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Monday
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Abstract

Tamar Greaves

Plenary Session - A journey through beamlines with ionic liquids

Ionic liquids (ILs) can be considered as both liquid salts and as novel solvents, and can be tailored to have properties suitable for a broad range of applications. They can also be combined with molecular solvents, such as water, to enable more control over the solvent environment. Over the last nearly 20 years I have explored the solvent properties of neat ILs and IL-solvent mixtures, with a focus on fundamental solvent properties, their use as amphiphile self-assembly media and more recently their use as solvents for biological molecules. The vast compositional space possible through cation-anion-water combinations has led to the use of high throughput approaches, including liquid handling robots, automated data acquisition and data analysis, and machine learning. This research has made significant use of many ANSTO beamlines, and in particular the SAXS/WAXS beamline has enabled large data sets to be collected. In this presentation, I will journey through the use of a selection of ANSTO beamlines and how they are aiding us in understanding IL solvation properties, along with the issues specific to using ILs and novel solvents instead of aqueous solvents. This will include the fundamental liquid nanostructure of the neat ILs and how these are modified by the addition of solutes, along with the crystal structure of solid ILs. The use of ILs as amphiphile self-assembly media has led to them supporting micellar, lamellar, hexagonal and cubic liquid crystal phases, with structure-property relationships developed between the IL structure and the phases identified. This has then led to their use as solvents for biological systems, including protein stability, protein crystallography, cryopreservation, drug delivery and understanding their interactions with cells. The opportunities which ILs are presenting for technique development, largely enabled due to their negligible vapour pressure, will be discussed.

Monday 27th

Abstract: 81

Aiswarya Pradeepkumar

Real-time monitoring of the epitaxial graphene growth with neutron reflectometry

The synthesis of epitaxial graphene (EG) on cubic silicon carbide (3C-SiC) on silicon substrates could enable tunable electronic and photonic devices that can directly integrate with existing silicon technologies. We have previously indicated that using Ni/Cu catalytic alloy [1] on the highly-defective 3C-SiC enables uniform graphene growth over large scales and a lower temperature process than the more conventional thermal decomposition of the 3C-SiC[2].

A thorough understanding of the epitaxial growth mechanism will inform future advances in grain size and layer control of this EG process. In this work, we performed an in-situ growth of EG on 3C-SiC/Si (1100°C, 10-5 hPa) and investigated the real-time kinetics of alloy-mediated graphene layer formation using neutron reflectometry, thanks to the neutron's ability to penetrate below the surface of heterostructures and probe light elements[3]. Neutron reflectometry measurements were performed on the Spatz time-of-flight neutron reflectometer at the ACNS, ANSTO. The time-resolved neutron measurements were conducted in situ during a controlled annealing process. The results indicate the start of a solid phase reaction at 600°C, where we expect that the Ni catalyst react with SiC forming NiSi2 and releasing atomic carbon. After 1 hour of annealing at 1100°C, a low-density surface layer forms, which may be related to molten copper and the liquid-phase growth conditions of EG [1] that lead to an increase in the density of the graphene layer. This work enables to understand the graphene growth mechanism on 3C-SiC/Si substrates and the catalytic role of the metallic layers to optimize the synthesis process for graphene-based electronics and photonics.

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Abstract: 122

Sajjad Seifi Mofarah

Ion Implantation for Surface Engineering of Heterojunction Nanostructures for Advanced Applications

Recent developments in advanced materials technology have focussed on addressing the increasing global demand for renewable energy sources to reduce dependency on exhaustible fossil fuels. The design of high-performance efficient materials at the nanoscale through surface engineering for batteries, pseudocapacitors, catalysts, and sensors is a crucial step in the advancement of renewable technologies. Surface engineering can assist in the development of heterojunction nanostructures and low-concentration solid solutions from doping which have significant potential in energy-related and low-power sensing applications.

One route for achieving controlled surface chemical modification is ion implantation. The NEMCAT group at UNSW Sydney in partnership with the Centre for Accelerator Science (CAS) at ANSTO has been undertaking collaborative projects on the use of low-energy ion implantation to modify the structural and chemical characteristics of nanostructures with unique architectures ranging from one-dimension (1D) to three-dimension (3D). The nanostructures are mainly formed through novel electrochemical deposition, controlled nano-assembly of nanoparticles, and/or conversion of metal-organic frameworks (MOFs), as precursors. The nanostructures can be decorated with metal heteroatoms by implantation followed by subsequent heat treatment under specific atmospheres to incorporate them as dopants in the lattice. The resultant heterojunction nanostructures showed exceptional performance in energy storage (pseudocapacitance), catalysis (dye degradation), and sensing applications (H2O2 detection). The heterojunction nanostructures, coupled with an increased density of structural defects introduced through controlled ion implantation processes, offer a promising approach for tailoring the electronic, chemical, and structural properties of these nanostructures. This represents a notable advancement, providing a simplified and tunable approach to developing functional materials suitable for energy generation and environmental remediation.

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Monday
27th

Abstract: 49

Jessica Merz

High-intensity in-situ neutron diffraction study of MAB phase ceramic synthesis

This high-intensity neutron diffraction study using Wombat has identified complex, multi-stage reaction pathways, including self-propagating reactions, in the formation of MAB phase ceramics. The reaction mechanisms of this group of advanced ceramics were previously poorly understood, preventing their large-scale production and potential use in a range of high-performance applications. These include as inert electrodes in green Al refinement, as nuclear shielding materials, and as catalysts in the form of 2D MBenes.

Using scan rates of up to 100 Hz during heating from room temperature to 1200 °C, samples were reacted in either a vacuum furnace, heating at 5 °C/min, or in an induction furnace at >400 °C/min. This allowed the analysis of the reaction mechanisms of the MAB phases, identifying intermediate phases and categorising reaction stages. Intermediate phases with lifespans of 1-30 s have been identified, as well as previously unknown low-temperature formation windows for ternary phases in at least two systems. This includes the formation of MoAlB at <600 °C, ~500 °C lower than what was previously believed to be required.

Understanding the reaction pathways of the MAB phases based on the results of this in-situ neutron diffraction study will allow improvements in MAB phase synthesis through the optimisation of sample preparation and heating conditions to suppress the formation of impurity phases. These results may also lead to the development of more energy efficient low-temperature synthesis.

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Monday
27th

Abstract: 99

Frederick Marlton

Examination of the local and average structure of the CaTi1-xFexO3-x/2 ionic conductor

The flexible structure of perovskites enables the incorporation of anion vacancies, making them attractive materials for ion conduction applications. Calcium titanate-based compounds exhibit oxygen ionic and electronic conductivity, and have the potential to be used in high-temperature electrochemical devices due to their moderate thermal expansion and stability in reducing atmospheres. The ionic conductivity can be altered by partially replacing the Ti^{4+} cations with lower valent cations, such as Fe^{3+}. This creates negative charges, which are compensated by the formation of oxygen vacancies. The perovskite system $CaTiO_3$ – $CaFeO_{2.5}$ exhibits an increase in oxygen vacancies, from zero in $CaTiO_3$ to 0.5 per formula unit in $CaFeO_{2.5}$ (or $Ca_2Fe_2O_5$), which adopts the brownmillerite structure. The brownmillerite structure can be considered a non-stoichiometric perovskite, derived from the perovskite structure by the addition of one oxygen vacancy per six anionic sites, ordered along [101] rows in each second (0k0).

Several studies have been conducted on the $CaTi_{1-x}Fe_xO_{3-x/2}$ system using a combination of Mössbauer spectroscopy, microscopy and diffraction techniques. An early study revealed that with increasing Fe content, the anion vacancies go from completely disordered at low Fe contents, to a fully ordered from. This evolution from a disordered to ordered arrangement of vacancies is important as it affects the structure of the system and, in turn, the ionic conductivity.

In this work we used a combination of high-resolution X-ray diffraction and neutron total scattering to understand the local and average structure of $CaTi_{1-x}Fe_xO_{3-x/2}$ for $x \leq 0.4$. This revealed significant disordering of the oxygen framework, which has implications for tuning the ionic conductivity.

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Monday
27th

Abstract: 133

Renjun Guo

Substrate Surface Morphology Regulation Enabling Highly-efficient p-i-n Perovskite Solar Cells

The engineering of the interface between thin films of perovskite absorbers and charge transport layers has been a driving force in advancing perovskite solar cells (PSCs) in the past decade. In the case of p-i-n PSCs, the progress and adoption of hole transport layers that utilize self-assembled monolayers (SAMs) have facilitated highly efficient contacts, effectively reducing interfacial recombination and enhancing power conversion efficiency in both single-junction and tandem solar cells. However, the performance and reproducibility of PSCs have been limited by the non-conformal growth of self-assembled monolayers. Here, we report a comprehensive study of the impact of substrate morphology on the growth modes of electron-blocking layers (EBLs) and relative PSCs. By investigating the domain distributions of EBLs through grazing-incidence small-angle X-ray scattering (GISAXS) methods, we identify the different growth modes of EBLs affected by the substrates. By substrate morphology regulations, we achieve a PCE of 24.8 % for the p-i-n PSC. The quasi-steady-state J-V scan performs a PCE of 23.5 %. The 500-h maximum power point tracking efficiency demonstrates that our approach shows good operational stability. Through sophisticated fluence-dependent time-resolved photoluminescence spectra and intensity-dependent photoluminescence quantum yield characterizations, the efficiency loss channels of solar cells could be suppressed by our strategies due to a more homogeneous SAMs distribution on the regulated indium tin oxide (ITO) morphology substrates. Our drift-diffusion simulation results confirmed that the suppressed interface energy loss could boost performance.

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Monday
27th

Abstract: 11

Matthew Teusner

New materials for battery electrodes are paramount to ensuring future battery supply can meet the ever increasing demand for energy storage. Furthermore, detailed investigations into the various physical and chemical aspects of these materials are required to allow the same level of nuanced microstructural and electrochemical tuning that is available for conventional electrode materials. Specifically, deeper insights into the relationship between the electrode nano and microstructure and electrochemical performance provide avenues for significantly increasing the performance of a material.

The research reported here is part of a larger project investigating metal-carboxylates, e.g., iron (ii) tartrate, as potential anode materials in lithium-ion batteries. This versatile family of materials not only demonstrate high capacities, but are typically non-toxic, environmentally benign, and easily synthesised from inexpensive and renewable/abundant feedstock chemicals. Additionally, use of these materials allows for a unique approach to controlling the electrode's nano and microstructure, due to their dissolution during electrode formulation; selective tuning of the electrode structure doubled the capacity of the material in some cases.

Small and ultra-small angle neutron scattering (SANS and USANS) was employed to better understand the electrode nano and microstructure and its relationship to the electrochemical performance. Use of these techniques to investigate battery electrode structure is relatively novel and as such, this research presents a foundational approach to the data interpretation and application.

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Wed
29th

Abstract: 134

Xiao-Qiang Liu

Hybrid improper ferroelectricity in A-site cation ordered Li2R2Ti3O10 ceramics with triple-layer Ruddlesden-Popper structures

Hybrid Improper Ferroelectrics (HIFs) have attracted considerable attention due to their potential for realizing room temperature multiferroicity with strong magnetoelectric coupling. HIFs exhibit a unique ferroelectric polarization induced by a complex distortion pattern involving two oxygen octahedral tilting modes. These materials are expected to be prevalent in perovskite and layered perovskite structures, as the ubiquitous distortions of oxygen octahedra occur in perovskite-related compounds.

While HIFs have been extensively studied in double-layer Ruddlesden-Popper oxides, their existence in oxides with an A-site cation ordered odd-layer Ruddlesden-Popper structures has thus far remained unexplored experimentally, despite theoretical predictions. In this study, we present the experimental observation of r oom-temperature ferroelectricity in the A-site cation ordered Li2R2Ti3O10 (R=La, Nd) ceramics with a triple-layer Ruddlesden-Popper structure. The polar phase was determined through a combination of first-principles calculations and powder diffraction analysis conducted at room temperature. The emergence of ferroelectricity in these materials was attributed to the triple-coupled irreps, including the A-site cation ordering. Our findings provide valuable insights into the design and realization of hybrid improper ferroelectrics in A-site ordered triple-layer Ruddlesden-Popper compounds.

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Wed
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Abstract: 165

BAOQI DONG

Investigating the role of Mo on precipitation in Mo-containing steel by ex-situ, in-situ SANS and APT

The precipitates in high strength low alloy steels have been historically studied by site specific Transmission electric Microscope (TEM) and Atom Probe Tomography (APT). However, these results are from very small regions which are sensitive to local composition changes and crystallography. Data that covers a wider field of view (which is, therefore, more statistically significant) is . In the present work, ex-situ and in-situ Small-Angle Neutron Scattering (SANS) combined with Atom Probe Tomography (APT) are employed for the first time to reveal the evolution of precipitation in Ti-Mo and Ti steels during tempering. The scattering signal clearly indicated that the size and volume fraction of precipitates changed dramatically after tempering. Due to the introduction of many atomic level and nanoscale precipitates after tempering, the average size of precipitate was refined, and the volume fraction was increased. The average size decreased from 3.72 to 2.82 nm in the Ti-Mo steel and from 5.08 to 3.07 nm in the Ti steel, respectively. At the same time, the volume fraction increased from 0.091 to 0.149 % in the Ti-Mo steel and from the 0.065 to 0.102 % in Ti steel after tempering, respectively. These larger scale statistically significant results provide evidence for the role of Mo in changing the precipitation behaviour and thereby the strength. More work is required to understand the mechanism by which this occurs and to develop a link between this new technique and established APT, which is currently underway.

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Wed
29th

Abstract: 120

Gary Bryant

Size, shape and self-assembly of Nanodiamonds in suspension

Nanodiamonds (NDs) are becoming increasingly important in science and technology with applications from drug delivery to sensing to tribology. NDs are generally made using two methods: by detonation (detonation nanodiamonds – DNDs) or using high-pressure high-temperature synthesis (HPHT NDs), and the two types of NDs have very different properties. HPHT NDs can be prepared with nitrogen-vacancy (NV) centres to make fluorescent nanodiamonds (FNDs), which can be used as nanoscale sensors for temperature and electromagnetic fields.

Many applications of NDs require suspension in aqueous solutions (for example biological media), however, to date there have been very few studies of their behaviour in suspension. Here we present two separate studies of NDs in suspension.
1. DND Self-assembly. DNDs consist of primary particles with sizes around 5 nm, but are known to self-assemble into fractal-like aggregates in water. Here we use small-angle scattering and light scattering to study the effects of salt and particle concentration on aggregate size and shape. The results suggest two aggregate populations with diameters of ~50 nm and ~300 nm, and we discuss the implications for DND applications.

2. Size and shape of FNDs. FND shape strongly affects fluorescent brightness and can limit sensor applications. Here, we use small-angle scattering, light scattering and AFM to demonstrate that FNDs have disk-like shapes with aspect ratios around 3. This high aspect ratio is important for many quantum sensing measurements as it enables enhanced sensitivities compared to spherical particles. We discuss the implications of FND particle shape for quantum sensing applications.

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Wed
29th

Abstract: 60

Joey Williamson

Structural and Magnetic properties of CoMoO4

The XMoO4 transition-metal molybdates (where X = a divalent transition metal ion) have received considerable investigation because of their interesting structural and optical properties, leading to potential applications that range from catalysts, to supercapacitors, to sensors [1]. These same structural properties have also led to interesting magnetic properties for several of the molybdates (Ni, Mn, and Cu): antiferromagnetic ordering at low temperature, with two notable spin flop transitions as field is increased [2].

This report investigates gaps in the literature, addressing the lack of magnetic data for CoMoO4, and exploring alternate forms of fabrication. Powder and thin film samples of CoMO4 were made by solid-state synthesis and RF sputtering respectively and annealed into their desired phases. Raman spectroscopy and X-ray diffraction were used to analyse synthesis routes for both optically active phases (α and β) in powder and thin film form. Magnetic measurements confirm the trend seen amongst the other molybdates, with varInstruments & Techniquesion in critical fields and transition temperatures seen between film and powder forms. Notably, the spin flop transitions for CoMoO4 are at a much lower critical fields than the other molybdates classified thus far and have a hysteresis loop that is not seen in other members of the family.

