed compounds in the A'-pocket of MR1. The crystal structure of MR1-lumichrome revealed that lumichrome formed a covalent “flavin bond” with MR1-Lys43 differing from the typical Schiff-base bond of MR1-Lys43-Ag complexes seen with riboflavin precursors. Collectively, we identified three-ringed isoalloxazine derivatives which can bind MR1 and downregulate cell surface expression levels, suggesting a potential role in dampening MAIT cell immunity.

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James Cayley, Eugene Tan

DAY 2

ABSTRACT 35

Dose-rate dependence of Gafchromic film within ultra-high dose-rate FLASH irradiation fields at PEER

Many FLASH studies employ Gafchromic films for dosimetry. The use is so prolific that these films are considered dose-rate independent. During development of the 100 MeV Pulsed Energetic Electrons for Research (PEER) beamline at the ANSTO ANSTO, ultra-high-dose-rate (UHDR) dosimetry investigations revealed an over-response of Gafchromic EBT-XD film as the dose-per-pulse (DPP) and dose-rate was increased. This effect was also discovered during independent characterization at a different facility, and for EBT3 under rigorous metrological conditions, traceable to primary standards.

Initial results at PEER demonstrated an overresponse relative to the charge delivered in each pulse of the linac. A complimentary experiment was conducted to deliver fixed charge and, therefore, DPP over different timescales. For all DPP, the lowest dose-rate deliveries converged to produce the same normalised values in units of Gy/nC. Extrapolating this value and comparing to the dose measured by EBT-XD confirmed the overresponse and allowed for correction factors to be calculated.

The observation of this dependence and the work that followed has important ramifications for the field as clinical FLASH treatments advance towards reality. The sparing often reported in high DPP preclinical research may be due to under-dosing when relying upon Gafchromic film measurements, rather than a FLASH sparing effect.

This talk presents initial results obtained at PEER, and further work conducted since to fully characterize EBT-XD for use in UHDR investigations at PEER and DESY, Germany. Further, investigations are currently underway to determine the physical phenomena responsible for this effect, to understand if it is possible to produce these films without a dose-rate dependence.

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Spencer Passmore

DAY 2

ABSTRACT 74

Optimizing the connectivity of alternate conformations to untangle protein ensemble models

Ensemble modeling offers a means of representing diffraction data collected in X-ray crystallography experiments that can account for the multitude of conformations that proteins realistically occupy inside a crystal. Despite this, ensemble models typically offer only minor reductions in R-free compared to single-conformation representations. It has recently become known that ensemble models introduce a unique kind of local minimum trap to refinement that cannot be avoided or resolved by contemporary approaches. A kind of connectivity issue, these traps frequently manifest as locally strained geometries in distant parts of the structure, and thus are rarely apparent from inspection. Here, we present a method to escape these traps by finding the energy-minimizing assignment of conformation labels to the alternate locations (altlocs) of atoms, thereby relieving geometric strain without changing the model structure factors. The efficacy of the method is demonstrated by application to a previously published synthetic dataset that traps modern refinement software.

When applied to real data, the approach is shown to improve Rfree and geometry validation metrics over controls. Applying this method in combination with conformation-aware water-picking to a deposited dataset for a 19 kDa protein, we produce a 0.77 Å 6-conformation model with R-work/R-free values of 4.7%/6.4%.

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Rabia Sandhu

DAY 2

ABSTRACT 77

High-Spatial-Resolution Dosimetry for Microbeam Radiotherapy with a Multi-Channel Hydrogenated Amorphous Silicon Detector

Microbeam radiation therapy (MRT) is an emerging spatially fractionated radiotherapy technique that delivers arrays of narrow, high-dose X-ray microbeams to enhance tumour control while reducing normal tissue toxicity. Clinical translation of MRT requires detectors capable of real-time dosimetry with high spatial resolution under ultra-high dose rate (UHDR) conditions. Existing dosimeters are unable to simultaneously provide real-time readout, high spatial resolution, and multi-channel operation, requiring mechanical scanning for peak-to-valley dose ratio (PVDR) measurements.

