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Concurrent Session 3: Industry & Innovation / 287

The Australian Synchrotron and Advanced Materials: Challenge/Opportunity/Solutions

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One of Australia's world class research facilities, the Australian Synchrotron, provides cutting edge tools to academic and industry researchers, empowering them to problem solve and innovate in a wide range of sectors. As well as servicing the traditional academic user base, the Australian Synchrotron has an Industry Engagement team focused on supporting commercial customers to utilise the synchrotron's capabilities. However, going beyond the academic user base presents some challenges as well as opportunities. This presentation will: [U+F0D8] Discuss how to raise awareness and understanding of technical capabilities to potential commercial clients [U+F0D8] Share ways to inspire businesses to explore applications and capitalise on the opportunities arising from our world class infrastructure [U+F0D8] Showcase existing case studies, demonstrating successful connections between science and industry Examples of case studies from the Australian Synchrotron will be presented that highlight the capabilities and advantages of the facility to commercial and academic users. Lessons learned will be shared as well as a practical approach to achieving "buy in" from key decision makers to achieve a mutually beneficial outcome.

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Discussion Panel

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Concurrent Session 3: Radiotherapy I / 281

Clinical synchrotron radiotherapy programs from a medical physicist point of view

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Therapeutic applications of synchrotron x-rays are becoming a reality. The first phase I/II clinical study of Synchrotron Stereotactic Radiation Therapy (SSRT), in place at the European Synchrotron Radiation Facility (ESRF) since 2012, consists of a dose escalation protocol to show the feasibility and safety of the technique. 13 patients have been treated using 80 keV high-flux quasi-parallel monochromatic x-ray beams, in the presence of iodinated compounds injected immediately before irradiation, for radiation dose enhancement purposes1,2. Even if the technique is still in its infancy, these promising technical results are allowing the clinical transfer of other synchrotron radiation therapy modalities for an improved healthy tissue sparing effect combined with an increased tumoricidal effect. One realistic option is the use of high dose rate arrays of synchrotron microbeams (Microbeam radiation therapy, MRT) for treating isolated small lesions3. MRT is based on the spatial fractionation of the dose using an array of parallel microbeams having a width comparable to that of a human hair (˜50 micrometres) and being separated by regions of almost zero radiation. Pre-clinical studies have demonstrated that MRT significantly improves the treatment outcome compared to conventional radiotherapy4,5. This is the result of preferential damage to cancer cells and high tolerance of healthy tissues within the irradiation pattern. Although MRT is currently confined to synchrotron radiation facilities because of the very high radiation dose rate required (5,000 times higher than clinical radiotherapy), clinicians and medical physicists are collaborating closely with synchrotron scientists to spearhead its development towards clinical trials.

Extensive methodological developments and rigorous medical physics codes of practice are required for its implementation in clinics. Such protocols are well established in conventional clinical radiotherapy but are not applicable to MRT due to the x-ray spectrum, high dose rates and radiation detector limitations. Recently, absolute real time dosimetry methods have been successfully benchmarked using a microdiamond detector6 or spectrometry techniques7. Moreover, rigorous and reproducible preclinical studies are now possible with the DynMRT system available at the Australian Synchrotron medical beamline. This is mandatory to strengthen the biological data available on healthy tissue tolerances and tumour responses to MRT.

Radiotherapy Workshop: Should we MRT Treat Canines / 296

The case for large animal data

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Concurrent Session 3: Industry & Innovation / 193

Optimal fly-scan trajectories at the AS

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Data acquisition at virtually every beamline at the AS involves scanning; however, none more so than the XFM beamline, where every pixel in an image is acquired serially by scanning a specimen through a tightly-focused beam. At XFM, faster scanning means more science. On-the-fly scanning has significantly improved scan speeds by removing overheads between pixels. However, developments in the past 15 years now require optimisation of the entire scan motion as a sequence of line scans. We have developed an approach which breaks the motion profile into two components, being a 'measurement motion' ('scan' moves), connected by 'transition motion' ('skip' moves). The Skip-Scan approach provides an efficient platform for implementation of generalised on-the-fly scans that are fully optimised for accuracy and speed. This approach is used for implementation of optimised raster scans at XFM.

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Merger, a Software Pipeline to Merge Datasets at the Australian Synchrotron MX beamlines

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The ability to determine the progress of an experiment is critical to efficiently use beamtime during synchrotron visits. While processing results from individual datasets are sufficient for many crystallography experiments, chemical crystallography experiments that require use of the minikappa to collect datasets from multiple orientations, and sensitive samples where partial datasets can be collected from multiple macromolecular crystals in particular would benefit from the ability to combine results from multiple data collections. With these applications in mind, we have developed a dataset merging pipeline.

The Merger pipeline is designed to automatically run dataset merging using three different programs – Phenix scale_and_merge, Blend, and XScale. The user simply selects the datasets to combine using the web application, selecting a reference dataset if desired, and press the 'Merge Selected Datasets' button to trigger the merging process. Written entirely using the Python programming language, the Merger pipeline is run within the Airflow pipeline framework which was originally developed by Airbnb. Several steps are first performed to sanitize the input to the different merging programs, removing incompatible (different space group/unit cell parameters) datasets, reindexing datasets if necessary, and after running XScale, further analysis software is run to derive dataset statistics. The merging results from XScale, the standard of dataset merging software, are inserted into the database to allow users to readily compare results using the web application.