References:
[1] Costa, R.K.S. et al. (2019) 'Influence of europium doping on the structural phase-transition temperature of beta- and alpha - CoMoO4 polymorphs', Materials Research Bulletin, 118, p. 110517.
[2] Ehrenberg, H., Schwarz, B. and Weitzel, H. (2006) 'Magnetic phase diagrams of -MnMoO4', Journal of Magnetism and Magnetic Materials, 305(1), pp. 57–62.

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Tuesday 28th

Abstract: 58

Olga Martin

The role of ultra-high dose rate in effectiveness of Microbeam Radiotherapy for breast cancer treatment

In preclinical studies, Microbeam Radiotherapy (MRT) has demonstrated a much-improved therapeutic ratio compared to conventional radiotherapy, i.e., better local tumour control with substantially reduced normal tissue toxicity. It has been proposed that the combination of microbeams with ultra-high dose-rates (UHDR) further enhances the therapeutic ratio of MRT, but this assumption has never been directly tested.
Recently, at the Imaging and Medical Beamline (IMBL), ANSTO Australian Synchrotron, we conducted experiments involving irradiation of triple-negative 4T1.2 mammary carcinomas in BALB/c mice. We tested various MRT and/or broad-beam daily fractionated regimens. We found that a combination of MRT and broad-beam treatments, both delivered at ultra-high dose rates, is safer for animals and effective for primary tumour control than either modality alone. Further, using this combined treatment scheme, we explored the impact of decreasing MRT dose-rates on the efficacy of MRT/broad-beam treatment. A single session of 285Gy peak-dose/7Gy valley-dose MRT, delivered at ~1000Gy/s, ~100Gy/s, or ~10Gy/s, was followed by two daily sessions of 8-Gy BB, delivered at 100Gy/s. We then compared primary tumour growth, overall survival, skin toxicity, and the tumour immune response.

The long-term local tumour control, survival, and normal skin sparing were superior with MRT delivered at the UHDR of ~1000Gy/s. The increased skin sparing is consistent with FLASH effect literature for treatment delivery at UHDRs, however improved tumour control and survival is interestingly, unique to MRT delivered at UHDR. Analysis of the tumour immune response at 2 and 9 days post-last irradiation allowed identification of potential targets for adjuvant immunotherapy in this irradiation setting, such as macrophage infiltration and increase of PD1/PD-L1.

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Tuesday 28th

Abstract: 17

Ronan Smith

Visualising In-Vivo Magnet-Assisted Treatment Delivery within the Airway using Ultra-Fast Phase-Contrast and Dark-Field X-ray Imaging

Gene therapy has the potential to permanently treat genetic disorders such as cystic fibrosis by using viral gene vectors to insert DNA correction into cells. Delivering the viral vectors is challenging as they must be guided to the areas of the lung that require treatment and held in place to allow transduction. Binding viral vectors to magnetic nanoparticles allows them to be controlled using external magnetic fields, helping overcome delivery challenges.

High-resolution propagation-based phase-contrast x-ray imaging allows us to see inside the airways of a rat and capture high-speed videos showing how paramagnetic particles can be manipulated. Here, we present our latest results from an in-situ experiment at the BL20XU beamline of the SPring-8 synchrotron (Japan).

We designed custom imaging setups to explore how different motions and orientations of external magnetic fields can move, hold, and distribute nanoparticles within the trachea of live rats. We discuss the challenges of imaging materials inside live animals at a sub-micron resolution, and some of the innovative solutions we have developed. As well as using propagation-based phase-contrast, we also demonstrate that ultra-fast beam-tracking methods can provide additional dark-field information for in-vivo and in-situ experiments, allowing us to detect events which were otherwise invisible.

We acknowledge travel funding provided by the International Synchrotron Access Program (ISAP), managed by the Australian Synchrotron. Australian Synchrotron's MCT offers a spatial resolution comparable to BL20XU, and the innovative techniques we developed may be of interest to its users, as well as users of the animal imaging facilities of IMBL.

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Monday
27th

Abstract: 23

Anna Roujeinikova

Structure and function of the bacterial flagellar motor

The bacterial flagellar motor is a membrane-embedded rotary macromolecular machine that converts the electrochemical energy of the proton gradient into the mechanical energy of rotation. The knowledge about the bacterial motor is a source of inspiration for nanotechnology and one of the first steps towards making artificial motors on the same scale.

Recent breakthrough electron cryotomography studies have revealed proteinaceous periplasmic structures adjacent to the stator (the powerhouse) of polar flagellar motors, which are essential for the stator assembly and function. function. These structures are either disk-shaped, as is the case with Vibrio spp., or form a round cage, as is the case with Helicobacter pylori. It is now recognized that such additional periplasmic components are a common feature of polar flagellar motors, which sustain higher torque and greater swimming speeds compared to peritrichous bacteria such as Escherichia coli and Salmonella enterica.

The presentation at the meeting will showcase the cutting-edge research on the structure, composition, and function of the periplasmic scaffold in the polar bacterial flagellar motor of Helicobacter pylori. This microorganism displays high motility in the very viscous mucous layer of the stomach, which enables us to use H. pylori as a model system to study the polar motor specialised for locomotion in highly viscous fluids.

The presented work will illustrate the advantages of an interdisciplinary approach combining biology and physics. The presentation will conclude with the discussion of the new paradigm for how the previously unseen accessory components control the function of the flagellar motor.

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Monday
27th

Abstract: 43

Anton Le Brun

Structural Analysis of Antimicrobial Peptide Binding to Biomimetic Bacterial Membranes Using Neutron Reflectometry

Multi-drug resistant (MDR) bacteria, commonly known as 'super bugs', are an increasing global health threat as existing treatments against common infections become evermore difficult to treat. One area of exploration in new treatments to combat MDR bacteria is using short membrane-active peptides. Antimicrobial peptides (AMPs) show promise as typically the damage inflicted on the bacterial cell is permanent, making it improbable that resistance to the treatment can occur. However, there are several challenges in the use of AMPs as a therapeutic agent including delivery and specificity amongst others. To understand how AMPs interact with cell membranes structural information is required. One method is to use biomimetic membranes immobilised to surfaces in combination with neutron reflectometry, which can probe the structure of surfaces and interfaces down to the nanometre scale and is useful for the study of biomimetic membranes as it can provide information on the thickness and composition of the different layers within the membrane system [1]. We have used biomimetic membranes to determine the location and orientation of the AMP maculatin 1.1 from the skin secretions of an Australian frog bound within the membrane using neutron reflectometry [2,3]. More recently we have investigated the binding of the AMP caerin 1.1 to membranes [4]. Caerin 1.1 is the longest AMP from Australian frog skin secretions, and its membrane activity is found to be pH dependent.

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[4] M.-A. Sani et al. Biophys. J. 122: 1058 (2023)

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Monday
27th

Abstract: 144

Leonie van 't Hag

Fusion Peptide-modified Nanoparticles as Therapeutic Delivery Vehicles

Nanostructured lipid cubic phases can be used as drug delivery systems for therapeutic proteins and peptides. However, there is a lack of understanding regarding the influence of cubic phases on therapeutic peptide secondary structure, representative of its function, and encapsulation efficiency. This study investigated the effect of cholesterol level, phospholipid addition, and fusion peptide origin (COVID, HIV and Influenza), as well as lipid membrane curvature. The study highlighted the significance of the secondary structure of peptides in influencing lipid encapsulation. Peptides adopting α-helical configurations were found to have better interactions with lipid bilayers, leading to improved lipid encapsulation properties. On the other hand, peptides with β-sheet structures demonstrated different interactions and may have different effects on lipid organization and stability. The research shed light on the relevance of higher-order structures, such as protein domains or multimeric assemblies. Higher-order structures of peptides were observed to influence their binding affinity and selectivity to specific regions of the lipid bilayer. Understanding these structural characteristics is essential in designing peptides with enhanced specificity and efficacy for viral fusion inhibition.

The study also explored the role of cholesterol in peptide binding to lipid bilayers. Cholesterol, as a key component of the lipid raft domain, was found to modulate peptide-membrane interactions. Peptides displayed varying affinities to cholesterol-rich liquid-ordered phases, suggesting that the presence of cholesterol influences their binding preferences within the lipid bilayer. This highlights the importance of considering cholesterol content in lipid bilayers when designing therapeutic peptides targeting viral membrane fusion. Fusion peptides and their fusion capabilities present a potential avenue to improve cell membrane fusion of cubosomes for biomedical applications.

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Monday
27th

Abstract: 123

Stewart Walker

"Examine well, thy blood" - at the Australian Synchrotron

The IR and Far-IR beam-lines at the Australian Synchrotron have been used to investigate blood and breakdown products that give blood and bruises their particular colour. This research - research that matters - could lead to improved analysis and determination of concentration of carboxy-haemoglobin to determine pre-mortem vs post-mortem exposure to carbon monoxide in fires and to determining the relative ages of bruises to aid investigations of violent crimes. Haemoglobin, oxy-haemoglobin and carboxy-haemoglobin can be detected by placing a mobile UV-Vis integrating sphere above the blood on the ATR and the FAR-IR beam-line below to obtain the combined spectra. As Shakespeare wrote in Midsummer Night's Dream on 8th October 1600, "Examine well thy blood".
Despite there being very little difference in chemical structure the FAR-IR spectra of the breakdown products that give bruises their changing colours over time, biliverdin (green), which breaks down to, bilirubin (orange), are very different. FAR-IR spectra from the 2023/2 beam time have shown that there are characteristic peaks attributed to pure biliverdin-biliverdin interactions, pure bilirubin-bilirubin interactions and also peaks that can be attributed to each individual compound in dilute mixtures so without interactions. This leads to the potential for FAR-IR analysis to be used in cases where the spectra of different bruises needs to be assessed to determine the relative age of bruises in 1) the deceased or 2) if a child was in the custody of one parent/carer or the other at the time of the bruise or 3) to aid an elderly person – those who can't speak for themselves. As Shakespeare also said, "Thrice-blessèd they that master so their blood."

Primary author
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Tuesday 28th

Abstract: 121

Elette Engels

The DAAD Australia – Germany exchange grant tool: 5 years of bench-to-bedside support for microbeam radiotherapy (MRT)

Microbeam radiotherapy (MRT) has been shown to increase the therapeutic window in small animal models of cancer entities which are very difficult to treat with current clinically established treatment options. This has been shown in small animal models simulating human disease and in canine veterinary patients (dogs) with spontaneous malignant brain tumours. Since canines suffer from malignant tumours very similar in size, histology and course of the disease like human patients, the successful treatment of veterinary patients is a good indicator for a successful bench-to-bedside-translation, provided the required technical environment for clinical MRT trials can be created.

Historically, the development of MRT has been an international interdisciplinary project. Since 2019, researchers from the University of Wollongong and the Rostock University Medical Center have developed several 'international first' research projects supported by the German Academic Exchange Service (DAAD), allowing Australian researchers to travel to Germany for researchers for collaborative studies in return, with the aim to advance MRT towards veterinary and human clinical trials.

We report on the international first MRT studies from this collaborative effort, including explanted beating hearts, an in-vivo study of MRT in the spinal cord, and the development of anthropomorphic phantoms for studies conducted at the Australian Synchrotron, and the commissioning of the first synchrotron-based MRT research tool at the PETRA III synchrotron on the DESY campus in Hamburg, Germany.

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Tuesday 28th

Abstract: 118

Lucy Costello

How the IMBL is Helping us Zoom in on Lung Cancer

Lung cancer is one of Australia's leading killers. At present the diagnostic tool for lung cancer in Australia is a two-dimensional (2D) chest x-ray, with the possibility of a three-dimensional (3D) chest CT if further information is required. There are a couple of issues here, 1) a 2D image does not tell us enough information about a 3D object and 2) the lung tissue is so weakly attenuating that the resulting image from a conventional medical x-ray or CT can be of limited value in identifying abnormalities.

This research presents the preliminary findings of an investigation at the Australian Synchrotron's Imaging and Medical Beamline (IMBL) into the use of Phase Contrast Computed Tomography (PC-CT) to better visualise the lungs and characterise suspicious areas. So far, we have imaged human-sized whole lungs and have seen that propagation-based x-ray phase effects improve the visibility of lung features, even at the high x-ray energy and large pixel size required for such a large object. In addition, we have investigated ways to improve non-invasive characterisation of suspicious areas in the lung using region-of interest (ROI) imaging. This ROI approach zooms in to capture a high-resolution image of a small volume (< 1%), deep within the fully intact lungs, resolving blood vessels, small airways and soft tissue structures.

Our primary aim is to take low radInstruments & Techniquesion dose, high-resolution 3D images for clinical cancer diagnostics. With the use of the Australian Synchrotron, we aim to transform the diagnosis of lung cancer using novel x-ray imaging methods.

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Tuesday 28th

Abstract: 106

Michael Rice

A subset of Vδ1+ CD1d reactive γδ T cells recognise CD1d in an auto-reactive manner

T cells are categorised via the expression of their T cell receptor (TCR) into either αβ or γδ T cells. Whilst αβ T cell functions are comprehensively understood γδ T cells are ill-defined but are increasingly realised to be an important T cell subset that display potent anti -bacterial, -viral and -cancer effector functions. The breadth of antigens recognized by γδ T cells is slowly being elucidated and broadly defined as non-peptide ligands independent of the Major Histocompatibility Complex (MHC). However, how γδ T cells recognise antigens is unclear, seemingly utilising recognition mechanisms unheralded by αβ T cells. To resolve how γδ T cells recognise antigens and clarify their role more broadly we investigated γδ T cells reactive to CD1d, an MHC-1 like antigen presenting molecule that typically presents antigens to Natural Killer αβ T cells (NKT).

Biochemical analysis of 5 Vδ1+ TCRs revealed a dichotomy in recognition modes, being either lipid dependent or lipid independent. This is stark contrast to the prototypical NKT TCR that displays exquisite lipid specificity. We then determined via X-ray crystallography, the structure of a γδ TCR-CD1d complex where the Vδ1-TCR adopted an auto-reactive like recognition strategy, solely recognising the CD1d molecule. This is stark contrast to NKT-TCR that directly recognises the head-group of the presented lipid antigen, further demonstrating the antibody-like ligand recognition exhibited by γδ T cells. Complementary small angle X-ray scattering, suggests the γδ TCRs investigated here all adopt similar top-docking recognition modes. Our investigations demonstrate, to our knowledge, the first lipid independent γδ TCR-CD1d ligand structure.

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Monday 27th

Abstract: 20

Mia Brennan

Ionic Conductivity and Disorder in Sodium Perovskite Solid-State Electrolytes

The growing need for safe, reliable energy storage has brought solid electrolytes to the forefront of battery material research. One approach to achieve these goals is to use the highly versatile perovskite structure. This structure, with the general formula ABX3, allows for the inclusion of a wide range of dopants to tailor the ionic conductivities of resultant solid electrolytes [1]. However, an overall mechanism remains elusive.

Recently, ionic conductivity of the sodium-based perovskite Na1/2La1/2ZrO3 was improved via Sr2+ substitution onto the A site, reaching a maximum ionic conductivity in Na1/2-xLa1/2-xSr2xZrO3 at x = 1/6. Zhao et al. propose that this increase in ionic conductivity is due to the widening of sodium conduction pathways caused by the addition of larger Sr2+ [2]. Our experiments have shown that doping the A site with even larger Ba2+ cations further increases the ionic conductivity and sodium mobility, confirming the mechanism proposed by Zhao et al. However, unlike the Sr2+ series, we have found that the ionic conductivity of the Ba2+ series reaches a local maximum at x = 1/6 but has a global maximum at x = 7/32, coinciding with disorder in the long-range structure as evidenced by X-ray diffraction. A structural model of the perovskites' long-range average structure will be presented, alongside total scattering data obtained at the Institut Laue-Langevin (ILL), Grenoble, and extended X-ray absorption fine structure (EXAFS) data collected at the Australian Synchrotron. These data have allowed for a better understanding of the local structure and how it deviates from the average. The insights obtained will be used to showcase a better understanding of ionic conductivity in these highly versatile systems.