This work presents the first experimental characterisation of a multi-channel hydrogenated amorphous silicon (a-Si:H) detector fabricated on a plastic substrate for synchrotron MRT dosimetry. The detector comprises eight strips arranged in an edge-on geometry, enabling simultaneous sampling of microbeam peak and valley regions. Detector performance was evaluated at the DESY P61A beamline through dose linearity, percentage depth dose, broadbeam and microbeam field profiling, and PVDR measurements. X-ray beam-induced current mapping at the ANSTO assessed charge collection efficiency, with performance benchmarked against the PTW microDiamond detector.

The detector demonstrated excellent dose linearity ($R^2 \geq 0.999$), reproduced percentage depth dose within ±3% of the reference detector, and simultaneously resolved five microbeams with a mean full-width at half-maximum of 51.6 ± 1.7 µm and a mean pitch of 397.8 ± 1.5 µm, consistent with nominal microbeam width and pitch. XBIC mapping confirmed uniform charge collection while identifying the connection pad as an unintended sensitive volume. These findings demonstrate the potential of the proposed a-Si:H detector array for real-time MRT quality assurance, providing high spatial resolution without sequential mechanical scanning.

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Christopher Szeto

DAY 2

ABSTRACT 76

Room-temperature serial crystallography of the antivirulence drug target DsbA by in-tray serial crystallography

Antimicrobial resistance is a major and growing cause of death worldwide. Antivirulence agents disarm pathogens without the selective pressure that drives resistance to antibiotics. Bacterial disulfide bond protein A (DsbA) folds virulence factors essential for Gram-negative invasion, so inhibiting DsbA should attenuate virulence without inducing resistance.

Twenty years of structure-guided effort on *E. coli* DsbA have produced inhibitor candidates that stall pre-clinically. Inhibitor optimisations are guided by cryogenic data, but cryocooling can alter structural conformations [1]. This matters for DsbA as its most promising inhibitor site is a cryptic pocket that opens only when the protein is dynamic [2].

We present the first serial synchrotron crystallography (SSX) structures from the ANSTO MX3 microfocus beamline. Rastering directly through 96-well MiTeGen in-situ plates gave complete room-temperature (RT) structures of apo *E. coli* DsbA and hen egg white lysozyme. No micro-crystallisation optimisation, bespoke scripting, or sample handling beyond tray setup was required. Radiation damage is why cryocooling became standard. SSX spreads dose across thousands of crystals, limiting global damage at RT, but disulfides are damaged roughly 5-fold faster than the bulk structure. Across DsbA datasets collected at 3%, 5%, and 20% transmission, the catalytic disulfide stayed intact even in sodium cacodylate, while an adventitious Cu site at a crystal contact lost density progressively with dose. We also show hot-off-the-press cryo/RT differences in a DsbA-inhibitor complex, and a practical guide to which drops are worth collecting, how many give a complete dataset, and what orientational sampling to expect.

1. Stachowski TR, Fischer M. Nat Chem Biol 2026;22:169–179.
2. Mohanty B et al. Angew Chem Int Ed 2025;64:e202515306.

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Vincent de Rover

DAY 2

ABSTRACT 45

Geant4 Modelling and Experimental Validation of Synchrotron Minibeam Radiation Therapy with Clinically Relevant Treatment Scenarios

Introduction: Synchrotron minibeam radiation therapy (MBRT) has demonstrated exceptional healthy tissue sparing and strong tumour control in pre clinical studies by spatially fractionating radiation into peak and valley doses. A Geant4 model of synchrotron MBRT delivered at the Imaging and Medical Beamline (IMBL) in hutch 3B at the ANSTO has been validated for clinically relevant treatment conditions.

Materials and Methods: To perform this validation, a range of broad beam (BB) and MBRT fields with varying sizes (up to 7×7 cm^2) and filtrations were delivered. Depth dose curves were measured using PTW PinPoint and microdiamond detectors, EBT XD films, and epitaxial silicon detectors, and compared with Geant4 simulations. Additionally, dose distribution in a heterogeneous 3D printed head phantom was assessed for a clinically relevant MBRT scenario.