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NEW OPTICS FOR SOFT X-RAY PTYCHOGRAPHY

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There is growing interest in combining soft X-ray ptychography with spectroscopy and applying it to the study of functional materials and biological systems in situ [1-3]. Realising the full potential of this method depends on efficient nanofocusing of the X-ray beam. Fresnel zone plates (FZP) are commonly employed, but their efficiency is typically less than 10% [4]. Achieving higher efficiency generally demands complex nanofabrication strategies that require replacing the radially concentric pattern of opaque and transparent zones with one that approximates a structure with continuous variation in thickness [5].

A linear tilted zone plate (LTZP) design based on a Kinoform optic [6], was optimised for use at the Soft X-ray Imaging (SXRI) beamline of the Australian Synchrotron [7]. The LTZP design aims to produce a continuous modulo 2π phase shift in the illumination using only planar nanofabrication methods. A continuous variation in projected thickness is achieved by tilting a particular planar geometric design with respect to the incident beam. By varying the tilt angle, high efficiency can be achieved over a wide X-ray energy range.

The LTZP was successfully fabricated using electron beam lithography (EBL). Efficiency better than 70% was demonstrated using a photon energy of 320 eV. We will describe the design and fabrication of the LTZP optics and outline the potential improvements to multi-dimensional ptychographic imaging experiments that they can provide. We will also outline plans for further developments that exploit new nanofabrication capabilities based on grey-scale (3D) electron beam lithography and thermal scanning probe lithography.

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Condensed Phase Techniques & Applications at the THz/Far-IR Beamline

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An increasingly wide variety of condensed phase studies have been successfully undertaken at the THz/Far-IR beamline over the past few years. The combination of a small, collimated, and bright synchrotron THz photons with traditional spectroscopic techniques can offer new opportunities to scientists from fields such as nanotechnology, geology, renewable energy sources, forensics, biology, engineering and environmental science. In this paper, we will present some of these applications and current techniques, as well as new techniques which are under consideration for the study of condensed phase materials. In particular, we will present our recent efforts using a diamond-transmission cell for liquids and the ATR technique.

Concurrent Session 4: Technique Development / 252

The MX2 goniometer story: the old, the current and the new one

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Sample positioning and rotation on the X-ray beam are critical experimental parameters for a successfully experiment . This becomes exacerbated when handling small crystals on a micro-focus beam like the one provided by the MX2 beamline at the Australian Synchrotron. Here it is paramount that the centre of rotation is on the same location as the X-ray beam. For one hand, any procession, particularly if asymmetric, around the X-ray beam will have an effect on data quality. On another hand parameters like temperature have a huge effect in changing the centre of rotation over a period of time meaning that regular check of its alignment as well as good control of temperature on the beamline hutch is required over the course of an experiment. We present here the challenges presented with wear and tear of the old MX2 goniometer, the setup we had after deployment of an emergency repair and what we have now as the final solution after installing an XFEL like goniometer in September 2016

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Elemental Contrast X-ray Tomography Using Ross Filter Pairs

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Here we present x-ray imaging experiments based on the use of Ross filter pairs. Although such Ross filter arrangements have been applied in proof-of-principle spectroscopy experiments, to date there have been no reports of this approach used for full-field x-ray imaging. Here we report on the experimental demonstration of Ross filter pairs being used for quasi-monochromatic, full-field imaging in current laboratory based x-ray sources which are polychromatic and not tuneable. This lack of monochromaticity limits the range of applications for these sources and in particular

it reduces the elemental specificity of laboratory based x-ray imaging experiments. However, Ross filter arrangement has several important benefits for laboratory based x-ray imaging including, as we demonstrate, elemental contrast enhancement. The method is demonstrated both for two-dimensional radiography and for three-dimensional x-ray tomography.

Concurrent Session 1: Earth & Environment / 235

Far-Infrared Synchrotron spectra of Titan's cyanide haze

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Titan is Saturn's largest moon and is the only planetary body in our solar system with a dense atmosphere that is comparable to Earth. Photochemical processing of the two major atmospheric components (N2 and CH4) produce a suite of hydrocarbon and nitrile species, from small hydrocarbons to large complex organic molecules (COMs) and polymeric nitriles (tholins). Tholins aggregate and coagulate to form suspended aerosols that descend in altitude from the stratosphere and settle on the surface of Titan. These complex molecular systems are responsible for the seasonal far-infrared absorption feature at 220 cm-1 that remains unassigned.
Despite the abundance of observational data from the recent Cassini-Huygens space probe to the Saturnian system, there are few experimental infrared analyses on nitrile aerosols under temperatures and pressures simulating Titan's atmosphere. Laboratory far-infrared studies can elucidate the temperature, pressure and particle size dependence on infrared signatures of pure and mixed aerosols. Without such experiments, the fundamental morphology and identification of the unassigned far-infrared band feature of these nitrile aerosols remain unresolved.
In this talk, we present the first infrared studies of nitrile-hydrocarbon and nitrile-water binary aerosols under conditions replicating the Titan atmosphere. We utilize the specialized enclosive-flow-cooling-cell (EFC cell) that is coupled to the THz/Far-IR beamline at the Australian Synchrotron. This is the only setup in the world that has the capabilities to study the far-infrared of aerosols like those detected on Titan. Here, our laboratory data will be compared and validated against Cassini mission data.