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Wed
29th

Abstract: 14

Haitao Yu

Inverse cubic and hexagonal mesophase evolution within ionizable lipid nanoparticles correlates with mRNA transfection in macrophages

mRNA lipid nanoparticle (LNP) technology presents enormous opportunities to prevent and treat various diseases. Here, we developed a novel series of LNPs containing ionizable amino-lipids showing a remarkable array of tunable and pH-sensitive lyotropic liquid crystalline mesophases including the inverse bicontinuous cubic and hexagonal phases characterized by high-throughput synchrotron radInstruments & Techniquesion X-ray scattering. Furthermore, with an interest to develop mRNA therapeutics for lung macrophage targeting, we discovered that there is a strong correlation between the mesophase transition of the LNPs during acidification and the macrophage assocInstruments & Techniquesion/ transfection efficiency of mRNAs. The slight molecular structural differences between the SM-102 and ALC-0315 ionizable lipids are linked to the LNP's ability to transform their internal structures from an amorphous state to the inverse micellar, hexagonal, and finally cubic structures during the endosomal maturation. SM-102 LNPs showed exceptionally improved transfection efficiency due to its ability to form the cubic structure at lower pH than the ALC-0315 analogues, which remained within the hexagonal structure, previously attributed to promote endosomal escape of the ionizable LNPs. Overall, the new knowledge draws our attention to the important role of mesophase transition in endosomal escape and the novel LNP libraries reported herein have broad prospects for advancing mRNA therapeutics.

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Monday 27th

Abstract: 18

Bryce Mullens

Seeing the Unseeable: Coupling Synchrotron X-Ray and Neutron Diffraction to Understand the Role of Vanadium

Vanadium is routinely used in a variety of functional metal oxide materials, such as BiVO4 photocatalysts for clean hydrogen gas generation, vanadium oxide-based redox flow batteries for energy storage, Bi4V2O11 as an oxygen ion conductor for solid oxide fuel cells, and Na0.33V2O5 superconductors for zero-loss power transmission. However, the exact chemistry of vanadium cations within these structures often remains elusive due to its weak X-ray scattering (Z = 23) in the presence of other metal cations, and it's almost-zero neutron scattering length (b = -0.38 fm).

Taking the well-known photocatalyst BiVO4 as our canvas, a combination of synchrotron X-ray and neutron powder diffraction has been used to devise a method to 'see' vanadium cations within these structures. BiVO4 undergoes a monoclinic-to-tetragonal phase transition at elevated temperatures associated with rotation of the VO4 tetrahedra. A variable temperature synchrotron X-ray diffraction experiment carried out on the Powder Diffraction beamline at the Australian Synchrotron was used to determine the atomic coordinates of V5+ with good precision and accuracy upon heating. This was then combined with variable temperature neutron powder diffraction data measured using the high intensity Wombat diffractometer at the Australian Centre for Neutron Scattering. Combining these datasets, a method was devised that finely balances the strongly scattering Bi3+ cations and the almost-zero scattering V5+ cations to determine information on the whole structure, as well as the anionic sublattice.

These results will be presented, along with a potential research direction for future studies containing vanadium cations and elucidating their role in potential energy materials.

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Monday 27th

Abstract: 129

Jennifer Stansby

The steam oxidation mechanism of U_2CrN_3/UN by in situ neutron diffraction

Uranium mononitride (UN) has been identified as a promising advanced nuclear fuel owing to its higher U density and thermal conductivity compared to standard fuel (UO_2). However, UN degrades upon exposure to steam, hindering its application in light water reactors i.e. 80% of the world's nuclear reactors. Incorporation of Cr is a widely used strategy to improve the corrosion resistance of materials, yet addition of Cr to UN yielding a U_2CrN_3/UN composite is reported to accelerate the oxidation process in steam.

Analysing when and how corrosion of composites occurs in realistic conditions is challenging because corrosion products may present temporarily. Moreover, conventional thermogravimetric analysis cannot be used to differentiate the crystallographic phases present, which might be reacting at different rates. Here, state-of-the-art in situ neutron diffraction data collection and analysis is used to monitor the real-time phase evolution of U_2CrN_3/UN in high temperature steam.

Previously, it was unclear why the steam oxidation progressed faster for the Cr-incorporated U_2CrN_3/UN fuel than for pure UN. Now, by observing the rates of mass loss from corrosion of the U_2CrN_3 and UN phases in U_2CrN_3/UN pellets, it is shown that the onset of corrosion in this duplex microstructure is led by the UN, which experiences enhanced corrosion rates in the presence of U_2CrN_3. A higher oxidation onset temperature of 430 °C is observed for the U_2CrN_3 phase, compared to 400 °C for UN. This quantitative and mechanistic understanding of steam oxidation from in situ neutron diffraction enables better defined operating regimes for next-generation reactors.

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Monday
27th

Abstract: 37

Callum Weir-Lavelle

Exploring Lithium-MedInstruments & Techniquesed Ammonia Electrosynthesis through In Situ Neutron Reflectometry

A major challenge preventing the uptake of renewables is their intermittent nature. Storing excess renewable energy as carbon-free fuels like hydrogen and ammonia offers a viable option to regulate the power supply. Ammonia is technologically simpler to liquify than hydrogen and has a well developed global transportation infrastructure. Current ammonia production relies on the centralised Haber-Bosch process, which is not feasible to use in the geographically isolated locations associated with renewable energy production. Hence, a sustainable alternative, like the electrochemical reduction of nitrogen gas, is required. Among these methods, the lithium-mediated nitrogen reduction reaction (Li-NRR) stands out for its viability.[1]

Monash University has made significant strides in the Li-NRR, achieving nearly 100% faradaic (current-to-ammonia) efficiency and practical rates.[2,3] The focus now shifts to enhancing energy efficiency and sustainability in the Li-NRR process. This necessitates designing electrodes and electrolytes, requiring a deep understanding of the solid electrolyte interphase (SEI) formed on the reactive lithium layer and its role in enhancing selectivity and curbing undesired reactions.

Our ongoing work employs *in situ* neutron reflectometry to unravel the Li-NRR mechanism by characterising the solid electrolyte interphase and determining its impact on the performance. For the first time, we were able to reveal dynamic changes in the surface's scattering length density profile during ammonia production. This approach aims to unravel the intricate processes occurring at the electrode surface facilitating the design of alternative pathways for efficient and sustainable ammonia production through lithium-mediated electrochemical nitrogen reduction.

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Monday
27th

Abstract: 34

Richard Mole

Crystal field splitting, magnetoelastic coupling and quantum tunneling: Inelastic Neutron Scattering as a tool in molecular magnetism

Single molecule and single ion magnets are molecules that display a magnetic bistability. Varying the structure and coordination environment of the magnetic ions in these materials using synthetic chemistry can tune the ground state and allow both the energy barrier for reorientation to be changed, and quantum tunneling through the barrier to be introduced. As such these molecules have been touted as potential candidates for molecular scale data storage, qubits and as components in spintronic applications. Inelastic neutron scattering is one of the most accurate techniques for studying these molecules, as it allows individual transitions between states to be measured rather than a thermal average of all states. Historically this has made it the most precise way to determine the crystal field splitting in the absence of an applied magnetic field.

Recently we have also demonstrated that magnetoelastic coupling is also encoded into the INS data. This has allowed us to explore vibrational relaxation mechanisms in candidate single ion magnets. However, there are multiple different relaxation mechanisms, in this contribution I will demonstrate, through recent results, that we can not only determine the magnitude of the crystal field splitting, but also that INS is also sensitive to the lifetime of quantum tunnelling and demonstrate that unique information can be extracted in this way.

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Wed
29th

Abstract: 4

Daniel Eriksson

MX3: A new macromolecular crystallography beamline at the Australian Synchrotron

The High-Performance Macromolecular Crystallography beamline (MX3) will be capable of providing high-flux, microfocus X-rays for small and weakly diffracting protein crystals. MX3 will provide three modes of data collection: goniometer (standard pin-mounted experiments), serial crystallography (fixed target and injector), and in-tray collection. The optical design allows users to rapidly change beam size by a combination of a secondary source aperture and compound refractive lenses.

A high degree of automation will support unattended data collection of entire projects. Given a set of expected outcomes, all samples attached to an experiment can go through screening, data collection and merging without user interaction. Results are entered in a database for easy comparisons across multiple experiments. In-tray screening and in-tray data collection are related but separate. In-tray screening will be achieved through a program aimed at synchrotron users and non-users alike. “Tray Tuesdays” will set aside beamtime for automated screening and evaluation of plate wells. The ScreenShot user interface developed in-house will serve as a portal for sending trays and evaluating the results.

Early X-ray diffraction screening of crystalline material can direct researchers’ efforts towards the most promising conditions, guiding optimisation and minimising wasted synchrotron time. In-tray data collection in contrast, aims to collect entire datasets without harvesting of crystals. This will be performed at room temperature and will merge data from multiple crystals to form a complete dataset. While screening can be done with most standard tray types, collecting full datasets requires special low-background trays that are commercially available.

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Wed
29th

Abstract: 135

Catriona Thomson

A supramolecular investigation of selenadiazole functionalized porphyrin nanotubes

Porphyrin and its derivatives are of growing continued interest owing to their π -conjugated electronic systems which can be exploited in a vast array of fields from light-harvesting to catalysis. Unfortunately, many porphyrin systems assemble in fibers, sheets and/or nanoparticles and thus cannot be explored crystallographically. This work will outline a novel crystalline porphyrin nanotube (PNT) which self-assembles under solvothermal conditions. These crystals incorporate tetrapyridyl-porphyrin, selenadiazole moieties, and Cd(II) metal centers as discrete, hexagonal nanotubes. Revealed by Single Crystal X-Ray Diffraction (SCXRD) data from MX1, each PNT comprises a large channel running through the c-axis, with a pore diameter greater than 10 Å, a void volume greater than 35 % of the unit cell and key selenadiazole functionality lining the voids. We have demonstrated the propensity of PNTs to uptake guest molecules which interact with key chalcogen bonding moieties within the pores of the nanotubes through non-covalent interactions. This has been demonstrated via SCXRD experiments and gas-sorbance measurements, proving PNT is capable of capturing DMSO, CS2, CBr4, Collidine, CO2 and Xe. These experiments are justified by solid-state NMR studies and illustrate PNT's potential for chemical sensing and storage for medical and environmental remedInstruments & Techniquesion purposes.

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Wed
29th

Abstract: 97

Hayden Robertson

Polymer brushes through the eyes of a Platypus and a Spatz

Stimulus-responsive polymers can alter their conformation as a function of external factors.[1] One such polymer is the thermoresponsive poly(*N*-isopropylacrylamide) (PNIPAM), which, when end-tethered to a substrate forms a brush that undergoes a phase transition from well- to poorly-solvated over a broad temperature range. The phase transition temperature of polymer brushes can be moderated by altering the properties of the solvent, such as the inclusion of ions. These resultant phenomena are known as specific ion effects (SIE), whereby the observed effect is dependent on ion identity rather than just concentration or valency.[2] To date, no all-inclusive theory regarding SIE exists. However, as natural environments are composed of complex mixtures of aqueous and non-aqueous electrolytes, understanding the interplay of ion and solvent identity is imperative for real-world technologies.

To probe the role of the solvent in SIE, we investigate changes in the behaviour of a PNIPAM brush in electrolytes composed various non-aqueous/aqueous solvent mixtures: dimethyl sulfoxide (DMSO)/water and methanol/water. Surface characterisation techniques such as spectroscopic ellipsometry (SE) and neutron reflectometry (NR: PLATYPUS; SPATZ) were employed to monitor changes in brush thickness and conformation, respectively, as a function of solvent and electrolyte composition.[3],[4] Interestingly in water-rich electrolytes (e.g., 10 mol% methanol), NR revealed polymer brush structures analogous to pure water. However, in water-limited electrolytes (e.g., 70 mol% DMSO), significantly modulated brush conformations revealed a Hofmeister series reversal; behaviour opposite to that observed in electrolytes of pure water. Here NR is aiding the deconvolution of the myriad interactions between the solvent, solute and substrate to elucidate the dominate drivers behind ion specificity.

1. 10.1039/D2PY01487D
2. 10.1039/D2CP00847E
3. 10.1016/j.softx.2022.101225
4. 10.1107/s160057672100251x

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Tuesday
28th

Abstract: 15

Jiali (Maggie) Zhai

Harnessing the Power of Synchrotron SAXS for Lipid Nanoparticle Design and Structure-Function Correlation

Ionisable amino-lipid is a key component in lipid nanoparticles (LNPs), which plays a crucial role in the encapsulation of RNA molecules, allowing efficient cellular uptake and then releasing RNA from acidic endosomes. Herein, we present direct evidence for the remarkable structural transitions, with decreasing membrane curvature, including from inverse micellar, to inverse hexagonal, to two distinct inverse bicontinuous cubic, and finally to a lamellar phase for the two mainstream COVID-19 vaccine ionisable ALC-0315 and SM-102 lipids, occurring upon gradual acidification as encountered in endosomes. The millisecond kinetic growth of the inverse cubic and hexagonal structures and the evolution of the ordered structure formation upon ionisable-lipid-RNA/DNA complexation are
quantitatively revealed by in-situ synchrotron radiation time-resolved small angle X-ray scattering coupled with rapid flow mixing. We found that the final self-assembled structural identity, and the formation kinetics, were controlled by the ionisable lipid molecular structure, acidic bulk environment, lipid compositions, and nucleic acid molecular structure/size. The implicated link between the inverse membrane curvature of LNP and LNP endosomal escape helps future optimisation of
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Tuesday 28th

Abstract: 128

Joseph Bevitt

A revolution in palaeontology with neutron and synchrotron X-ray imaging at ANSTO

Fossils of dinosaurs and other extinct organisms yield insights into ancient biology and behaviour. They provide detailed information on contemporary environmental conditions, fossilisation and evolutionary processes. X-ray computed tomography (XCT) is a critical tool for the digital excavation of delicate fossils to determine these evolutionary relationships and other details.

Using the intense beam of X-rays at the Australian Synchrotron's Imaging and Medical Beamline, we have uncovered extraordinary new Australian dinosaur species, brought to light soft-tissue remains of 100 million-year old organisms trapped in amber, and corrected major inaccuracies in the fossil record.

The applicability of XCT to solving some queries in the fossil record has been hampered by the inability of X-rays to penetrate through large, and dense samples, and poor contrast between many fossils and matrix. When X-rays fail, neutrons provide an opportunity for improved penetration and contrast. Concerns for the potential to radioactivate specimens inhibited museums from exploring the use of neutron tomography (NCT) in palaeontology.

Since first demonstrating the non-destructive application of neutron imaging to fossils at ANSTO using the DINGO, we have actively led a global revolution in palaeontology.

This talk will illustrate how NCT has revealed the stomach content of dinosaurs, seed dispersal mechanisms in polar Cretaceous conifers, proved that crocodiles ate dinosaurs [1], and unveiling unpreceded soft-tissue remains including the world's oldest fossil heart [2]. Further, by a unique one-stop-shop approach, we are combining the benefits of both neutron and synchrotron X-ray tomography to guide the physical excavation of nationally significant fossils, rejuvenate palaeontology in Australia and attract projects from around the world.

[1] Gondwana Res 106, 281-302 (2022)
[2] Science 377(6612) 1311-1314 (2022)

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Tuesday 28th

Abstract: 142

Ivan Herrera Benzaquen

Adelaide ATOM Trap Trace Analysis; A new facility for Groundwater dating

Water is an increasingly precious natural resource, and there is a growing need to provide a better understanding of environmental systems, such as the hydrology of groundwater aquifers. Groundwater access and management is a major and growing issue in Australia. A complete understanding of our groundwater resources is neccessary.

One powerful tool available to address these challenges, and for developing more sophisticated resource and impact assessment models, is the dating of environmental systems using natural and anthropogenic radionuclides. Geoscientists and hydrogeologists use these radionuclides as tracers for understanding mixing and transport processes in hydrological systems. The longlived RNGs, ^{85}Kr, ^{81}Kr, and ^{49}Ar, are among the most powerful tracers available, with each isotope covering a distinct age range around its respective half-life, ^{85}Kr=10.739±0.014 years, ^{81}Kr =229.000±11.000 years, and ^{39}Ar=269±3 years. These noble gas tracers have geophysical and geochemical properties that simplify data interpretation; they have uniform or very well-known distributions in the atmosphere, and relatively simple transport processes underground.

Atom Trap Trace Analysis (ATTA) takes advantage of one of the techniques used in quantum technologies, laser cooling, to cool down, trap, and count the trace isotopes. With ATTA we are able to measure trace concentrations of RNG isotopes with a reduction in the required sample volumes and processing times by multiple orders of magnitude.