Results: The Geant4 model showed excellent agreement with experimental BB measurements in solid water, remaining within 4%. For MBRT fields, film measurements demonstrated strong consistency, with peak doses matching within 6% and most valley doses within 10%, falling inside measurement uncertainty. In the heterogeneous head phantom, the peak to valley dose ratio (PVDR) was maintained even after traversing bone equivalent material, yielding a PVDR of 5.1 ± 0.2 compared with 5.5 ± 0.6 at similar depth in solid water. Conclusion: Overall, the Geant4 model has been successfully validated for synchrotron MBRT fields. Preservation of PVDR in a realistic 3D printed head phantom further, using clinically relevant treatment fields supports the efficacy synchrotron MBRT, with ongoing work extending model validation to additional heterogeneous phantoms.

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Ben Krinkel

DAY 2

ABSTRACT 1

Targeting cancer's metabolic rewiring: structure-guided discovery of malic enzyme inhibitors at the AS

Cancer remains a global challenge that urgently needs therapies to improve outcomes and quality of life. Tumour cells rewire metabolism, increasing glutamine dependence and upregulating mitochondrial malic enzyme 2 (ME2), which generates pyruvate and NAD(P)H. ME2 is overexpressed in pancreatic, melanoma, and lung cancers, making mitochondrial malic enzymes compelling, underexplored targets for structure-guided drug discovery.

We expressed and kinetically characterised recombinant human ME1, ME2, and ME3, with and without inhibitors, and then solved a complete set of X-ray crystal structures at the ANSTO. High-resolution crystallography revealed a potent malic enzyme inhibitor bound with a clear ligand and metal coordination, and captured an unexpected enzyme conformation, opening new structural hypotheses for inhibition.

Guided by these structures, we performed virtual screening of a curated library of up to 14 million drug-like and fragment molecules, advancing biochemical hits into cellular assays. Structure-based screening against the novel conformation identified multiple scaffolds; lead compounds NPD 389 and FLA showed distinct inhibition profiles. NPD 389 binds in a metal-coordinating mode, while FLA occupies a previously cryptic pocket adjacent to the NAD+ and malate sites that rearranges upon ligand engagement. We also investigated malic enzyme binding partners using BioSAXS, revealing unexpected protein-protein interactions.

In melanoma and triple negative breast cancer cell panels, NPD 389 and FLA reduced proliferation in most models, supporting their potential as chemical leads. These results establish ME2/ME3 as tractable targets and reveal metal binding modes and cryptic allosteric pockets, providing a powerful platform for rational optimisation of potency, isoform selectivity, and mitochondrially targeted cancer therapeutics.

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Samuel Nitschke

DAY 2

ABSTRACT 69

Heavy element-tagged fluorescent probes for correlative optical and X-ray fluorescence microscopy

Cells are highly compartmentalised, yet assigning elemental distributions to specific subcellular regions remains challenging. Fluorescent probes can be directed to cellular compartments, but fluorescence alone does not provide an elemental landmark within an X-ray fluorescence microscopy (XFM) map. We are developing a toolbox of fluorescent probes containing heavy element tags that can be imaged independently by fluorescence microscopy and XFM. Correlation between the optical and elemental signals allows probe localisation to be validated across modalities and provides landmarks for compartment-resolved elemental analysis.

We first established this approach using brominated 4-amino-1,8-naphthalimides, whose intracellular fluorescence distributions were reflected in their bromine XFM maps. Having demonstrated that bromine could act as an XFM tag, we extended the platform towards subcellular mapping by introducing organelle-directing groups. A brominated naphthalimide-Hoechst conjugate produced nuclear localisation by fluorescence microscopy and nuclear enrichment of bromine by XFM, showing that intentional localisation could be recovered by both modalities.

Lanthanide-containing probes expanded this strategy by incorporating intrinsic elemental labels as DOTA-chelated complexes. Untargeted coumarin-based lanthanide probes showed broad intracellular distributions, with spatial agreement between their fluorescence and corresponding elemental maps. Appending a Hoechst targeting group to an ytterbium-DOTA probe redirected its distribution to the nucleus, with the nuclear fluorescence reflected in the corresponding ytterbium XFM map. Together, these results trace a progression from mapping general cellular uptake to resolving designed subcellular localisation. Expanding this strategy across different targeting groups and elemental labels will provide a toolkit for mapping distinct cellular regions using two complementary imaging modalities.