Concurrent Session 4: Radiotherapy II / 191

A pre-clinical sample positioning system for microbeam radiotherapy at the Australian Synchrotron

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Microbeam radiation therapy (MRT), using X-rays from a synchrotron, is a novel, preclinical form of radiotherapy that shows promise of providing a major advance in cancer control if successfully translated to clinical practice (Brauer-Krisch et al, 2010; Crosbie et al, 2010). Clinical translation of MRT requires developing a protocol for a patient positioning system (PPS). Following recent developments in image-guided synchrotron MRT (Pelliccia et al, 2016a and 2016b), we present the implementation of a pre-clinical protocol at the Imaging and Medical Beamline of the Australian Synchrotron.

The synchrotron PPS will be composed of three key elements: 1) Treatment planning 2) Synchrotron imaging 3) Image registration and patient alignment. The treatment plan, available before the synchrotron session, is imported into the synchrotron control system. Imaging of the patient is done at the beam line, using either the synchrotron beam or a conventional x-ray tube unit. The images are registered with the existing treatment plan and the patient is aligned according to the registration. Verification is performed after alignment and before the treatment is initiated.
We have developed a functional positioning system protocol using a small animal phantom, namely a plastinated mouse. A CT of the phantom is taken using a medical CT machine and then imaged again at the beam line. The image is registered with a Digitally Reconstructed Radiography (DRR) from the CT and the registration prompts a sample alignment and image verification. The registration process allows for anatomical landmarks or fiducial markers to be used for alignment. This preclinical sample positioning system protocol for synchrotron microbeam radiotherapy (MRT) has been realised at the Australian Synchrotron with scalability included to allow for patient positioning chairs and couches with many more degrees of freedom. The protocol marks a further step towards the clinical translation of synchrotron MRT.

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Single Molecule Magnetism in a Series of Dysprosium 5,7-Dibromo-8-Hydroxyquinolinolato Complexes

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Modern hard drive disks (HDDs) store information in the form of magnetic field orientation combinations. Information density / size of HDDS are hence limited by the size of the magnets used to construct the device. Molecules and single ions capable of magnetic hysteresis, termed single molecule magnets (SMMs) and single ion magnets (SIMs), respectively, are of interest then as a means to miniaturize HDDs. Widespread adoption of SMMs or SIMs in HDDs however is not currently feasible as the phenomenon requires liquid helium cooling in order to be observed. Current challenges for the field then include the discovery of SMMs or SIMs capable of retaining magnetization at temperatures above that of liquid nitrogen. Lanthanoid complexes are currently of interest then as the near degenerate 4f orbitals contribute greatly to ion anisotropy and hence the stability (Ueff) of single molecule / ion magnet magnetic hysteresis. Recent work within the Deacon group regarding a series of single ion / molecule magnets featuring the 5,7-dibromo-8-quinolinolate ligand will be presented.

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Controlling size and chirality of supramolecular cage complexes

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A series of chiral coordination cage complexes has been synthesised using amino acid substituted diimide ligands. Using a biphenylsulfonediimide core (BPSD) substituted with amino acids, a series of quadruple stranded Cu4L4 cages have been formed. The cages contain two copper paddlewheel units connected by four ligands. Analogous chiral complexes (helicates) and achiral complexes (mesocates) can be formed by controlling or removing the stereocentres within the ligands(1). Enantiopure leucine-substituted ligands (LeuBPSD) form helicates, complexes which have supramolecular chirality due to a twist in the ligands. Swapping the handedness of the amino acid ligand forms the opposite handedness helicate cage complex. The helicate cages are self-selecting, as the reaction of the (R,R) and (S,S) ligands with Cu(II) forms a mixture of enantiopure cages, with no product containing both ligands. Removing the chirality of the ligand, by using a BPSD ligand substituted with achiral amino acid, glycine (GlyBPSD), or using the (S,R)-LeuBPSD ligand, leads to the formation of mesocates, which lack supramolecular chirality. The cage complexes formed with BPSD ligands have an internal void volume of ˜300 Å3. The use of alternative diimide amino acid substituted ligands have also been shown to form larger and more complex chiral supramolecular cages, which have an internal void volume of up to 1000 Å3, establishing the possibility of chiral catalysis and separation applications for these complexes.