We report here on the progress towards an Australian ATTA facility, one of only four such facilities worldwide. The first measurements by an ATTA facility in the Southern Hemisphere of ^{85}Kr and ^{81}Kr in an atmospheric air sample will be presented, along with progress toward the measurement and dating of groundwater samples taken from the Eromanga Basin in Australia.

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Tuesday 28th

Abstract: 114

Sherryn MacLeod

3D Isotopic Reconstruction in Bulk Samples Using Post-Neutron-Tomography SPECT

TThe non-destructive assessment of interior elemental composition and spatial distribution in bulk samples (greater than a few hundred μm) is essential across various domains such as archaeometry, palaeontology and cultural heritage. Traditional neutron activation analysis (NAA) techniques offer elemental identification but lack the 3D spatial context. Similarly, advanced imaging techniques like X-ray and neutron tomography provide 3D structural information but often fall short in extrapolating internal elemental distributions.

To address this issue, we propose a novel method: post-neutron-tomography SPECT, that combines neutron scattering and molecular imaging. Using ANSTO's thermal neutron imaging beamline (DINGO), samples are irradiated, resulting in temporary activation through neutron capture. Like NAA, the characteristic gamma lines from these decaying radionuclides can be used to identify the created isotopes. By performing single-photon emission computed tomography (SPECT) of the neutron-irradiated samples over an extended period, the spatial distribution of elements, determined by their radioisotopes, can reconstructed. Energy and time-windowing techniques allow for quantification and discrimination of radio-isotope with overlapping half-lives and gamma lines. Successful 3D reconstructions of copper (Cu-64) and gold (Au-198) samples demonstrate the method's potential in rendering 3D isotopic views within bulk objects. Combined with structural imaging modalities and simulation modelling, this approach enhances our capacity to estimate elemental distributions in bulk samples of unknown compositions.

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Tuesday 28th

Abstract: 57

Jiani Sheng

Synchrotron MCT illuminates uniquely preserved 445 Ma bituminous radiolarian fossils from the Wufeng Formation, China

Novel taphonomy begets new imaging technology. Ghost radiolarians preserved as hollow molds infilled by bitumen and dolomite in uppermost Ordovician marine shales record a unique taphonomic history. First observed in thin sections, bituminous casts of radiolarian skeletal tests preserved in Wufeng Formation oil shales from the Sichuan Basin, China proved inextricable from their host strata. X-ray micro-computed tomography using the new BRIGHT beamline at the ANSTO Australian Synchrotron facilitates non-destructive, high-resolution *in-petro* imaging of lagerstätten quality radiolarian assemblage within minicore 'biscuits'. Employing a spatial resolution of 1.3 µm and unparalleled phase contrast achieved via synchrotron, we unveiled >20 radiolarians representing seven species within a single slice of minicore smaller than a rice grain. Despite the minute sample size, this assemblage considerably enriches knowledge of uppermost Katian radiolarian biodiversity in China. The unveiling of this mode of preservation in radiolarians and the powerful visualisation capacity of synchrotron MCT, opens new avenues for pioneering paleontological studies on this critical plankton group. Moreover, with heightening climate concerns, black shales assocInstruments & Techniquesed with Oceanic Anoxic Events, which are frequently correlated with episodes of climate change are of increasing interest. The fossil records within these rock formations provide crucial insights into ecosystem responses including mass extinctions to past extreme conditions, as well as giving insights how they influence the global climate regulatory systems, such as the carbon and silica cycles. The complex nature of the taphonomy and the remarkable fossils it yields continue to surprise and provide renewed insights for a deeper understanding of Earth's systems.

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Monday
27th

Abstract: 180

Jamie Schulz

Facility Update: Australian Centre for Neutron Scattering (ACNS)

The Australian Centre for Neutron Scattering (ACNS) utilises neutrons from Australia's multi-purpose research reactor, OPAL, to solve complex research and industrial problems for Australian and international users via merit-based access and user-pays programs. The neutron beam facilities of OPAL consist of neutron beam tubes that penetrate the reflector vessel, a cold neutron source, beam shutters and neutron guides. A suite of 15 neutron beams instruments utilise both the thermal and cold neutron beams for both atomic and molecular structure determination and dynamics measurements, residual stress measurement and neutron imaging. An update will be given on the OPAL reactor and its neutron beam facilities, recent upgrades, user program, and future plans.

Monday
27th

Abstract: 181

Danielle Martin

Facility Update: Australian Synchrotron (AS)

The Australia Synchrotron achieved first light in August 2006, and since then has operated 10 individual beamlines as part of Australia's largest standalone scientific research facility. In a typical year, ANSTO Australia Synchrotron conducts up to 1000 individual experiment and hosts more than 5500 User visits. Although one of the smaller 3rd generation facilities, operating at 3 GeV and 200 mA, the Australian Synchrotron's research community is prolific: generating 591 peer-reviewed journal articles in 2022 alone. In 2018, the facility embarked on an ambitious program to build 8 new beamlines. As part of project BRIGHT, 33 funding organisations from across Australia and New Zealand have contributed $102M, to deliver new capability and add to our suite of beamlines. With at least 3 of these beamlines now in operations, this presentation will provide an overview of major activities across our beamlines and an update on the remaining BRIGHT beamlines still under construction.

Monday
27th

Abstract: 182

Tamim Darwish

Facility Update: National Deuteration Facility (NDF)

The National Deuteration Facility at ANSTO provides deuterium and other stable isotope labelling through both biological and chemical techniques for a diversity of molecules and applications. The molecular deuteration and labelling of molecules is an essential prerequisite in many spectroscopic and neutron scattering studies, including NMR and IR spectroscopic methods. The use of deuterated molecules in neutron scattering experiments for investigating the relationship between molecular structure and function expands the range and complexity of science that can be conducted at reactor and spallation-source neutron facilities. This presentation will detail the recent advancements occurring at the NDF, and the impact of the bespoke deuterated and labelled compounds produced by the facility. Key developments and investigations will be discussed that reveal the exciting and diverse research opportunities which are now available at the NDF.

Monday
27th

Abstract: 183

David Child

Facility Update: Centre for Accelerator Science (CAS)

The Centre for Accelerator Science (CAS) at ANSTO's Lucas Heights campus operates four tandem accelerators, ANTARES, STAR, Vega and Sirius, delivering ion beams for a wide range of research and applications. CAS capabilities include accelerator mass spectrometry, ion beam analysis and ion beam irradiations. Our science themes are: exploring the past, understanding the present, design for the future.

The range of applications that CAS covers is extremely wide, including these examples: nuclear astrophysics (the first detection on Earth of material from recent r-process nucleosynthesis), cultural heritage (dating some of the world's oldest rock art), electronics development (testing radiation hardness of electronics for satellites), water resources research (dating and tracing groundwaters in Australia), pollution monitoring (tracing the sources of airborne dust), food safety (PFAS screening of food packaging), and many more.

CAS receives support from the Commonwealth government's National Collaborative Research Infrastructure Strategy (NCRIS) to ensure that CAS capabilities are made accessible to researchers on the basis of scientific merit. Many of our capabilities currently operate at maximum capacity. CAS has received a boost this year with additional funding through the 2023 NCRIS funding round. This will enable CAS to expand capacity and deliver faster results across all our major capabilities.

Monday 27th

Abstract: 75

Jitendra Mata

Charged colloidal particles interaction in the microgravity environment of space: A USANS and SANS study

We conducted an experiment involving the aggregation of colloidal particles with both positive and negative charges in an aqueous solution. This experiment took place within a microgravity environment at the International Space Station. To facilitate this process, a specialised setup was employed to blend the colloid particles under conditions of microgravity. Subsequently, these arrangements were solidified within a gel matrix using ultraviolet (UV) light exposure. Upon their return to Earth, the samples were subjected to analysis using optical microscopy and small and ultra-small angle neutron scattering along with their controlled ground samples.

The experimental results revealed intriguing insights*. For instance, the space-based samples composed of polystyrene particles, which possessed a specific gravity (ρ) almost identical to that of the surrounding medium (ρ= 1.05), displayed an average association number approximately 50% greater than the control samples from the ground. Moreover, the structural symmetry of these space samples was notably enhanced. This suggests that the formation of colloidal structures can be notably affected by even slight factors such as gravitational settling and ground-based convection. The impact of electrostatic interactions on clustering behaviour was also demonstrated through the example of titania particles (ρ ~ 3), which typically experience sedimentation-related challenges when studied on Earth due to their relatively high density. However, within the microgravity environment of the space station, these particles formed association structures without encountering the sedimentation issues prevalent on the ground.

These findings carry implications beyond the confines of the experiment. The knowledge acquired from this study could prove instrumental in the development of a model that aids in the design of advanced photonic materials as well as improved pharmaceuticals.

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Wed
29th

Abstract: 21

Christine Browne

Controlling the liquid crystal formation of cellulose nanocrystals with electrolyte

Cellulose is the most abundant naturally occurring polymer on Earth and has garnered much interest in creating products which are biodegradable, environmentally friendly and recyclable. Cellulose nanocrystals (CNC) are liberated from these materials through an acid hydrolysis process and typically are 100-500 nm long and have diameters of 3-5 nm. This renders the surface with a negative charge and makes them highly stable in aqueous suspensions. Due to these properties CNCs form chiral nematic liquid structures with can be exploited in applications such as sensors, optical devices and as viscosity modifiers.

The effect of electrolyte addition on the chiral nematic structures was investigated by varying the atomic size, valency and concentration. The bulk suspension properties were investigated using rheology, polarised optical photography and microscopy. While the further detailed investigation of the chiral nematic and subsequent tactoid formation upon the addition of electrolyte was quantified using SAXS completed at the Australian Synchrotron and USANS/SANS at ACNS. The addition of electrolyte to a CNC suspension containing chiral nematic structures increases the nematic pitch indicating the suspension has a weaker structure. Further increases in electrolyte causes the aggregation and complete breakdown of the chiral nematic structures. The univalent species have a greater effect on the chiral nematic structures with the onset and magnitude of structure breakdown occurring at a lower ionic strength compared with the divalent species. Cation type and size also influences the effect of the chiral nematic structure.

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Monday 27th

Abstract: 76

Paul Michalski

Application of Neutron Spectroscopy and Imaging to Reveal Drying Behaviour and Preservation of Australian Native Fruits

Food production is being challenged by population growth and increased drought. One way to manage these challenges is with Australian native food crops, which have unique sensory and nutritional properties, while being inherently well-adapted to Australian climate and in which there is emerging a local industry and global interest [1, 2]. A barrier to the industry's growth, however, is understanding how to maximise the retention of quality attributes over the course of preservative processes. This is particularly true for those processes which manipulate food moisture, prompting the need to also understand the behaviour of water in these fruits as they are processed. Measuring the drying kinetics and water sorption isotherms and how these change with processing and temperature has revealed bound water physics in these fruits different to what has been observed for commonly known foods. The extent to which hydrogen (and thus water) scatters neutrons makes them ideal to study moisture in food. By subjecting Australian native fruits, processed in different ways, to neutron backscattering spectroscopy by using Emu in ANSTO, the dynamics of bound water in these unique foods has been characterised. The use of neutron tomography with Dingo in ANSTO has also revealed the local moisture transport and structural changes in these fruits as they are processed under different conditions. The combination of these techniques has given more rigorous insight into the water transport mechanisms in Australian native fruits and allowed for improved understanding of how their preservation can be optimised for longer shelf-life and nutritional/quality retention.

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Monday
27th

Abstract: 26

Grant Webber

Combining neutron reflection and computations to unravel the behaviour of (multi-)responsive polymer brushes in electrolyte solution

Responsive polymer brushes provide a robust platform to study the manifestation of specific ion effects due to the ability to collect data in conditions where the polymer is notionally in a poor solvent environment. Specific ion effects are phenomena where observed behaviour is influenced by ion identity, not merely valency and concentration. We have shown specific ion effects on the temperature range over which brushes of poly(N-isopropylacrylamide) (PNIPAM) [1] and poly(oligoethylene glycol methacrylate) (POEGMA) [2] transition from swollen to collapsed, where anions can either increase or decrease transition temperature.

Here we examine the effect of three potassium salts from across the Hofmeister series on the thermoresponsive behaviour of a multi-responsive poly((2-2(-methoxyethoxy)ethyl methacrylate)-stat-(2-(diethylamino)ethyl methacrylate)) (P(MEO_2MA-*stat*-DEA)) 90:10 mol% copolymer brush at pH 4 and 9. The structure of the P(MEO2MA-*stat*-DEA) is influenced by temperature (*via* MEO_2MA), solution pH (*via* DEA) and electrolyte (both). Rigorous analysis of neutron reflection data (PLATYPUS, SPATZ) using the refnx package reveals non-monotonic polymer volume fraction profiles are the predominant fit to the reflectivity curves. This surprising outcome is supported by numerical self-consistent field (nSCF) theory calculations. It was found that whether an anion salted-in or salted-out the brush (increase or decrease transition temperature, respectively) can be switched by changing the pH. This is attributed to a change in the strength of interactions between the ions and each monomer upon discharging/charging of the DEA tertiary amine groups [3,4].

1. B. A. Humphreys, et al., doi:10.1039/c5cp07468a.
2. T. J. Murdoch, et al., doi:10.1016/j.polymer.2018.01.053.
3. E. C. Johnson, et al., doi:10.1016/j.polymer.2020.123287.
4. E. C. Johnson, et al., doi:10.1021/acs.langmuir.0c01502.

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Monday
27th

Abstract: 145

Livia Salvati Manni

SAS to elucidate the phase behaviour of phospholipids in protic ionic liquids

Protic ionic liquids (ILs) are liquid salts with a melting point below 100 °C, they can form a 3-D hydrogen-bond network, they can self-assemble in nanostructures and support amphiphilic self-assembly. For this reason, they have been identified as a possible alternative solvent to host life. In this work we investigated the effect of protic ionic liquids on phospholipids self-assembly. Phospholipids are among the main building blocks of life, and they can self-assemble in a variety of geometries. We characterized and compared the structure and stability of self-assembled phases formed by four phospholipids with identical phosphocholine head groups and different alkyl tails, DSPC, POPC, DSPC and DPPC in protic ILs with different amphiphilicity: ethylammonium nitrate (EAN), Propylammonium nitrate (PAN) and Ethanolammonium nitrate (EtAN).

Employing a combination of small- and wide-angle x-ray scattering and small-angle neutron scattering we discovered complex and unexpected phase behaviours with transitions that have never been observed in water. We can rationalise such behaviours with the amphiphilic nature of the solvents and the chain melting temperature of the lipids. These results provide new insight for the design of lipid based nanostructured materials in ionic liquids.

Monday 27th

Abstract: 48

SENLIN GU

Enhancing Nanofiltration Performance through Aligned Hexagonal Lyotropic Liquid Crystal

Overcoming the permeance-selectivity trade-off in membrane fabrication is a long-standing challenge. Hexagonal lyotropic liquid crystal (HLLC) emerges as a transformative candidate, offering a solution. The key lies in precisely preserving and orienting the HLLC structure on substrates. By harnessing the influence of the HLLC precursor mesophase, a breakthrough method utilizing cold-pressing was introduced to coat the HLLC template onto an ultrafiltration substrate. Intriguingly, the integration of a hydrophilic crosslinker ensures impeccable structure retention and alignment, forming hexagonal cylinders perfectly aligned on the substrate surface, as revealed by cutting-edge SAXS techniques. This strategic approach, empowered by the interaction between hydrophilic crosslinkers and cylinders characterized by 13C solid NMR, not only enhances hexagonal structure preservation but also optimizes system processibility by reducing the clearing point. As a result, an impressive leap in nanofiltration and mechanical performance is realized, showcasing a remarkable 30 L/m2*h*bar thickness normalized permeance alongside a remarkable 90% sodium ion rejection rate. This achievement significantly surpasses the capabilities of existing commercial nanofiltration membranes, opening new horizons for fabricating advanced nanofiltration lyotropic liquid crystal membrane with the assistance of SAXS and solid NMR techniques.

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Wed
29th

Abstract: 86

Alice Tiong

Pulse protein gels: understanding the role of soluble proteins and protein particles in the gelation mechanisms through SANS/USANS

Protein demand has been increasing the past few decades, and this has led to the growth of the plant-based protein market as more sustainable protein sources. Plant proteins have ~4 times lower water use and ~6 times lower land use in comparison to animal-based proteins [1, 2]. Plant proteins can form texturized products, by going through gelation, which is most commonly induced with heating and cooling of the proteins. Pulse proteins have been proposed to be great candidates to produce meat analogues, however, the gelation mechanism that can exist between different plant sources is not understood.