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Usman Faryad

DAY 2

ABSTRACT 34

Thermal Transformation of Scorodite (FeAsO4.2H2O) During Bushfire-Relevant Conditions: An Impact on Arsenic Transformation and Mineral Stability

Climate change is increasing the frequency of bushfires globally and is increasingly believed to drive arsenic (As) cycling. Arsenic is a notorious redox-sensitive metalloid that is sensitive to fire-driven thermal processes, which in turn has impacts on structural stability. However, the geochemical response of arsenate-bearing iron (Fe) minerals under low-to-moderate bushfires remains poorly resolved. To investigate this, we simulated low-to-moderate bushfires (175–350°C) on scorodite (FeAsO4·2H2O), with and without organic matter (5% C w/w citric acid and humic acid). Findings from XRD, Synchrotron Powder Diffraction (PD), XAS, Mössbauer spectroscopy and TEM indicated crystallinity loss after heating at 275 and 350°C.

FTIR analyses showed the absence of structural-water O-H bands from the structure (consistent with TGA), suggesting an anhydrous ferric arsenate-like phase. Mössbauer spectroscopy indicated a broad Fe(III)-doublet, suggesting ferrihydrite, and a second Fe(III) paramagnetic-doublet, which is identified as an amorphous ferric arsenate phase. Arsenic K-edge XANES revealed partial As(V) reduction to As(III) with 6-8% at 275°C and 13-15% at 350°C in the humic and citric acid systems, respectively. Arsenic and Fe K-edge EXAFS shell fitting indicated the formation of a predominantly poorly ordered, anhydrous ferric arsenate phase, in which Fe exhibited neither well-defined Fe-O tetrahedral nor octahedral local coordination.

These findings indicate that bushfire heating promotes structural and redox changes, which results in novel nano-crystalline phases with implications for As solubilisation in post-fire contaminated landscapes.

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Kilahney Murphy

DAY 2

ABSTRACT 117

Benchmarking Naturally Weathered Polysiloxane and Polyurethane Coatings using Synchrotron IRM, XFM and GiSAXS/GiWAXS against Tabletop Techniques

The Royal Australian Navy replaced exterior polyurethane-based topside topcoat systems with a polysiloxane based topcoat. The polyurethane coatings, requiring an isocyanate curing agent that poses significant WH&S hazards, displayed chalking (breakdown products) in service and required regular re-coating. Polysiloxane coatings removed the need for hazardous isocyanate curing agents while providing greater exterior weathering durability (compared to polyurethanes), due to a greater content of silicon-oxygen bonds in the polymer backbone.

To demonstrate the improved exterior weathering of polysiloxane coatings, a commercial polyurethane-based topcoat and a commercial polysiloxane-based topcoat containing equivalent tinting pigments were placed in comparative natural weathering environments continuously for 5 years. The effects of high-UV, high-humidity tropical and high-UV temperate weathering conditions were compared to unexposed samples. The degree of weathering of the samples was characterised by SEM/EDS and FTIR tabletop instruments. These tabletop measurements were subsequently benchmarked against results obtained from highly sensitive and spatially precise XRM, IRM and SAXS/WAXS analyses using synchrotron light.

The greater resolution and capabilities of synchrotron-based analytical techniques were found to support and enhance the findings of tabletop instruments through the ability to conduct spatial mapping and define microstructures more precisely. For example: • Molecular changes in each coating examined with IRM, both spatially and with principal component analysis, provided evidence that the polyurethane coating exhibited greater bulk degradation compared to polysiloxane. • XANES results via XFM suggested that the oxidation state of coating components, with emphasis on chromium state changes within pigments, were relatively stable. These findings were consistent with nano-structure/crystalline structure, as determined by GiSAXS/GiWAXS.

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Nathan Collins

DAY 2

ABSTRACT 18

Reconstructing Late Holocene eruption histories at Mt Taranaki using synchrotron X-ray fluorescence microscopy of speleothems

Speleothems are emerging as valuable archives of volcanic activity, yet their potential for preserving primary tephra deposits remains largely unexplored. Here, we used the X-ray Fluorescence Microscopy (XFM) beamline at the ANSTO to investigate the depositional origin of volcanic particles and associated geochemical proxies within four Late Holocene speleothems from a tufa cave located proximal (<13 km) to New Zealand's highest risk volcano, Mt Taranaki. Quantitative XFM elemental maps acquired at 2–20 µm spatial resolution resolved multiple volcanic particle-rich laminae throughout the speleothems. The origin of volcanic particle-rich laminae was evaluated by integrating particle distributions with spatial variations in environmentally sensitive trace elements (e.g., Mn, Br, Sr, Zn and Cu).