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Using Synchrotrons to unravel the Chemistry of Nucleation

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The formation and growth of nanoparticles is of critical importance in a variety of scientific areas and in everyday life. The prevailing models used to describe these processes have mainly been based on thermodynamic arguments and by the use of concepts such as “monomers” or “particles”, thereby omitting to incorporate the important influence of differences in the chemical nature of different systems. One of the main reasons for this lack of incorporation of the chemistry into these models has been the lack of quantitative information on an atomistic level obtained in situ during nanoparticle formation, i.e., characterization methods that enable the extraction of atomic level structural information, preferably at a suitable time resolution under real experimental conditions. I will present an overview numerous in situ studies we have performed using numerous different tools that enable extraction of atomistic structural information about the formation and growth of nanoparticles during Sovothermal synthesis. The main characterization methods have been synchrotron based in and ex situ PXRD, total X-ray scattering, PDF-analysis and EXAFS. The data has been analyzed by sequential Rietveld refinement, real space Rietveld refinement, curve fitting, Debye scattering equation based techniques and other methods. Our studies have revealed a fascinating chemical richness spanning from mono-metal to complex polymer precursor species, which through a specific system-dependent multistep mechanism develop into pristine nanomaterials. The results have led us to call for a paradigm shift in how nucleation of nanoparticles is conceived – it is imperative to move away from a one-fits-all approach and instead consider many-fit-many models that incorporate the true chemistry of different systems, rooted in atomistic chemical insight obtainable to a large degree by the use of Synchrotron radiation.
Reference: The chemistry of nucleation, Bøjesen et al. CrystEngComm, 2016,18, 8332-8353

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Proposal for Ultra-low Emittance Measurements on IMBL with an X-ray Interferometer

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The Australian Synchrotron storage ring has achieved a world record low vertical emittance below 1 pm rad. These beam parameters produce very small beam sizes which are hard to accurately measure. This proposal is to test an Young's Double slit X-ray interferometer on the long baseline of the IMBL to measure vertical electron beam sizes down to 1.6 μm. These measurements will be part of the vertical emittance reduction research program with the goal of reaching the quantum limit of vertical emittance.

Concurrent Session 2: Advanced Materials II / 233

Structure of Concentrated Colloidal Suspensions using SAXS and SANS

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Colloidal suspensions of hard spheres are valuable experimental model systems for exploring phase behaviour and dynamics in condensed matter. Such colloids form colloidal crystals at concentrations above the freezing volume fraction of 0.494, allowing the investigation of the kinetics and dynamics of crystallization. As colloidal particles are much bigger than atoms, processes are correspondingly slower, and metastable states can be studied in real-time using the well-established technique of dynamic light scattering (DLS), or the more recently developed technique of x-ray photon correlation spectroscopy (XPCS). In this work we explore how the use of Synchrotron Small Angle X-ray (SAXS) and Neutron (SANS) scattering can be applied to the study of structure in colloidal suspensions near the freezing volume fraction. In particular we explore their advantages and disadvantages relative to traditional light scattering techniques.

Concurrent Session 4: Radiotherapy II / 186

How big is that diamond?

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Detectors using diamond for the active layer are becoming more popular in radiotherapy because they have a relatively flat energy response and can be small. Recently published modelling of a

new solid-state diamond detector (PTW model 60019) suggests that only a region of diameter 0.6 mm responds to radiation. The manufacturer's specifications indicate that the active area is a disk of diameter 2.2 mm. We measured the active area by collimating a synchrotron beam of average energy 95 keV to spatial dimensions of 0.1 mm and scanning the diamond through the beam. The measured area had a diameter of 2.4 mm, in good agreement with the specifications when the beam size is considered. 2D plots of the diamond spatial response also confirm the shape of the active area.

Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 241

Application of 3D MESA Silicon Strip Detector for use in MRT Dosimetry at the Australian Synchrotron.

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Microbeam Radiation Therapy (MRT) is a promising preclinical radiotherapy modality that uses micron-sized, spatially fractionated radiation fields to treat radioresistant and otherwise untreatable tumours. A typical MRT configuration consists of arrays of 25-75 μm wide high-dose 'peaks' separated by 100-400 μm wide low-dose 'valleys' that are produced by an x-ray spectrum from a synchrotron light source. A synchrotron light source is essential as the concept of MRT dose delivery requires very low divergence and a high dose rate (>20kGy/s) to deliver treatment doses quickly enough to minimize dose blurring due to motion of the target. The high dose rate, high dose gradients and small field sizes present a challenge for Quality Assurance and dosimetry. To address these issues CMRP have produced a novel n-type SOI silicon single strip detector (SSD) - the 3D MESA SSD – that aims to improve spatial resolution via construction of an isolated sensitive volume (SV). This is accomplished by using ion plasma etching techniques to remove the silicon surrounding the SV until it protrudes 10 μm above a SiO2 insulating layer. Two options of the 3D MESA SSD have been produced– named 'one sided' (22.5 μm wide) and 'two sided' (36 μm wide). Each option was fabricated with three different lengths of the SV: 50, 100, or 250 μm. Detector Topology was examined using a scanning electron microscope at the Australian Institute of Innovative Materials (AIIM). Electrical characterisation of samples mounted on Dual-In-Line (DIL) package was performed at CMRP using a Keithley 237 high voltage source measure unit and a Boonton 7200 capacitance bridge to produce IV and CV curves to determine optimal bias and leakage current. Charge collection studies on those samples using Ion Beam Induced Charge Collection (IBICC) with 5.5 MeV 2He4 ions were carried out at the ANSTO ANTARES 10MV tandem accelerator in conjunction with TCAD modelling. Radiation damage studies, detector bias studies, and acquisition of microbeam dose profiles were performed at the Australian Synchrotron's Imaging and Medical Beamline (IMBL) hutch 2B using CMRP's X-Tream dosimetry system. The impact of charge collection from under the bridge that connects the SV to the readout pad has been studied. Investigation into methods of mitigating and eliminating excess charge collection are presented and discussed. Electrical and charge collection characteristics, topology, and microbeam dose profiles will be presented in this poster.

Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 234

High Data Rate MX at the Australian Synchrotron.

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The advent of the Eiger family of detectors has pushed the speed of MX experiments to new heights with SAD phasing datasets being collected in as little as 1 second. The Eiger16M can produce 10Tb of data per day at a bandwidth of 40Gb/s. These high data rates come with a range of benefits and challenges for synchrotron facilities. With an Eiger 16M detector scheduled for delivery in December 2016 the MX2 beamline needs to be ready to meet these challenges. The requirements for beam and crystal stability, robot speed, network bandwidth, fast processing and storage will be discussed and the Australian Synchrotron's plan to deal with these requirements. The likely improvements in data quality and collection speed will be significant, changing the way the MX2 beamline is used. Due to the high frame rate (133Hz full frame and 750Hz for 4M mode) significant high-frequency fluctuations in beam position and/or intensity can have an adverse effect on data quality. The measures being undertaken to characterise the current beam motion and upgrades to the MX2 optics (such as the MHFM mirror) will be discussed. From international experience beamlines upgrading from CCD to pixel-array detectors can experience issues where users are unfamiliar with the new detectors. As Eiger frames will look radically different to CCD images the "rule-of-eye" can no longer be used as a solid judge of crystal quality. Data representations from hundreds of summed frames may be required to produce a single CCD-equivalent image for visualisation. Tools for the graphical representation of Eiger data in a user-friendly manner are being developed. Finally, the planned collection modes and user automation will be presented. The Eiger16M detector can transform the capabilities of the MX2 beamline but requires a parallel transformation in the other beamline components so that it can deliver the maximum benefit to the user community.

Concurrent Session 2: Surfaces / 293

Photo-Switchable Block Copolymer Self Assembly

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Block copolymers can self-assemble into well-defined, nanoscale morphologies, which are typically isotropic and lack long range order. Chemical or physical templates generated through optical lithography can direct self assembly to create morphologies with enhanced long range order and fashion them into hierarchical patterns. This ability allows the patterns formed to be optimized to be more suitable for a desired application. Alternatively, the incorporation of stimuli-responsiveness into these materials has the potential to exert similar control over long range order and pattern complexity, while also creating dynamic nanostructures with expanded functionality. Here, photo-responsive block copolymers are synthesized and their ability to undergo a change in morphology triggered by light exposure is investigated. This will allow direct spatial control to be exerted over self-assembled nanostructures produced in thin block copolymer films.
Photo-responsive block copolymers were synthesized through successive RAFT polymerisations and post-polymerisation modification reactions to yield poly(benzyl methacrylate)-b-poly(o-nitrobenzyl methacrylate). When the o-nitrobenzyl group is exposed to UV light, it degrades to reveal a carboxylic acid functional group, allowing the polymer to be switched from a structure with two aromatic blocks and low segregation strength to an aromatic and polar acid block with a large segregation strength and induce self-assembly as a result.
Samples of this material were exposed to UV radiation for varying amounts of time to achieve different degrees of o-nitrobenzyl group deprotection and different levels of segregation strength

as a result. GISAXS was used to characterize the evolution of morphology during this process, taking advantage of the high sample throughput achievable through the use of a synchrotron X-ray source to characterize a large number of samples and optimize annealing conditions for the controlled evolution of nanoscale architectures in these materials.
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Concurrent Session 1: Advanced Materials I / 219

Understanding the Formation of Bimetallic Pd-Au Co-catalysts on TiO2

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Transition metal modified titania (M/TiO2, M = Pd, Pt or Au) photocatalysts have shown excellent activity for H2 production in alcohol-water mixtures under UV excitation [1, 2]. Recently, we have found that a 0.25 wt.% Pd-0.25 wt.% Au/TiO2 photocatalyst demonstrated a superior H2 production rate of 68 mmol g-1 h-1 compared to monometallic 0.50 wt.% Pd/TiO2 (43.0 mmol g-1 h-1) or 1.00 wt.% Au/TiO2 (34.2 mmol g-1 h-1) photocatalysts evaluated in 80 vol.% ethanol solutions at a UV flux (365 nm, 6.5 mW cm-2) comparable to that present in sunlight at the Earth's surface. To rationalise the high H2 production activities of the Pd-Au/TiO2 photocatalysts, we characterize the materials using UV-Vis absorbance, TEM, XRD, XRF, N2 physisorption and lab-XPS. Preliminary data strongly suggests the formation of bimetallic Pd-Au nanoparticles on the surface of TiO2 responsible for the increased H2 evolution rates. Using higher resolution instrumentation, such as synchrotron XPS, XAS and HR-STEM, we further probed the question of 'what is the Pd-Au nanoparticle structure (random, core-shell, ordered binary alloy)?' Synchrotron Pd 3d and Au 4f XPS data (hν = 1486.7 eV) confirmed the presence of Pd(0)-Au(0), whilst HR-STEM/EDS showed Pd-Au nanoparticles of size 2-5 nm composed of randomly arranged Pd and Au atoms with a near 1:1 atomic ratio. Pd K-edge and Au L3-edge EXAFS analyses found the onset of alloy formation to occur around 160 °C in a 1 vol.% H2 atmosphere and nearest neighbour Pd-Au bond lengths of 2.08-2.35 Å were intermediate to that of Pd and Au metal in good agreement with HR-STEM data (Figure 1). Results here guide the rational design of new and improved M/TiO2 photocatalysts for H2 production.
Figure 1. A-HRTEM, B-STEM-EDS, C-Pd and D-Au L3 FT-EXAFS.
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Low Emittance Electron Beams for Free Electron Lasers