In this project, plant protein isolates that were extracted using different methods were used to understand how the extraction methods and salt content can affect protein solubility and protein composition, which in turn affects the gelation behavior. With techniques such as dynamic light scattering and circular dichroism, it was found that extraction method heavily influences average protein particle size and protein structure where more intensive procedures led to larger particle sizes and higher amounts of unstructured proteins. In combination with scattering techniques, it was seen that the gelation mechanism depends on both the soluble protein and protein aggregates. Despite exhibiting different gelation pathways, the gelation strength for the plant proteins were similar to each other, demonstrating the potential of different gelation pathways.

1. Reijnders, L. and S. Soret, Quantification of the environmental impact of different dietary protein choices. The American journal of clinical nutrition, 2003. 78(3): p. 664S-668S.
2. Xu, X., et al., Global greenhouse gas emissions from animal-based foods are twice those of plant-based foods. Nature Food, 2021. 2(9): p. 724-732.

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Wed
29th

Abstract: 138

Woojeong Kim

Surface composition of β-carotene microcapsules comprising pea/whey protein complexes by synchrotron-FTIR microspectroscopy

Plant/dairy protein blends show sufficient potential as novel ingredients suitable for food application with improved functionality. This study aims to elucidate the stability of spray dried β-carotene microcapsules by identifying the surface composition using synchrotron-Fourier transform infrared (FTIR) microspectroscopy. To investigate the impact of enzymatic cross-linking and polysaccharide addition on heteroprotein, three wall materials were prepared: pea/whey protein blends (Con), cross-linked pea/whey protein blends (TG), and cross-linked pea/whey protein blends-maltodextrin complex (TG-MD). Uniform β-carotene microcapsules were prepared using mono-disperse spray dryer. Feed emulsion properties, encapsulation efficiency for 8-week storage, morphology, and synchrotron FTIR spectroscopy were measured to establish a relationship between the surface composition and the chemical stability of β-carotene microcapsules. Both enzymatic cross-linking and polysaccharide addition improved the stability of β-carotene microcapsules. The TG-MD exhibited the highest encapsulation efficiency (> 90%) after 8 weeks of storage followed by TG and Con. Chemical images obtained using synchrotron-FTIR microspectroscopy confirmed that the TG-MD displayed the least amount of surface oil, followed by TG and Con, due to increasing amphiphilic β-sheet structure of the proteins led by cross-linking and maltodextrin addition. The synchrotron-FTIR results revealed distribution of the protein and lipid on the surface of the microcapsules, proving that enzymatic cross-linking between heteroproteins with the addition of a small amount of maltodextrin (0.5%) led to a substantial reduction of the surface oil. This result provided insights into designing wall materials in transition from major dairy proteins to plant proteins for encapsulating and protecting oil-based bioactive compounds.

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Wed
29th

Abstract: 51

Vikram Singh Raghuwanshi

Characterisation of poly(N-isopropylacrylamide) (PNIPAM)-grafted nanocellulose hydrogels

Poly(N-isopropylacrylamide)-grafted cellulose nanofibers (PNIPAM-g-CNFs) are novel thermo-responsive polymer hybrids with unique properties. PNIPAM-g-CNFs exhibits a lower critical solution temperature (LCST) at 35 oC in water. The themo-responsive property depends on the conformation of PNIPAM on the CNF during temperature variation. Below and above the LCST, the conformation of PNIPAM on the CNF surface changes due to its temperature dependent hydrophobic and hydrophilic switching properties.

The nano to microscale structural changes, optical and rheological properties with temperature of PNIPAM-g-CNF suspensions are compared with pure PNIPAM and PNIPAM blended CNF (PNIPAM-b-CNF). Small angle neutron scattering (SANS) combined with Ultra-SANS (USANS) reveal the nano to microscale conformation changes of these polymer hybrids as a function of temperature. Below LCST the PNIPAM-g-CNF exhibit water like behavior due to the PNIPAM chains sustain open conformation and poor interaction with CNF. Above LCST, the PNIPAM chains change their conformation to entangle and aggregate nearby CNFs and formed large CNF voids. Grafted PNIPAM chains inhibits the free movement of CNF which increases the strength of the gel as confirmed by rheology.

In comparison, PNIPAM-b-CNF sustains similar water like behaviour below LCST. Above LCST, the blended PNIPAM chains phase separated from the CNF to form large aggregates of micrometre size. The fundamental understanding of temperature-dependent conformation of PNIPAM-CNFs enables engineering of thermo-responsive hydrogels for biomedical applications.

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Tuesday 28th

Abstract: 94

Stefania Peracchi

From Space to Medical Research: Australia's unique ion microbeam capabilities to investigate radInstruments & Techniquesion effects with micro-precision.

The Centre for Accelerator Science (CAS) provides a sovereign ANSTO capability of customized precision irradiation with focused ion microbeam in vacuum for applications to advanced materials, devices and technologies and interdisciplinary science.

Cosmic radiation can impact space technology, leading to events like Single Event Upsets (SEUs) that can temporarily or permanently disrupt essential instrumentation crucial for mission success, testing, or regular service operation. Understanding the causes and frequencies of such events is vital to mitigating component failure risks and optimizing electronics performance. The structural components of spacecraft and power systems, including photovoltaic technologies, stand susceptible to space radiation, which has demonstrated its propensity to worsen properties and performances. Furthermore, prolonged human exposure to the severe space radiation environment poses health hazards. It is evident that ground-based tests are essential to foster a safer and further exploration, mitigating the risk of failure and the investment loss.

Two ANSTO Heavy Ion Microprobes on the 10MV ANTARES and 6 MV SIRIUS accelerators provide to Australian users, from both academia and industry, unique capabilities to investigate the radiation effects on electronics, shielding materials, and power technologies. The ion microbeams precision irradiation in both vacuum and air conditions, allow the irradiation of living biological samples, expanding the horizon in medical research areas such as fundamental radiobiology, particle therapy, drugs development and many more.

The presentation will show the recent development of expanding our irradiation capability in both vacuum and in enclosed ambient on the ANTARES Heavy Ion Microprobe system targeting users interested in space and radiobiology research.

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Tuesday 28th

Abstract: 101

Annaleise Klein

Advancements at the Australian Synchrotron Infrared Micro= spectroscopy (IRM) beamline: a new field of research, a cross-beamline sample holder, and (potentially) going sub-micron

The Infrared Microspectroscopy (IRM) beamline at the Australian Synchrotron is primarily used for mapping chemical functional groups in 2D space at the resolution of a few micron in a non-destructive manner. A diverse range of samples can be analysed, including biological, biomedical, materials, food science, cultural heritage, and geology. Here, we showcase our latest research into a new area of study for the beamline: electrochemistry and catalysis. Also, the results of a cross-beamline collaboration with the X-ray Fluorescence Microscopy (XFM) team to develop a compatible sample holder for measurements at both beamlines. We present a major upgrade the IRM beamline team is looking towards - the potential purchase of a nano-IR instrument, with the goal of coupling synchrotron radiation with the instrument. Finally, we discuss the potential benefits and new areas of research the recent advancements at the IRM beamline and the nano-IR instrument may open up for the scientific community.

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Tuesday 28th

Abstract: 139

Peter Kappen

A 4th Generation Synchrotron for Australasia

The Australian Synchrotron has been going strong since it opened its doors in 2007, and we expect the facility to keep delivering benefit well into the late 2030s. By that time, science drivers will demand more than the current facility can technologically deliver. Essentially, synchrotron science and technology will have moved on significantly, and several 4th generation synchrotrons will have materialised around the world. It is thus time to think about how we could move from third to fourth generation synchrotron science in Australia and the Region.

In this contribution we will discuss science and technology parameters for a new synchrotron lightsource. As next generation synchrotrons deliver significantly smaller emittance and thus higher brightness and better photon beam coherence than our current facility, they open the door to tackling science problems in a better or smarter way. This will be driven by boosting the current methods we have, as well as going far beyond. A future synchrotron will give us access to time-resolved measurements at the millisecond scale, microscopy at low- or sub-nm resolution, streamlined in-operando measurements in seconds, rapid diffraction off weakly diffracting micro-crystals, and more.

This presentation seeks to drive a dialogue with the broader community and solicit input into plans and proposals for a 4th generation synchrotron for Australasia.

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Wed
29th

Abstract: 154

Karyn Wilde

Isotopic labelling strategies of the National Deuteration Facility enabling biomolecular investigations using NMR spectroscopy.

Molecular deuteration of organic compounds and biomolecules is an essential prerequisite in many NMR, infrared, mass spectroscopy, and neutron scattering studies. To reduce spectral complexity and signal linewidths in both solution and solid-state NMR spectra, the application of various stable isotope labelling schemes for proteins has been well established within the biomolecular NMR community. The National Deuteration Facility (NDF) at ANSTO is the only facility of its kind in the Southern Hemisphere, with the specialised expertise and infrastructure to produce a broad range of deuterated molecules through both biological and chemical techniques that may otherwise not be available commercially. The NDF enables biomolecular investigations using NMR through the operation of a proposal-based user program (offering different modes of access) for provision of bespoke deuterated and multiple-isotope labelled molecules to researchers and industry.

The NDF utilises their reliable and robust methods for the deuteration of a broad range of proteins by high-cell density, high-yield recombinant expression in Escherichia coli BL21 using a simple defined method [1]. These methods have been adapted to produce uniformly double (13C/15N, 2H/15N) and triple labelled (2H/13C/15N) proteins, as well as selective amino-acid labelling, for the support of structural and functional investigations. Molecules produced through chemical deuteration and used in neutron studies such as ionic liquids, unsaturated lipids, uncommon surfactants, sugars, and heterocyclic and aromatic compounds can also be applied to NMR studies, enabling different and complementary experimental approaches for your research. The deuteration of novel molecules by the NDF with NMR applications will be described, with selected examples of protein labelling and their application highlighted.

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Wed
29th

Abstract: 16

Anita D'Angelo

New gas system and mass spectrometer for the Powder Diffraction beamline at the Australian Synchrotron

The Powder Diffraction (PD) beamline at the Australian Synchrotron is located on a bending magnet and is optimised for in-situ, in-operando and time resolved structural studies of materials. Experiments that mimic how the material functions under 'real world' conditions can be carried out to address scientific challenges in energy, medical and mineral fields using a variety of beamline sample environments. This includes battery tester, heating or cooling stages, and cells to enable gases to be passed over the material to observe phase transitions while diffraction data is collected.

The Powder Diffraction beamline is continually looking to expand the capabilities offered to the user community. This work details the commissioning of a new Hiden XCS gas system that will allow gases to flow over a sample and to make gas mixtures, as well as a Hiden QGA mass spectrometer to identify the gases generated from reactions. The development of an improved flow through cell design will be discussed. The gas system is primarily used for catalysis and gas absorption experiments and replaces the existing manifold used at the beamline. Positive impacts on user science include (1) increased efficiency through minimising the experiment setup time, (2) increased accuracy in experiments as it will allow users to obtain precise mixtures of gases, and ability to set accurate flow rates, (3) increased safety through equipment standardisation and (4) addition of a new capability through the acquisition of a mass spectrometer. Examples of the equipment's use will also be presented. This information can be used as a guide for researchers considering in-situ and in-operando experiments at the Powder Diffraction beamline.

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Monday
27th

Abstract: 111

Ulf Garbe

10 years of open shutter at DINGO at OPAL

The neutron radiography / tomography / imaging instrument DINGO is operational since October 2014 to support research at ANSTO. DINGO provides a useful tool to give a different insight into objects because of different contrast compared to X-rays and high sensitivity to light elements. Since starting hot commissioning with first friendly users the research community is constantly growing with a strong boost from the World Conference for Neutron Radiogrpahy (WCNR-11) in 2018. A major part of applications from both sides of the community, research and industrial user, was demanding the high-resolution setup and fast scans on DINGO. In the original design DINGO could provide a minimum pixel size of 27 µm with 2k x 2k pixel. Upgrades of the past ten years involved a neutron microscope setting to achieve 1.7 µm pixel size. In addition, we upgraded to new cameras moving from CCD to scientific CMOS and finally using astronomy CMOS cameras with 26 or 60 mega pixel chips. A new graphical user interface was developed for these astronomy cameras. These new cameras are demanding on computing and data storage as well. We developed a custom-made CT reconstruction package to streamline the data reduction process and offer a variety of rendering software like VGStudio, AVIZO and Dragonfly. Next to all technical upgrades, we like to present a collection of scientific and commercial high lights over the last ten years. These highlights cover a large variety of scientific field like materials science, engineering science, palaeontology, cultural heritage and many more.

Finally I give an outlook on further planned upgrades to keep DINGO competitive for another ten years of great science.

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Monday 27th

Abstract: 130

Jaydeep Patel

Implementation of machine vision based automatic feedback control and analysis of Liquid sample delivery at European XFEL.

One of the most significant factors in a successful serial crystallography experiment is the sample delivery system. There are two main types of sample delivery systems, fixed and moving targets. However, for Megahertz crystallography a moving target system is required as the sample delivery rate needs to match the pulse rate. Thus, a liquid sample jet which is a moving target is used. A stable liquid jet is required for high-speed crystallography. As there are several jetting characteristics, like sample size or flow rate and gas pressure, etc, are required to be set optimally for achieving a stable jet at higher speeds. A liquid jet can be unstable because of a change in any one of these jetting characteristics during the experiment.

The aim of this project is to develop a pipeline supporting an automated feedback loop for liquid-jet sample delivery via real-time analysis of optical microscopy images which are typically collected during serial crystallography data collection. The goal is to enable unsupervised correction of the jet position and motor parameters to maintain the alignment between the liquid sample stream and the x-ray beam. The implementation of this system will maximize the use of the available beam time at the European XFEL whilst keeping sample consumption to a minimum. As a precursor to achieving these aims, we have first developed a method for automatically extracting key parameters related to the jet behaviour using optical microscopy images collected at the beamline and tried to correlate this information to the jetting characteristics. This tool provides seamless control of the nozzle position-controlling motors, ensuring maintained interaction region overlap during experimental data collection.

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Monday
27th

Abstract: 52

Jannis Ahlers

Zero-optics dark-field imaging with multi-energy X-rays

Diffusive dark-field X-ray imaging is a burgeoning modality which enables full-field quantification of sub-resolution scattering in the sample. This has a variety of promising applications, including in the diagnosis of lung disease; the many small air-sacs in the lung strongly scatter X-rays, and when these break down the dark-field signal is reduced. State-of-the-art diffusive dark-field imaging techniques rely on the use of optics, for example by introducing grid or random speckle masks into the beam, and measuring the loss of visibility of this pattern. Propagation-based imaging is an experimental configuration that does not include any optics, instead using downstream self-interference of a scattered coherent wavefield to convert in-sample phase-shifts into detectable intensity fringes. It has recently been shown that diffusive dark-field effects can be present in propagation-based images, and can be well-described using the X-ray Fokker–Planck equation [1]. Previous work used two images taken at different distances to solve the inverse problem of propagation-based diffusion retrieval [2]. In this work we consider the related problem of dual-energy retrieval, relying on the strong spectral dependence of scattering. We show that diffusive dark-field varies significantly at clinical energies. An algorithm for dual-energy diffusive dark-field retrieval for single-material samples, based on the Fokker–Planck equation, is developed under assumptions of slowly-varying dark-field and a-priori spectral dependence. We compare the advantages and disadvantages of different methods of reconstructing the dark-field signal using our method. Dual-energy diffusion retrieval opens the door to single-exposure and time-resolved propagation-based diffusive dark-field imaging using energy-resolving detectors.

[1] Paganin, D. M., & Morgan, K. S. (2019).
[2] Leatham, T. A., Paganin, D. M., & Morgan, K. S. (2023).

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Monday 27th

Abstract: 102

Josie Auckett

High-energy X-ray diffraction is coming soon to the Australian Synchrotron

We are excited to introduce the new high-energy Advanced Diffraction and Scattering (ADS) beamlines, which are the first beamlines at the Australian Synchrotron to offer very hard X-rays (45–150 keV; □ = 0.08–0.27 Å) for diffraction experiments. ADS-1 and ADS-2 are projected to join the Synchrotron user program in late 2024.