Comparisons between particle-rich laminae deposited before and after the last known eruption of Mt Taranaki (~AD 1790) provided an analogue for sediment remobilisation associated with historical land clearance, allowing geochemical signatures indicative of primary fallout and secondary reworking to be differentiated. Candidate tephra horizons identified by XFM were subsequently targeted for electron probe microanalysis (EPMA), confirming multiple primary tephra layers and enabling correlation with individual eruptive episodes spanning the past ~1500 years. Integration of XFM-derived annual Sr lamina counts with refined U–Th chronologies constrained eruption ages to annual and, in some cases, sub-annual precision, resolving individual eruptive pulses and providing unprecedented constraints on eruptive timing and tempo.

These results highlight the capability of synchrotron-based XFM to combine high resolution particle imaging with quantitative two-dimensional geochemical mapping, providing a powerful new approach for reconstructing eruptive histories from speleothem archives.

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DAY 2

ABSTRACT 21

Thermal evolution of amorphous ferric arsenate in the presence of inorganic and organic phosphorus

The thermal stability of arsenic (As)-bearing iron (Fe) phases, such as amorphous ferric arsenate (AFA), is critical for understanding the long-term stability of As immobilisation under changing environmental conditions. However, the influence of inorganic and organic phosphorus (P) species during thermal events remains poorly resolved. Here, AFA stability and phase transitions in the presence of inorganic and organic-P species at 25, 40, 50, 60, and 70°C are examined. Synchrotron-based X-ray diffraction indicated that higher organic-P loading promoted the formation of ferric phytate-like structural features at 25 °C, whereas inorganic P inhibited crystallisation up to and including 60°C. Iron K-edge and As K-edge XAS further demonstrated temperature-dependent changes in the local structural environments in response to P reaction. Fe K-edge EXAFS reveals that organic P induces structural modifications, as indicated by the appearance of a Fe-P shell at 3.24Å (CN 1), even at 25°C. Conversely, inorganic P induces substantial structural rearrangements at 70°C, again demonstrated by the appearance of an Fe-P shell at 3.22Å (CN 1). The As K-edge EXAFS also shows the concurrent evolution of the local As coordination environment with increasing temperature, consistent with progressive reorganisation of the Fe–As coordination environment and release to solution.

The data demonstrate the evolution of Fe–P coordination environments during thermal transformation, depending on the temperature, while retaining a mixed Fe–P–As coordination environment. Collectively, these findings demonstrate that phosphorus speciation modifies the thermal transformation pathway of AFA and consequently influences As retention in iron-rich systems under elevated thermal conditions.

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DAY 2

ABSTRACT 61

Prompt gamma ghost imaging on the DINGO beamline

Prompt-gamma neutron activation analysis (PGAA) is a technique based on neutron-nucleus interaction. The interaction is unique for each element and isotope, and the measured gamma spectrum emitted by the target object can identify its atomic composition. Here, we explore the possibility of using ghost imaging (GI) to add spatial information to PGAA. Ghost imaging is a recent and unconventional imaging technique where the photons or particles that interact with the object can be recorded using a spectrometer without position information. Image formation relies on the correlation between two light beams or particle streams, one of which interacts with the object and the other acts as a reference beam. Ghost imaging has the potential to revolutionise neutron-based imaging in terms of achievable spatial resolution, dose reduction, and adding imaging capabilities where none currently exist.

To our knowledge, quantitative two-dimensional elemental mapping using PGAA has so far been demonstrated only with scanning-pinhole neutron illumination. We propose replacing sequential scanning with structured neutron illumination combined with computational imaging. This approach can produce high-resolution images from fewer measurements using compressed sensing and prior information obtained from simulation neutron radiography and tomography, potentially improving imaging efficiency and spatial resolution.

We set up a classical GI experiment on the Dingo neutron imaging beamline. The GI mask was designed with an S-cyclic matrix pattern and fabricated with boric acid to provide attenuation. We measured the peak energies for Ti and Cl given each patterned illumination and were successfully able to reconstruct the position of each element in Sample 1. A sensitivity study was conducted with Sample 2 to determine the ability to identify different concentrations of Cl.

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