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Free Electron Laser (FEL) facilities are capable of producing a peak brightness 10 orders of magnitude above 3rd generation light sources, with 10^{11} to 10^{13} photons per pulse. With ultra-fast pulse durations of 100 fs down to <10 fs, these FELs are capable of imaging structures at the molecular and atomic size level and investigating dynamical processes over timescales that take place on the order of femtoseconds. In order to achieve the high current values required for FEL lasing, strong bunch compression is required, which often results in double-horned current profile structures. These current spikes are responsible for large Coherent Synchrotron Radiation (CSR) production and the consequence is significant transverse projected emittance growth. The Linac Coherent Light Source (LCLS) has reported improved FEL performance from collimating the head and tail current spikes. In this paper we present a technique of CSR-suppression which involves including higher order magnets within the bunch compressors, to ultimately produce higher brightness photon beams.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 164

The design and synthesis of stabilised classical and non-classsical Platinum(IV) pro-drugs for targeted drug delivery

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Platinum(II) based anti-cancer drugs are the most successful class of chemotherapy drugs in clinical use and are used to treat half of all patients undergoing chemotherapy. Despite their success they are often associated with dose limited toxicities, severe side effects and drug resistance.[1-3] Platinum(IV) complexes are a promising class of pro-drugs which may bypass the problems associated with their platinum(II) counterparts. However, any pharmacokinetic advantages conferred by the platinum(IV) oxidation state is often lost due to the rapid reduction of these complexes en route to the tumour site.[4] Recently, Zhang et al. reported that platinum(IV) complexes containing cis-diamminetetracarboxylato coordination sphere exhibited unusual stability to reduction by L-ascorbate that did not correlate with their electrochemical reduction potential.[5] In this study, we further investigate the influence and relationship of structure, coordination and geometry on reduction stability, mechanism and metabolism of classical and non-classical platinum(IV) complexes in a range of endogenous and biological reductants and biological environments, using various spectroscopic and biological techniques such as XANES, SXFM, XRF μCT, 1D and 2D NMR and GF-AAS. Recently, we have reported reduction stability exhibited by cis diamminetetracarboxylato platinum(IV) complexes, using 1H NMR and XANES spectroscopy. Interestingly, this class of platinum(IV) complex appears to be usually stable to reduction in the presence of excess endogenous reductants but are rapidly reduced within DLD-1 human colon cancer cells.[6] Finally, we report several design and synthetic strategies for the development of targeted drug delivery for classical and non-classical platinum(IV) pro-drugs. These preliminary results potentially provide insights into the development of new design strategies for platinum(IV) based chemotherapeutic therapies that have enhanced reduction stabilities in the extracellular environment; such as the blood stream, but are easily and selectively activated at the tumour site.

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Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 267

Structural and Functional Insight into the Epigenetic Regulator SMCHD1

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Structural Maintenance of Chromosomes flexible Hinge Domain-containing 1 (SMCHD1) is a non-canonical SMC protein that plays critical roles in epigenetic regulation. Recently, heterozygous loss of function mutations in *SMCHD1* were identified in facioscapulohumeral muscular dystrophy (FSHD) patients, leading to failure of epigenetic silencing of the disease-causing gene *DUX4* in muscle cells. While the importance of SMCHD1 is well-described, there is limited understanding about how SMCHD1 protein mediates epigenetic control at the molecular level.
We performed small-angle X-ray scattering (SAXS) studies of the two recognisable domains of SMCHD1, namely the SMC hinge domain that is responsible for nucleic acid binding and the putative GHKL ATPase domain. We demonstrated that the hinge domain of SMCHD1 assembles into an unconventional dimeric arrangement flanked by intermolecular coiled-coil. Furthermore, we showed the N-terminal region of SMCHD1 that encapsulates the ATPase domain grossly resembles the crystal structure of full-length Hsp90 protein. Importantly, we found the ATPase domain of SMCHD1 is catalytically active. Therefore, similar to Hsp90's ATP-binding dependent conformational changes, we envisage that SMCHD1 dimer may undergo energy-dependent conformational changes to engage with chromatin. Additionally, ongoing characterisation of recombinant proteins incorporating patient-derived *SMCHD1* mutations have provided potential explanations for the underlying pathogenesis. Finally, our study has formed the basis of exploring activation of SMCHD1 as a potential therapeutic treatment for FSHD.