High-energy X-ray diffraction is particularly suited to strongly-absorbing samples or sample environments, or where access to high momentum transfer (large Q/short d-spacings) is desirable. Pair distribution function (PDF) analysis to study local structure will be a standard offering on ADS-2. The ADS beamlines will also cater to complex in situ experimental setups, with space provided in the endstations for user-supplied equipment in addition to standard non-ambient sample environments. Single-crystal diffraction experiments will be accommodated using a two-axis sample goniometer capable of supporting payloads up to ~2 kg. ADS-1 will offer both mono-chromatic and polychromatic beam modes for advanced material characterisations, including depth-resolved energy-dispersive diffraction, poly-grain texture and strain studies in bulk metals, and X-ray imaging of diffraction samples.

This presentation gives an overview of the planned capabilities and timeline for delivery of the ADS beamlines.

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Tuesday 28th

Abstract: 107

Robert du Toit

Validation of the Unified Tomographic Reconstruction (UTR) algorithm for Propagation-Based X-ray Phase-Contrast Breast Imaging

Early detection of breast cancer is key for improving health outcomes for patients. When detected during screening, 10-year survival rates increase from 85% to 95% compared to when symptoms present. Mammography, used in screening, delivers a relatively high dose to healthy tissue to create adequate absorption-based contrast between soft tissues. Phase-contrast imaging utilises absorption and phase change of X-ray waves as they traverse through the sample to improve image quality. We evaluate the quality of reconstruction for a new phase-contrast computed tomography (PCT) algorithm, Unified Tomographic Reconstruction (UTR), by comparing it to conventional Filtered Back Projection (FBP) for a set of mastectomy samples.

Nine samples were imaged in a complete, intact, unfixed state at the Imaging and Medical Beamline (IMBL) at the Australian Synchrotron using propagation-based PCT. Thick (3 mm) and thin (100 um) slices were analysed with Signal-to-Noise ratio divided by resolution (SNR/res) and Contrast-to-Noise ratio divided by resolution (CNR/res) as metrics for objective image quality. SNR/res was measured in adipose tissue, and CNR/res was measured across a glandular-adipose boundary, in three thick slices and 90 thin slices per sample.

UTR reconstructions produced an average SNR/res improvement of 39% for thick and 10% for thin slices as well as an average CNR/res improvement of 18% and 4%, respectively, compared to FBP.

The continued work in developing an improved reconstruction algorithm for phase-contrast breast imaging supports the development of a medical X-ray imaging facility at the Australian Synchrotron. Improvements in image quality will give improved diagnostic results for cancer patients.

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Tuesday 28th

Abstract: 77

Klaudiusz Jakubowski

Advancements in Creating a Digital Twin: Modeling and Analysis of the Dingo Thermal Neutron Imaging Beamline

The Australian Centre for Neutron Scattering's (ACNS) Dingo beamline is the sole high-flux thermal neutron source in Australasia. Currently its primary application is neutron imaging. Previous spectroscopic measurements revealed a broad spectrum of epithermal and fast neutrons and gamma background, which have not been directly characterised due to the high neutron flux. This introduces significant uncertainties into the quantitative interpretation of radiobiological experiments conducted on the beamline.

We have developed a Monte Carlo simulation model of the Dingo beamline, incorporating CAD drawings of the entire beam transport system and shielding structures. This model aims to accurately predict neutron and gamma spectra at the sample stage for all beam configurations. The model achieves very good agreement with experimental planar thermal neutron distribution measurements performed in-beam with gold foils and B4C-coated microdosimeters (within 8.1% and 2.1%, respectively), and out-of-beam spectra obtained via Bonner sphere spectroscopy (mean logarithmic neutron fluence ratios in thermal, epithermal and fast neutron regions within 0.1, 0.2 and 0.4). Our model estimates that the neutron spectrum at the sample stage consists of approximately 18% thermal, 64% epithermal and 18% fast neutrons. Additionally, the model provides an estimate of the gamma spectrum present at the sample stage.

Once fully validated, the Dingo digital twin will be a key enabler for future radio-biological research and detector advancement by providing accurate dosimetric and spectroscopic data across various positions in the beam, as well as predicting radiation damage and activation of samples irradiated at Dingo.

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Tuesday 28th

Abstract: 27

Andrew Nelson

Freeform modelling of Reflectometry data with Maximum Entropy

Modelling of neutron reflectometry data typically approximates an interface using a series of slabs (layers) of uniform scattering length density (SLD). Whilst this works well for simple systems it breaks down for complex structures, particularly when the structure is continuously varying or diffuse. One example is modelling extended polymer brushes, whose concentration gradually decays as a function of distance from a surface. Various approaches have been used to model such systems.

Analytical profiles can be used when apporprInstruments & Techniquese, but sometimes a freeform model is required – one that obeys no preconceived idea of what the structure should be. Various freeform techniques have been employed in the past, mainly via summed basis functions, such as Chebyshev/cubic B splines and Fourier series. Typically, these approaches can produce rapidly varying SLD profiles, so some method of stabilisation is required to make the profiles smooth. Recently we have had great success using PCHIP interpolating splines to describe the structure of polymer brushes, but these also have modelling artefacts. Here we revisit the maximum entropy approach, that approximates structures via a series of pixels. These pixels are smoothed via an entropic probability term, which is easily included in Bayesian modelling engines. This approach isn't new, but hasn't been widely used due to the absence of available tools, and computational requirements. We demonstrate that MaxEnt reproduces profiles determined in earlier brush work, and show how MaxEnt can be leveraged by the wider reflectometry community.

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Tuesday 28th

Abstract: 126

James Vohradsky

Investigation of the SOI microdosimeter for high LET ion measurements

In this work, a 3D silicon-on-insulator (SOI) microdosimeter was investigated during high LET ion irradiation using a 24 MeV carbon ion microbeam and a 500 MeV/u argon ion therapeutic beam.

The charge collection properties of the Mushroom microdosimeter with 24 MeV 12C ions was investigated using the ion beam-induced charge collection (IBIC) technique at the 6-MV accelerator SIRIUS, ANSTO. The microdosimeter was connected to a CSA and shaping amplifier with two different gains, covering two dynamic ranges of energies. A microbeam of 24 MeV 12C ions were raster scanned over the microdosimeter (spot size ⊠1.2 µm), with x-y charge collection median energy maps produced. The irradiated sensitive volume regions of the microdosimeter demonstrated full yield and well-defined charge collection efficiency (CCE), with observed radiation hardness. To reduce the 12C ion energy (and increase LET), 30 µm of polyethylene was placed in front of the microdosimeter.

Similar LET of ions were studied in additional experiments performed using 500 MeV/u 40Ar ions at HIMAC, Japan. In this experiment, the response of the SOI micro dosimeter to Ar ions was investigated when the microdosimeter was placed behind different thicknesses of PMMA layers.

The results demonstrate the performance of the SOI microdosimeter when measuring high LET particles, with some attributing low energy events observed in the extremely low energy region. However, it did not affect substantially to the micro dosimetric spectra nor the yD value. This demonstrates that the SOI microdosimeter is suitable for high LET ion QA applications.

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Tuesday 28th

Abstract: 146

Simon James

The BRIGHT future of X-ray Spectroscopy at the Australian Synchrotron

The Australian Synchrotron initially had only one high-flux beamline dedicated to X-ray absorption spectroscopy (XAS). However, the BRIGHT upgrade project has led to the creation of eight new beamlines at the facility. Among these, two are specifically designed for medium energy X-ray absorption spectroscopy (MEX). These new MEX beamlines, named MEX1 (covering energy range 3.3 - 13.6 keV) and MEX2 (covering energy range 1.7 - 3.3 keV), share a common bend magnet source.

As MEX1 and MEX2 transition from the commissioning and testing into being operational for Users, the number of available X-ray spectroscopy endstations will triple, significantly expanding the Australian Synchrotron's capabilities.

The introduction of the MEX beamlines addresses a gap in the existing beamline setup and offers distinct advantages for X-ray absorption spectroscopy across various scientific fields. Researchers in biology, material chemistry, geology, and environmental science can benefit from the ability to investigate the local structure, speciation, and chemistry of a wide range of compounds, spanning elements from silicon to uranium.

In the near future, additional features like high-energy resolution fluorescence detection (HERFD) and a medium-energy scanning microprobe will become accessible to Users.

These enhancements greatly enhance the facility's offerings and provide a valuable new resource for the user community. Through practical examples and a focus on relevant techniques, the presentation will introduce MEX beamlines, outlining their capabilities, current status, and planned development.

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Tuesday
28th

Abstract: 89

Anton Stampfl

Determining the neutron scattering function, using a semiempirical Hartree-Fock electronic structure calculation

The scattering function, S(Q,w), representing the interaction between the incident neutron and the pseudopotential representing an ensemble of atoms may be determined in a variety of ways: Via classical force-field approaches, through electronic structure calculations, through analytical approaches and through a combination of one or both of the first two approaches and applying molecular dynamics to study systems under non-equilibrium conditions. Electronic structure calculations quickly become computationally intensive once more than several hundred atoms are involved in a cluster or unit cell that represents the system under investigation.
In the case of neutron spectroscopy many systems investigated are dominated by hydrogen vibrations as the total scattering coefficient is approximately an order of magnitude larger than most total scattering coefficients from other elements. Scatter from hydrogen is mainly incoherent and therefore may be considered localised allowing potentially simple molecular models to be employed in the study of hydrogenous materials. Here a well known Hartree-Fock semiemperical calculation scheme is presented that is lightning fast for small molecules and adequate for large molecules, clusters, and dynamical studies.

Force constants are obtained by diagonalisation of the mass-weighted Hessian matrix to obtain the vibrational frequency for each mode assuming that each atomic-pair vibrates in a simple-harmonic fashion. The scattering function, S(Q,w), is then calculated firstly assuming a one-atom oscillator and then secondly more thoroughly for each atom-pair vibration within the molecule/cluster. A number of benchmark molecules are reported on. Interestingly these rapid calculations give a very good estimation of the scattering function that can be used for initial peak identification and further analysis of the detailed electronic and vibrational structure.

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Tuesday 28th

Abstract: 84

Jeremy Stockdill

Microstructure decomposition using propagation-based dark-field x-ray imaging

X-ray imaging plays an important role in diagnosing clinical pathologies, as absorption-based x-ray imaging is commonly used to produce images of bones, contrasted against the surrounding, weakly attenuating soft tissue. In a dark-field image, small-angle x-ray scattering can distinguish structures smaller than a detector can resolve (Paganin and Morgan, 2019; Pavlov et al, 2020). In the context of clinical x-ray imaging, these effects can be used to distinguish pathological phenomena such as emphysema of the lungs and cancerous tumour growth (Kitchen et al, 2020). Using images of two samples with differing microscopic structure (microspheres of different diameter), acquired using propagation-based x-ray phase-contrast imaging at the SPring-8 synchrotron in Japan, our research has focused on validating the mathematical model under which this modality of x-ray imaging is based. An algorithm developed by our research team has allowed for the extraction of scattering and refraction information from the microscopic structures within scattering samples using the Fokker-Planck equation (Paganin and Morgan, 2019). We have been able to characterise materials based on the strength of their scattering signatures from image reconstruction. Experimental values for this scattering strength have been reconstructed at the same order of magnitude as the theoretical values. As this reconstruction is dependent on the microscopic structures within a sample, we can use it to distinguish between two distinct scattering objects, such as a lung tumour from the surrounding healthy tissue. We hope this research can evolve to clinical application and provide a reliable tool for doctors to diagnose life-threatening medical conditions.

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Tuesday 28th

Abstract: 30

David Paterson

Turbo charging the X-ray fluorescence microscopy beamline at the Australian Synchrotron

The X-ray fluorescence microscopy beamline (XFM) at the Australian Synchrotron saw first light in 2008 and has been serving a diverse user research community since. The beamline was delivered with a unique horizontal-bounce double crystal monochromator (DCM) at the heart of its design. Several major upgrades to the X-ray fluorescence detection schemes, scanning microprobe architecture have been made. Most improvements focused on maximizing X-ray fluorescence detection efficiency alongside a hyper-efficient motion-controlled raster scan. Recently, ptychography has been added to the suite of imaging modes available, providing complementary nanoscale morphological context to fluorescence data. The photon delivery optics have remained unchanged, and we increasingly find that experiments are flux and/or coherent flux limited. Consequently, we have formed a strategic plan to enable science in the upper energy range of the beamline, i.e., 20–30 keV where the in-vacuum undulator source flux output declines. Target science includes the investigation of cadmium in agriculture and human health, e.g., in cereal grains, and silver in material science improving detection limits by accessing the K line emissions of these heavy metals.

We describe our funded upgrade plan to “turbo charge” the beamline by incorporating a horizontal-bounce double multilayer monochromator (DMM), increasing flux delivered to the endstation across the 4 to 30 keV energy range of the beamline. The original beamline design foresaw this upgrade, allowing space in the first optics enclosure for a DMM. Installation scheduled for early 2023. The expected flux gains will be presented along with design constraint to ensure the same horizontal offset as the DCM allowing quick efficient changeover between narrow (DCM) and broadband (DMM) monochromation.

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Tuesday 28th

Abstract: 38

James Cayley

MOS*kin* dosimetry in a synchrotron FLASH radInstruments & Techniquesion environment using very high energy electrons at PEER

Delivering radiation with treatment dose-rates above 40 Gy/s (FLASH) has been shown to spare healthy tissue while providing an equal or greater dose to the tumour. The MOS*kin* detector, designed at the Centre for Medical Radiation Physics at University of Wollongong is used in conventional radiotherapy and considered dose-rate independent over a limited range. We show that dose-rate independence also exists when exposed to an ultra-high dose-rate, very high energy electron beam at PEER.

The Australian Synchrotron uses a LINAC to inject 100 MeV electrons, capable of delivering pulses with expected dose-rates of 10^7 Gy/s. An array of five detectors was designed placed in the beam, with a scintillating screen positioned behind the array and imaged with a camera, to collect spatial data and relative beam intensity between pulses. 13 beam currents were used to deliver single 300 pC pulses from 20 to 400 ns in length.

An average response for the MOS*kin* detectors was calculated for each beam current. Dose-rates for each pulse were estimated using a standard MOS*kin* calibration factor and range from approximately 7×10^5–2.5×10^7 Gy/s. A steep drop off in response was observed at beam currents below 2 mA. Beam profiles were created using the camera data, with a Moffat distribution fitted to determine relative intensity between pulses at the detector's estimated location. The distribution was sampled at the estimated location of detectors and normalised to one, which enabled plotting against normalised MOS*kin* data to evaluate detector response against the charge delivered.

The MOS*kin* response is shown to be consistent with the scintillating screen, confirming the MOS*kin* exhibits dose-rate independence.

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Wed
29th

Abstract: 149

Matthew Large

Hydrogenated amorphous silicon dosimeters built on flexible kapton substrates for Microbeam RadInstruments & Techniquesion Therapy

Hydrogenated amorphous silicon (a-Si:H) is a novel candidate for high-flux x-ray dosimetry. The amorphous nature results in an improved radInstruments & Techniquesion hardness over traditional materials such as crystalline silicon. The synthesis of a-Si:H via Plasma Enhanced Chemical Vapour Deposition allows for a-Si:H to be deposited over large areas and directly onto a variety of substrates, including flexible materials such as polyimide (Kapton). Previous works from the authors have demonstrated the successful use of a-Si:H dosimeters in kV and MV fields for radiotherapy, as well as for dosimetry for Microbeam RadInstruments & Techniquesion Therapy (MRT) at the Australian Synchrotron's Imaging and Medical Beamline (IMBL). In this work, a series of flexible a-Si:H planar p-i-n diodes fabricated directly on Kapton substrates are characterized for dosimetry of Microbeam RadInstruments & Techniquesion Therapy (MRT) modalities. The fabrication of these detectors on Kapton substrates with thin metallic and diode layers results in fully flexible, radInstruments & Techniquesion-hard dosimeters. Detectors were characterized at IMBL for both broad-beam and microbeam dosimetry. For percentage depth dose (PDD) in broad beam, results show less than ±5 % varInstruments & Techniquesion from the reference PTW microDiamond dosimeter for 3T wiggler field and beam filtrations Mo-Mo through to Al-Cu. In MRT modality, detectors are operated in edge-on orientation to utilise the 2.5 µm active layer to reconstruct the microbeam profiles with extreme accuracy. Improved packaging and design of the detectors have resulted in accurate measurements of the Peak-to-Valley Dose Ratio (PVDR) of the MRT field. Complete results will be presented at the 2023 ANSTO User Meeting.

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Wed
29th

Abstract: 61

Michelle Croughan

Development and application of time-resolved directional dark-field retrieval at IMBL and MCT.

The ability to observe small structures is often limited by the spatial resolution of the imaging system. However, unresolved structures can scatter the x-ray beam creating a dark-field signal. Measuring dark-field provides sub-pixel information with less radiation dose than would typically be required to directly resolve those features, and typically with less time and equipment. Additionally, aligned elongated micro-structures in a sample will create a dark-field signal that is stronger perpendicular to the orientation of the structures than in the parallel direction. This is known as the directional dark field, and provides information about the orientation of micro structures.

Several techniques have recently emerged for the extraction of the directional dark field. We focus on the single-grid technique, extending it to quantitatively retrieve the directional dark field. Single-grid x-ray imaging is an x-ray phase contrast technique where the x-ray illumination is patterned using a grid and local changes to that pattern are measured when a sample is introduced. The dark-field scattering of the x-ray beam manifests itself as a localised smoothing of the grid pattern. By creating analytical models, we developed an algorithm that can extract dark-field parameters such as the dominant scattering direction, and the semi-major and -minor scattering angles. Importantly, as single-grid imaging only requires one sample exposure, this approach allows for low-dose and fast dynamic imaging. We show that this method is effective even in the presence of high image noise and demonstrate a number of applications with biological samples, such as the airway cilia, teeth and bones.

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Wed
29th

Abstract: 85

Nicolas de Souza

Emu neutron backscattering spectrometer: capabilities and applications

The Australian Centre for Neutron Scattering operates the Emu backscattering spectrometer at OPAL since 2016. Emu enables measurements at correlation times from tens of ps to a few ns.
Emu is set up with Si(111) analyzers in nearperfect backscattering on the primary and secondary neutron flight paths, delivering 1μeV FWHM energy-transfer resolution, and with a Doppler drive offsetting the incident energy by up to ±31μeV [1]. It is well-suited for quasielastic neutron scattering and low-lying excitation spectroscopy, with good sensitivity to hydrogenous species. In favorable cases, sensitivity to weaker scattering elements such as e.g. D, Na, O, ... is achieved [2,3]. The most-requested sample environment is a 1.5...750K cryofurnace in optional combination with other sample conditioning schemes such as gas delivery, pressure, light irradiation, electrical field, ...
Applications to various areas will be presented to highlight the versatility of the spectrometer. At present studies addressed solid-state dynamic disorder to liquid-state dynamics [2-7], including a variety of soft-matter and composite phases from the polymer and bio- sciences, from the fundamental to the applied domains. While Emu data are typically combined with data from other (neutron) techniques, soft-matter studies account for the bulk of experiments to date.

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Wed
29th

Abstract: 80

Melody Ranger

The development of in situ nuclear fuel studies on Wombat diffractometer

Licensing new fuel demands new approaches to test nuclear reactor fuel in realistic conditions. Our work has put nuclear fuel in a neutron beam to perform in-situ corrosion experiments in the Wombat diffractometer. This new capability underpins nuclear fuel studies involving the exposure of fuel pellets in steam to understand the corrosion mechanisms in nuclear accident conditions. Neutrons provide superior penetration depth, hence bulk, engineering-relevant characterisation, and are sensitive to light elements such as H and N in the presence of heavy U – particularly useful for the study of advanced fuels such as U_3Si_2 and UN. Representative data of both surface oxidation and the pellet interior provide industry-relevant conclusions for whole fuel pellets. 0.7 atomic % U-235 will fission in the thermal neutron beam, and calculations are presented to show how (a) criticality is not possible, (b) fission product concentration is below limits for safe handling and storage, and (c) dose rates can be managed, whilst (d) powder and fission product containment is effective. With our set-up, in-situ data enabled real time tracking of fuel corrosion, showing evolution of phase fraction and lattice parameters as the reaction progressed. We demonstrated hydriding behaviour in U_3Si_2 in steam, followed by its decomposition into UO_2 and U_3Si_5, and detailed analysis of steam oxidation for UN. Further plans include adding an in-situ mass spectrometer to analyse off gases, but already, our new approach described here is showing new ways to approach screening, licensing, safety assessment, and development pathways for new nuclear fuels.

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Wed
29th

Abstract: 119

Jay Archer

A Two-Dimensional Characterisation of Low Gain Avalanche Diodes for Low-LET Microdosimetry

A low gain avalanche diode (LGAD) achieves intrinsic gain and is thus of interest for low linear energy transfer (LET) microdosimetry. A novel LGAD device with two geometric configurations was characterised using an ion microprobe with protons energies of 1, 1.8, 3 and 8 MeV as well as carbon ions with an energy of 2 MeV/u using the SIRIUS accelerator at the Australian Nuclear Science and Technology Organisation (ANSTO). A two-dimensional assessment of charge collection in the device showed distinct regions in the detector with gain and without gain. The gain of the device was characterised for all ion configurations and at different reverse bias'. The gain did not monotonically increase with larger reverse bias' and was also observed to reduce with lower proton energies and carbon ions. This is due to an increase of the induced charge density in the device for higher LET ions resulting in charges being screened from the strong localised electric field in the gain layer. Thus, due to the non-linear behaviour of these devices with the deposited energy, a thorough investigation is required for the assessment of these devices for microdosimetry in proton therapy, heavy ion therapy and space radiation.

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Wed
29th

Abstract: 8

Samantha Alloo

Using sandpaper to capture multi-dimensional X-ray dark-field images

Sandpaper can double as a highly-sensitive optical element in the technique of speckle-based X-ray imaging. Random intensity modulations imposed by sandpaper act as X-ray wavefront markers which can be traced to recover sample information [1, 2]. The technique captures a reference-speckle wavefield and looks how propagation of the X-ray wavefield through a sample alters that pattern. Speckle alterations are characterised by attenuation, speckle shifts, and blurring, which align with X-ray transmission, phase-shift, and dark-field signals, respectively. Dark-field is particularly useful as the contrast is generated by small-angle X-ray scattering, hence the images reveal information about structures beneath the spatial resolution. We have developed theoretical methods, experimental procedures, and software implementations of an approach named “Multimodal Intrinsic Speckle-Tracking (MIST)” [3]. The appeal of our approach is that it makes the already experimentally simple speckle-imaging approach relatively low-dose (in comparison to alternative speckle-tracking algorithms) and computationally rapid (as signal extraction is performed on the whole-image). Pavlov et al. [4] derived a 2D anisotropic MIST approach that retrieves local orientations of unresolved sample microstructure. Our current objective is to develop a multi-dimensional speckle-imaging approach that reconstructs local microstructure correlation ellipsoids for each sample voxel – so-called X-ray dark-field tensor tomography. We recently performed preliminary experiments at the Australian Synchrotron’s Micro-CT beamline. Here, we describe our experimental protocols and present in-progress results from this beamtime where we imaged resin-encased carbon fibres.

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Wed
29th

Abstract: 151

Kathleen Wood

Quokka, the Monochromatic Small Angle Neutron Scattering instrument at ANSTO: Planned Upgrades & Scientific Highlights

Quokka is a 40 m pinhole Small Angle Neutron Scattering instrument, operating with a neutron velocity selector, an adjustable collimation system providing source-sample distances of up to 20 m and a high-count rate 1 m2 detector, capable of measuring neutrons over a flight path up to 20 m. Quokka routinely operates with focusing lens optics, capable of measuring down to a minimum Q value of 6 x 10-4 Å-1. The instrument is also equipped with incident beam polarisation and analysis capability and features a unique detector capable of countrates in excess of 5 MHz.

Quokka is designed as a general-purpose SANS instrument, with a large sample area, capable of accommodating a variety of sample environments, suitable for in-situ studies in both hard and soft matter. Grazing incidence geometry is also available through a project funded by the Taiwanese National Synchrotron Radiation Research Center.

We present current planned upgrades, including replacement of our guide system, along with a selection of recent research highlights.

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Tuesday 28th

Abstract: 42

Gail Iles

Effectiveness of an electromagnetic Space RadInstruments & Techniquesion Shield upon impact by high-energy protons and ions

The RMIT Space Physics Research Group is researching radiation shielding for space-craft and habitats for the crewed Artemis missions to the Moon. The 1U payload, “RADICALS” (Radiation Deflector of Ionising Charges using a Lorentz Shield) consists of an electromagnetic shield and an instrument suite of sensors. Bench testing and thermal modelling of the shield have been conducted in house and the instrument suite comprised of magnetometers, Geiger counters and a GPS receiver is fully operational. The payload will be launched by the Swedish Space Corporation in 2024 on a Sub-Orbital Express sounding rocket to test the effectiveness of the shield at 250 km altitude above the Earth’s surface, close to the magnetic pole in the Northern hemisphere.

The ANTARES heavy ion irradiation beamline at the ANSTO Centre for Accelerator Science (CAS) has been used to irradiate the RADICALS device as a pre-spaceflight qualification. High-precision, high-energy proton and carbon microbeams with different energies were directed towards the electromagnetic shield inside the RADICALS payload. When the magnetic shield was powered on, the charged particl es with differing beam energies were deflected successfully. Geiger counters mounted behind the shield registered a change in overall counts when the shield was OFF compared to ON. In parallel, magnetic models of the shield and radiation particle transport simulations have been generated which correlate well with the experimental data. The high-quality data obtained at ANSTO also helped to identify areas for improvement to the payload which will be implemented before the rocket flight into space.

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Tuesday 28th

Abstract: 35

Dongdong Qu

In-situ synchrotron X-ray diffraction analysis on the phase stability of dross particles in hot-dip Zn-55wt%Al-1.6wt%Si galvanizing bath

Low-carbon steel sheets are coated with Zn-55%Al-1.6%Si alloy to protect the steel against aqueous corrosion. The coated steel product is produced in a continuous galvanizing line resulting in a multi-layered microstructure consisting of the sub-strate steel, a thin intermetallic compound (IMC) layer, ⊠5c-Al20Fe5Si2 (+Zn), at the interface between the steel substrate and the coating overlay and the alloy overlay itself. Since the galvanizing bath is saturated with Fe, from the reaction between the strip and the bath, any additional Fe that dissolves from the strip will precipitate as fine particles of the IMC phase. When the fine dispersions of IMCs grow and/or ag-glomerate and reach some critical size, the IMC particles will settle to the bottom of the coating bath due to density differences between the IMCs and the coating bath. The settled IMCs will accumulate and form a consolidated layer of hard bottom dross which must be removed, and the dross removal process impacts both production efficiency and the safety of operations. In this study, the thermal stability of the dross particles from room temperature to 660 °C is investigated using in-situ synchrotron X-ray diffraction (XRD). Synchrotron powder XRD reveals that the dross contains τ5c (Im-3), FeAl3 (C2/m), α-Al (Fm-3m) and β-Zn (P63/mmc). We found that the crys-tal lattice structure of τ5c and FeAl3 is maintained during the heating process, while the reaction α-Al+β-Zn→Al(Zn) occurs between 270 and 330 °C and Al(Zn) dissolves into τ5c above 450 °C.

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Tuesday 28th

Abstract: 7

Yunhui Chen

Envisioning Laser Additive Manufacturing through X-ray - case studies at Australian Synchrotron

Laser Additive Manufacturing (LAM) is an emerging technique for the fabrication of complex 3D components directly from computer design. It has the potential to revolutionize manufacturing processes. However, its wider industrialisation is currently inhibited by solidification cracking, residual stress and distortion, anisotropic microstructures and most importantly a large distribution of entrained defects. It is critical to establish a scientific understanding of how to control defect formation and thus optimise mechanical performance in LAM. This presentation shows a pathway to tackle the porosity issues in a new 'hot-tear-free' new alloy system. Taking advantage of the recent BRIGHT upgrade of the Australian synchrtron, we utilise the MCT beamline to understand the pore elimination mechanism by direct evaluation of the porosity density and distribution in the product and correlate them with processing conditions and the quality of the feedstock. Correlating with previous in situ X-ray imaging results, we provide new insights into the LAM process with relevance to microstructure and defects control in AM fabricated components. These information can contribute directly to industrial practice while producing quantitative data to inform and validate physical models in support of digital twins.

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Tuesday 28th

Abstract: 131

Jiawei (Jade) Tu

Analysis of residual stresses, microstructure, and hardness of steels after laser cleaning

The effectiveness of non-destructive laser cleaning technology has been established in the restoration of architectural heritage sites and artistic pieces, such as sculptures and building exteriors. This technology's applicability can be extended to various sectors, including automotive, marine, rail, aircraft, and other infrastructure domains. Recent advancements in ultra-short pulse lasers have enabled efficient large-scale cleaning, potentially enhancing the long-term preservation of iconic structures like the Sydney Harbour Bridge. The lasers could efficiently eliminate contamination and rust from structures without producing secondary solid waste. The technology also mitigates and minimizes the adverse impacts on the steel substrate by preserving the microstructure of the underlying steel.

This study aims to investigate the impacts of nanosecond and femtosecond laser ablation treatments on steel samples by evaluating residual stress, characterizing microstructural changes, and conducting comprehensive mechanical tests. The assessment of non-destructive residual stress through neutron and X-ray diffraction was conducted using the Kowari strain scanner at the Australian Nuclear Science and Technology Organisation. Simultaneously, microstructure analysis and mechanical testing, including hardness testing, took place at the University of Sydney.

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Tuesday 28th

Abstract: 50

Shafaq Shafaq

Investigation of Crystallinity Distribution of In-situ Consolidated CF/PEEK Composites with Wide Angle X-ray Scattering (WAXS)

The formation of crystals in semi-crystalline thermoplastics depends primarily upon their thermal history1. In-situ consolidation of carbon fibre polyetheretherketone (CF/PEEK) composites using automated fibre placement (AFP) yields higher heating and cooling rates than other fabrication methods. Open literature suggest that the lay-up speed affects the cooling rate which in turn affects crystallinity2. However, no studies have been performed to correlate the AFP processing parameters with a detailed crystallinity analysis of in-situ consolidated CF/PEEK laminates. This research investigation presents the effect of AFP process parameters along with tool temperature on crystallinity distribution of each ply in the quasi-isotropic laminate. The crystallinity content was analysed using differential scanning calorimetry (DSC) as well as wide-angle X-ray scattering using the SAXS/WAXS beamline at the Australian Synchrotron (ANSTO). The analysis of the through-thickness crystallinity distribution in a laminate obtained from WAXS data revealed that the degree of crystallinity varies with distance from the metal tool surface. When a cool tool surface was used, the bottom plies received more consolidation and an extremely high cooling rate in the initial layer due to being in direct contact with the cold highly conductive tool surface, resulting in lower crystallinity (~16%) whilst upper plies experienced a slower cooling rate during lay-up, resulting in higher crystallinity (~24%). Conversely, when a heated tool surface was used, the plies near the heated surface exhibited higher crystallinity (~36%). Hence, this study demonstrates that the cooling rates can be adjusted by varying process parameters to control the crystalline regions, thereby tailoring the laminate's mechanical properties.

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Tuesday 28th

Abstract: 41

He Tian

Characterisation of Fe distribution in Al-Zn-Mg-Si coating alloys using synchrotron X-ray fluorescence

Low carbon cold rolled steel sheets are coated with Al-Zn-Mg-Si alloy to provide galvanic and cut-edge corrosion protection to the substrate steel sheet. A fundamental understanding of the alloy system and the nature of the microstructure of the coating is necessary to develop the underlying corrosion mechanisms of the various phases present in the microstructure of the coating. This work focusses on the effect of Fe additions on the microstructures of Al-Zn-Mg-Si coatings. We used a Bridgman directional solidification technique and prepared alloys containing 0.1wt% to 0.4 wt% Fe. The Bridgeman solidification experiments were conducted in the temperature range from 300 to 660oC. By controlling the temperature gradient and the descending rate in the furnace, a directionally solidified microstructure was obtained by quenching the samples in chilled recirculating ethylene glycol coolant. The directionally solidified samples alongside the air-cooled bulk samples were initially analyzed by scanning electron microscopy and energy dispersive x-ray spectroscopy (SEM/EDS). To assess the effect of Fe content on the distribution and morphology of the phases present in the coating alloy, thin film samples of nominal 30 µm thickness were prepared from the directionally solidified samples and further characterized by x-ray fluorescence at the Australian Synchrotron using the Maia array detector. The thin film samples were scanned at 7.05 keV and 18.5 keV. The effects of Fe content on the morphology and distribution Fe bearing intermetallic compound particles in the microstructure of the coating were determined.