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Ni/TiO2 - Low Cost Photocatalysts for Solar H2 Production

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This work targets the development of efficient metal co-catalyst modified titania photocatalysts for alcohol photoreforming to H2 that function under direct sunlight. Conventionally, noble metals such as platinum, palladium or gold have been used co-catalysts to activate TiO2 for hydrogen production, though the use of such co-catalysts for industrial scale H2 manufacture is not feasible due to their high cost and low natural abundance, motivating the search for low cost alternatives. This study compares the performance of 3 different Ni/TiO2 photocatalysts for H2 production in alcohol-water mixtures, placing particular emphasis on the role of the TiO2 support and alcohol sacrificial reagent. P25 TiO2 (85% Anatase, 15% Rutile), isolate anatase from P25 TiO2, isolate rutile from P25 TiO2, commercial brookite and physical mixed P25 TiO2 were used as the support phase. XPS and Ni L-edge NEXAFS analyses verified that metallic Ni was the dominant nickel species in the near surface region of the photocatalysts. Ti L-edge NEXAFS spectra show L3-edge and L2-edge features with two sublevels (t2g and eg) which arise from crystal-field splitting caused by the octahedral ligand fields about the Ti4+ cations. The difference between the three TiO2 polymorphs (anatase, rutile and brookite) was seen in the eg feature at the L3 edge, which is split into two unresolved components (i.e. dz2 and dx2-y2 states). This change in the relative intensity of the dz2 and dx2-y2 peaks on going from anatase to rutile is explained by distortion of the Ti4+ site from D2h (in anatase) to D2d (in rutile). For brookite, the dz2 and dx2-y2 peaks have similar intensities. These observations are in good

accord with Ti L-edge data reported for mineral and synthetic titanias (Fig. 1). The Ni/P25 TiO2 photocatalysts were very active for H2 production in 10 vol.% alcohol-water mixtures under UV excitation, with the optimal Ni loading being ˜0.5 wt.%. Ni/anatase and Ni/physical mixed P25 photocatalysts showed a diminution in the photocatalytic H2 production performance, which confirmed the importance of interfacial electron transfer at the rutile:anatase interface.

Concurrent Session 1: Earth & Environment / 217

RADIOACTIVE PARTICLES AS CONCENTRATED SOURCES RELATED TO UPTAKE AND DOSE IN MAMMALS

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The radiological residues at the former weapons testing sites in Australia, at Maralinga, Emu and the Monte Bello Islands, often occur in particulate form ("hot particles"). Large numbers of these particles were emitted from nuclear test detonations and non-nuclear tests. For example, more than 3000 readily identifiable particles can occur in the soil of a single square meter, in a plume that extends for tens of kilometres at the Taranaki site (Maralinga). The physical and chemical characteristics of these particles affect their mobility and availability for uptake into living organisms. These particles, which are weathering slowly, may contain long-lived radionuclides (e.g. 239Pu) and thus will provide persistent sources of smaller, more readily respirable hot-particles, as well as ionic forms of radionuclides, for many thousands of years. From these Australian sites, we have gathered a series of particles that have weathered and interacted with the environment for 50+ years since their initial formation and release events. The particles are being evaluated using a range of methods including gamma spectrometry, PSL autoradiography, Accelerator Mass Spectrometry analysis (AMS), leaching studies, and X-ray fluorescence microscopy (XFM) at the Australian Synchrotron. Significant findings include the clustering of 137Cs on the exterior of a glassy fission fragment, with 90Sr occurring in the nearby interior, suggesting the 137Cs may be more available for weathering processes, and the beta emissions from the 90Sr may be largely self-shielded within the particle. In contrast, a different particle from a nearby site lacked any fission products, but contained Pu(IV) oxyhydroxides, consistent with weathering in a semi-arid environment. The 239Pu would impart significant dose to nearby tissue. However, XFM data, including X-ray absorption near edge structure (XANES), and extended X-ray absorption fine structure (EXAFS) indicate particles with a "core-shell" structure, with most Pu(IV) oxyhydroxide clustered in the core surrounded by an external layer containing Ca, Fe, and U. Detailed dose modelling suggests most of the alpha emissions from particles $> 5\mu$m are self-shielded within the particles themselves, and therefore impart lower dose than the equivalent dissolved Pu. However, when Pu exists on exterior surfaces, a hot particle that has been internalised (e.g. lodged in a mammalian lung) may produce relatively intense dose rates to adjacent tissues.

Concurrent Session 2: Advanced Materials II / 197

Biomimetic nanostructured lipidic materials for encapsulation of therapeutic proteins

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Proteins and peptides represent the fastest growing class of pharmaceuticals with application as drugs, vaccines and diagnostics. However, they present significant challenges for drug delivery due to their complexity and fragile nature. Hybrid protein-lipid materials are highly prospective bionanomaterials for the long-term storage and controlled release of therapeutic proteins and peptides. The lipid nanostructure offers the potential for targeted and controlled release of the bioactive molecule, while retaining the protein in a functionally active form. In order to advance the use of such materials we must understand the relationship between the nanostructure of the lipidic material, the encapsulated protein and their end use in drug delivery. The research presented aims to elucidate the fundamental physicochemical interactions between encapsulated proteins and peptides and lipidic materials suitable for drug delivery. In order to screen the large compositional space associated with the design of such materials, the project makes use of high-throughput methodologies, and employs large national and international facilities such as the Australian Synchrotron, the Bragg Institute and ASTRID 2 synchrotron, Denmark. The impact of encapsulated protein on the lipid nanostructure has been determined for a wide range of proteins and peptides. In addition the effect of the lipid nanostructure on the conformation and activity of the proteins has been determined directly within the lipidic material. Small-angle neutron scattering data on contrast matched lipidic materials has allowed the determination of protein location within the material for the first time. Results presented will guide the development of novel lipidic materials for the encapsulation and controlled release of protein and peptide based therapeutics.