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Tuesday 28th

Abstract: 141

Chris Wensrich

Direct inversion of the Longitudinal Ray Transform for Bragg-edge strain tomography

The natural tomography problem posed by Bragg-edge neutron strain imaging is examined from the point of view of inversion formulas for the Longitudinal Ray Transform (LRT). This problem is well known to be ill-posed with a null-space formed by compatible strain fields with fixed boundary conditions. Mathematically speaking, this is related to the usual Helmholtz decomposition of tensor fields into solenoidal (i.e. divergence-free) and potential (i.e. curl-free) parts.

In this presentation, we examine this relationship in the context of Airy stress functions and in the process define a Filtered (Tensor) Back Projection algorithm for inversion of the LRT in the case of 2D plane-stress and plane-strain residual strain fields. The technique is demonstrated for two-dimensional plane-stress systems in both simulation, and on real experimental data. We also demonstrate that application of the standard scalar filtered back projection algorithm to the LRT in these systems recovers the trace of the solenoidal component of strain and we provide physical meaning for this quantity in limited special cases.

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Tuesday 28th

Abstract: 136

Fernando Valiente Dies

Mesoscale numerical simulations for WAAM additively printed structures for prediction of temperature, microstructure and its effect on mechanical properties

Wire Arc Additive Manufacturing (WAAM) is a type of Direct Energy Deposition additive manufacturing process which takes advantage of well-established welding technology. It is consisting of a sequential deposition of weld passes and layers to form bases of engineering components later machined to the final shape. The WAAM process is characterised by high heat input, high deposition rate, high surface roughness and the anisotropy of material properties.

The high heat input leads to significant development of distortion and residual stresses, which can negatively affect the performance of the final component. At the same time, the high input can lead to the development of a highly textured micro-structure. Hence, significant effort is underway to address the development of residual stresses, distortion, or anisotropy in the mechanical properties, which depend on the microstructure texture. It is, however, impractical and expensive to test all manufactured components. Therefore, the development of validated numerical models is vital to obtain the required information.

In this project, the WAAM process has been employed to manufacture multipass, multilayer walls made using 316Si stainless steel consumable on a 316L substrate at the University of Wollongong. The transient temperature field during the WAAM process has been monitor by an array of thermocouples located on the substrate. The theremocouples readings are then used to calibrate the thermal numerical model which is later used in a phase-field model to predict resulting weld-like micro-strucre, and in mechanical model to predict resulting distortion and residual stresses. The modelling work is further supported by microstrucrual analysis, while the residual stresses will be measured using ANSTO's neutron diffraction technique, and contour cutting method.

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Tuesday
28th

Abstract: 54

Qichao Hao

The effect of In concentration and temperature on dissolution and precipitation in Sn-Bi alloys

Low temperature solder alloys based on the Sn-Bi system are currently undergoing development to provide the electronics manufacturing with a path to lower temperature processes. One distinguishing feature of these alloys is that there are significant changes in microstructure and crystallography at the temperatures to which solder joints are exposed in normal service. Previous studies have shown that a major factor influencing properties at these temperatures is the variable solubility of Bi in the Sn phase. The influence of alloying additions in improving the performance of these alloys is the subject of much research. In this study, in-situ heating synchrotron powder X-ray diffraction (PXRD) was adopted to further investigate the change in the lattice parameters of the Sn phase in Sn-57Bi-xIn (x=0.2, 0.5, 1, and 3, in weight percent) alloys during heating to study the dissolution of Bi in Sn and the effect of In. This study revealed that the introduction of In to the alloy can change the lattice parameters of the Sn and promote the dissolution of Bi in the Sn phase. In addition, there is an alloy-dependent temperature above which the dissolution speed of Bi in Sn increases significantly. Additions of In lower this temperature. The results offer profound insight into Bi dissolution in Sn phase in Sn-Bi based solder alloys and the effect of In on this phenomenon. The increased understanding of these phenomena provided by these results is a significant contribution the data base on which the ongoing effort to improve the reliability of the Sn-Bi based solder alloys is based, opening up for the electronics manufacturing industry a path to lower temperature processes.

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Tuesday 28th

Abstract: 132

Yutaka Tsumura

Application of finite element simulations to nanosecond laser ablation process

Surface preparation for steelwork repainting often involves sandblasting, which can damage the substrate's mechanical performance. Laser cleaning, an environmentally friendly alternative, applies laser ablation to remove paint and corrosion efficiently but can cause heat-related damages, such as crack formation and flaking. Selecting proper laser parameters is a complex process requiring multiple tests, and residual stress measurement through methods like X-ray or neutron diffraction can be costly.

This research explores the residual stresses of laser-ablated steel samples using finite element modeling. The comprehensive model encompasses complex multi-physics phenomena, including laser-substance interactions and melting/re-solidification processes. Simulations were conducted to identify the areas subjected to phase transformation and how residual stresses change during laser ablation. Experimental measurements using a nanosecond laser on steel plates were carried out for residual stress testing and microstructure characterization. X-ray diffraction and scanning electron microscopy were employed, with a comparison between the finite element model and experimental results presented.

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Wed
29th

Abstract: 112

Clemens Ulrich

Scaling Behaviour and Stability of Magnetic Skyrmions in Cu2OSeO3

A skyrmion is a topological stable particle-like object comparable to spin vortex at the nanometre scale. It consists of an about 50 nm large spin rotation which order in a 2 dimensional, typically hexagonal superstructure perpendicular to an applied external magnetic field. Its dynamics has links to flux line vortices as in high temperature superconductors. Cu2OSeO3 is a unique case of a multiferroic materials where the skyrmion dynamics could be controlled through the application of an external electric field. The direct control of the skyrmion dynamics through a non-dissipative method would offer technological benefits.

Important for technological applications would be a stability range of the skyrmion phase up to room temperature. While room temperature skyrmion materials exist, Cu2OSeO3 orders magnetically below 60 K. Our combined small angle neutron scattering and SQUID magnetization measurements did provide direct evidence that the stability range of the skyrmion phase can be extended in Te-doped Cu2OSeO3. Besides the information about the skyrmion range in the H-T phase diagram, neutron scattering provides also the full information about the orientation and skyrmion distances in the skyrmion lattice. Our systematic investigation offers new aspects about the scaling behaviour of the skyrmion and helical distances as a function of temperature and magnetic field. It is interesting to note that the changes in skyrmion distances are quite distinct for the different skyrmion phases, observed for different crystal orientations. The results provide new valuable information on the parameters in the spin Hamiltonian, which are responsible for the formation of the fascination quantum protected objects.

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Wed
29th

Abstract: 90

Caleb Stamper

The Unique Lattice Dynamics of Nanodiamond – a Molecular Dynamics and Inelastic Neutron Scattering Investigation

Nanoparticles exhibit remarkable properties due to their size-dependent quantum effects and high surface-to-volume ratio. Among these particles, carbon-based nanoparticles stand out for their extreme and diverse characteristics. Nanodiamond, in particular, has garnered significant attention owing to its unique combination of an extremely high surface-to-volume ratio, distinctive thermal, optical, and structural properties, and biocompatibility. Notably, recent focus has centered on nitrogen vacancy (NV) centers within nanodiamonds, holding promise for applications in quantum sensing, nanoscale imaging, and thermometry.

Understanding and controlling the intrinsic lattice vibrations (phonons) in nanodiamonds, including their interaction with NV centers, becomes pivotal for advancing nanodiamond-based technologies. To contribute to these advancements, our study presents a comprehensive exploration of nanodiamond's lattice dynamics through a synergistic approach that combines inelastic neutron scattering (INS) and molecular dynamics (MD) simulations. This presentation highlights nanodiamond's distinct vibrational modes in comparison to bulk diamond.

In our MD simulations, notable features emerge: shifts and broadening of phonon modes in energy (acoustic and optical), excess vibrational modes at lower energies deviating from the Debye relationship in the density of states, and additional vibrational modes above observed optical phonons. Many of these observations find confirmation through INS measurements conducted on Pelican. Our work underscores the critical importance of understanding size-dependent lattice dynamics to unlock the full potential of nanodiamonds across diverse technological applications.

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Wed
29th

Abstract: 5

Guochu Deng

Study Multiferroic/Magnetoelectric Materials with Inelastic Neutron Scattering

Multiferroic and magnetoelectric materials have been extensively studied in the past two decades due to their interesting properties and potential versatile applications. Magnetoelectric coupling is the fundamental mechanism of multiferroic and magnetoelectric properties in these materials. However, detailed magnetoelectric coupling mechanisms in multiferroic and magnetoelectric materials could be highly elusive, especially for those single-phase multiferroic and magnetoelectric materials. Magnetoelectric coupling mechanisms are highly dependent on their magnetic structures and exchange interactions. Neutron diffraction and inelastic neutron scattering are powerful tools to study the magnetic structure and spin dynamics in magnets, helping us to reveal the hidden magnetoelectric coupling mechanism in multiferroic and magnetoelectric materials. In this talk, two magnetoelectric materials

$Co_4Nb_2O_9$and $Mn_4Nb_2O_9$ were studied using neutron powder diffraction on Wombat[1] and inelastic neutron scattering technique on Taipan[2]and Sika[3] at ACNS, ANSTO. It was revealed that Co^{2+} ions have strong in-plane magnetic anisotropy and canted magnetic configuration due to the Dzyaloshinskii-Moriya (DM) interaction[4]. In contrast, $Mn_4Nb_2O_9$ demonstrates a collinear magnetic structure with magnetostriction as its magnetoelectric coupling mechanism due to the absence of DM interaction.[5,6] These two case studies in the multiferroic/magnetoelectric materials demonstrate that inelastic neutron scattering, and neutron powder diffraction are powerful tools to study microscopic mechanisms in these materials.

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Wed
29th

Abstract: 28

Chris Ling

A “Partial” Spin-liquid Candidate with a Perfectly Isotropic 2-D Kagomé Lattice

FeMn3GeSn7O16 [1] is a fully ordered stoichiometric phase with a complex composite layered structure that incorporates an undistorted hexagonal kagomé lattice of Mn2+ cations. Its discovery expands the chemistry of the hitherto singular FeFe3Si2Sn7O16 structure type [2] and improves on the perfection of its kagomé lattice by replacing anisotropic high-spin Fe2+ (d6, L = 2) with isotropic high-spin Mn2+ (d5, L = 0), achieved by the size-matched replacement of SiO44− with GeO44− polyanions in the bridging layer. Single-ion anisotropy of HS Fe2+ sites was suspected of playing a role in the unique “striped” magnetic structure of FeFe3Si2Sn7O16 below TN = 3.5 K,[3] which breaks hexagonal symmetry and leaves 1/3 of the spins geometrically frustrated in an apparent “partial spin-liquid” state down to at least 40 mK. We can now rule that out by observing the same magnetic structure in FeMn3Ge2Sn7O16. We will discuss the potential for further chemical variation and physical modification, and present new neutron scattering data that shed light on the nature of the magnetic ground state.

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[3] C. D. Ling, M. C. Allison, S. A. Schmid, M. Avdeev, J. S. Gardner, C. W. Wang, D. H. Ryan, M. Zbiri, T. Söhnel, Phys. Rev. B 9, 180410 (2017)

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Wed
29th

Abstract: 78

Shinichiro Yano

Magnetic structures and spin reorientations in the 2D triangular antiferromagnets.

A two-dimensional (2D) triangular lattice Heisenberg antiferromagnet (2D-THA) is one of the simplest examples of geometrically frustrated antiferromagnets. A novel spin state originated from low dimensionality and competing for magnetic interaction is expected. The materials of interest in this study are (Lu, Y)MnO3, (Lu, Sc)FeO3, and (Yb, Sc)FeO3. These compounds have P63cm symmetry and 120 degrees antiferromagnetic structures but the exchange interactions in nearest neighbors are J ~ 2.5 meV with S = 2 (Mn3+) and J ~ 4.0 meV with S = 5/2 (Fe3+). We have made a systematic investigation of polycrystalline and single-crystal samples by using neutron diffraction, inelastic scattering, and polarized neutron scattering experiments to understand the 2D-THA system. We focus on these results in this presentation

1. Determining the magnetic structure of 2D-THAs
2. Revealing the origin of the spin reorientation in the 2D-THAs

Under the P63cm symmetry, there are four possible 120-degree antiferromagnetic structures Γ1, Γ2, Γ3 or Γ4. They cannot be distinguished using unpolarised neutron scattering techniques only. By using polarised neutron scattering techniques, we developed techniques to solve it uniquely. For example, the magnetic structures of Lu0.3Y0.7MnO3 and Lu0.47Sc0.53FeO3 were determined as C3Γ3 + C4Γ4 and C1Γ1 + C2Γ2 respectively.

Based on the determined the magnetic structures, we have studied magnon dispersion of Lu0.3Y0.7MnO3 and Lu0.47Sc0.53FeO3 and analyzed based on the Hamiltonian with exchange parameters (intra-plane and inter-plane) and isotropic parameters (in-plane and out-of-plane). We found inter-layer interactions are important to understand the spin reorientations of 2D-THAs.

S. Yano, Chin-Wei Wang, Jason S. Gardner, Wei-Tin Chen, Kazuki Iida, R. A. Mole, and Despina Louca, Phys. Rev. B 107, 214407 (2023)

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Posters

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3	Characterising the phase transformation behaviour in In-Sn-Bi low temperature solder alloys by in-situ synchrotron powder X-ray diffraction	Jiye Zhou
5	Quantitative relationship between small-angle x-ray scattering (SAXS) and x-ray diffusive dark-field in single-grid imaging	Ying Ying How
8	Biochemical Mapping of Lipid-Iron Interplay in Pancreatic Islets Using ATR-FTIR Microspectroscopy	Keea Inder-Smith
9	Exploring underscreening through re-entrant behaviour of poly-electrolyte brushes in hypersaline solutions	Geran Dunlop
10	Synchrotron X-ray tomographic characterization of fracture pattern in veined rocks under triaxial compression	Haojun Wang
11	Characterising thin films by neutron/X-ray/light scattering: A brief history of refellips and refnx analysis tools	Hayden Robertson
12	Structures of electrochemical liquid/liquid interfaces studied using neutron reflectometry : ionic compositions and protein monolayers	Kosuke Ishii
14	Towards the Generation of MOF based Heterogenous Catalysts for Hydrogen Gas Production	Adam Stewart
15	Measurements of porosity in Martian mineral analogues using Small Angle Neutron Scattering and molecular modelling	Nicholas Florent
18	Thermal Treatment on Vertical Morphology of PffBT4T-2OD: ITIC Non-fullerene Bulk Heterojunction Thin Films	Tzu-Yen (Ian) Huang
19	Utilizing Neutron Powder Diffraction to Explore the Characteristics of Porous Silicon Materials Synthesized from Al-Si Alloy Powder for Hydrogen Storage	Honghao Li

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21	Unlocking Hydrogen Storage in high entropy alloys TiZrTaSiSnCo: An In-Depth Investigation with Neutron Powder Diffraction (NPD)	Ruiran Guo
22	Neutron vibrational spectroscopy of a Metal-organic Framework and Computer Simulations	Ferensa Oemry
23	2D Ferromagnetic M3GeTe2 (M = Ni/Fe) for Boosting Hydroxyl Adsorption toward Highly Efficient Water Oxidation Reaction	Guyue Bo
24	Atomic-Scale Exploration of NTD-Ga2O3 for Extreme Environments Applications	Samaneh Sadat Setayandeh
26	Analysis of the Degradation of Organophosphate Molecules Over Zr-Based Metal Organic Frameworks	jhair pena prada
27	Exploring Melanin Absorption Properties at Ambient Terrestrial Black Body Radiation Frequencies	Negin Foroughimehr
29	Translocation and fate of nanospheres in pheochromocytoma cells following exposure to synchrotron sourced terahertz radiation	Palalle Gamaarachchige Tharushi Perera
30	Hydration dependant structural phase transitions of platinum vacancy ordered double perovskites	Caleb Bennett
31	Radiolytic stability of metal (IV) phosphonate sorbents designed for nuclear waste treatment	Taren Cataldo
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