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Multilayer Gratings – New Possibilities for Efficient, Flexible, Monochromators in the Tender X-ray range from 1.5 to 4 KeV

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The higher and lower ends of the "Tender" X-ray region are not well defined in photon energy but the core of the range can be considered to be the point at which the two common X-ray monochromator types start to swop over; at present that swop over point is between 1.5 to 2 KeV. The two common monochromators are the double crystal monochromator (DCM) and the grating monochromator. The DCM relies on the availability of perfect single crystals cut to give diffracting planes with suitable lattice spacing such that a single photon energy is diffracted, with very high efficiency (60 to 90%) at angles between 3 to 80 degrees. For the lower photon energies the perfect single crystal has to work at very large angles close to normal incidence and at least for the first crystal generally has to absorb a very high power load without distorting or breaking down. For synchrotrons the only materials that work well in DCMs are semiconductor crystals, for silicon the lowest photon energy that could be monochromated is around 2 KeV. For grating monochromators they rely on the fact that X rays will reflect off a surface with efficiencies in the range 60 to 90%, if the X-ray angle of incidence to the surface is sufficiently shallow. The high reflectivity of the surface is a function of the photon energy, the angle of the surface and the total effective electron density of the material of the surface. To push towards higher photon energies the incidence angle of the surface has to be less than 2 degrees and the surface is generally coated with platinum, gold or rhodium. The monochromation is made by a single reflection grating that can have efficiencies in the range 30% at low photon energies to 5% above 2 KeV, Recently multilayers have been applied to gratings that can increase their total efficiency from 5% to over 50%. This allows grating monochromators to have efficiencies that are similar to DCMs and they become much more competitive in the range from 1.5 to 3 KeV, this could become the monochromator of choice in the range 2 to 3 KeV.

Concurrent Session 1: Earth & Environment / 170

Uranium (VI) absorption by tree bark in a column leaching experiment

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The relationship between uranium (U) and organic matter (OM) has received increasing attention in the fields of mining and remediation. Sediments and wetlands with high (%) OM content can accumulate U from groundwater, and over geological timescales lead to ore formations. The Mulga Rock deposit (13K tonnes of U) near Kalgoorlie, WA is one example in Australia, with many other examples found globally. Despite many occurrences of U-OM deposits, U accumulation within the OM is not yet fully understood. Initial mechanisms may include; U sorption, cation exchange and bonding to carboxyl, phenolic or hydroxyl functional groups. Sorption may later be followed by reduction of the U(VI) to more insoluble U(IV) for more permanent U fixation. The aim of this work was to test the sorption efficiency of U onto solid OM and examine the material for change in U speciation and reduction of the uranyl ion by means of a column experiment. Ground up tree bark (TB) from *Eucalyptus Globulus* was selected for the solid OM fraction due to its well characterized phenolic and carboxylic groups for binding to uranyl-type compounds. A comparison control was comprised of quartz-sand only. For the experiment 80 mg/L U(VI) uranyl nitrate was passed through columns containing either sand, or sand with 20% TB (S-TB) at a rate of 1.25 mL/min. Outflow was monitored using in-situ probes (EC, pH, ORP) to obtain breakthrough curves and fractions collected every 6 minutes for U concentration. Breakthrough curves were more retarded in S-TB columns compared to sand only. U concentration of collected liquid fractions was ˜ppb or not detected, implying high U retention by the S-TB. Furthermore, XFM images and XRF analysis revealed that U sorption occurred within the first third of the column. XFM also revealed that sorption occurred to OM in preference to quartz-sand. XAS-XANES analysis (U L3 edge) determined no change in U oxidation state on subsamples for either sand or S-TB. The U:Ca relationship, obtained from XRF on S-TB subsamples, was negative where U had absorbed within the column, and could be suggestive of ion-exchange. These results show that eucalyptus tree bark is a powerful absorbent for soluble uranium nitrate and provides a suitable solid organic material for use in U deposit formation and remediation studies.

Concurrent Session 4: Radiotherapy II / 263

Treatment planning for synchrotron microbeam radiotherapy

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Introduction
Synchrotron microbeam radiation therapy (MRT) is a novel radiotherapy modality with significant clinical potential. We have produced a simple dose calculation algorithm for MRT using the Eclipse Treatment Planning System (TPS), by Varian Medical Systems.

Method
The calculation engine in Eclipse was configured to directly evaluate 'peak' doses. Monte Carlo-simulated Peak-to-Valley Dose Ratios were used to obtain the 'valley' dose displayed in Eclipse. We compared dose profiles generated by Eclipse with Geant4 Monte Carlo simulations and measurements from the Imaging & Medical Beamline at The Australian Synchrotron. We also performed a plan comparison study using anonymised patient datasets, comparing kilovoltage MRT plans with clinical megavoltage treatment plans.
Results
The Eclipse TPS performed well in calculating 'peak' doses in a water phantom. Considering the simplicity of the algorithm, the 'valley' dose and field profiles were also produced with reasonable accuracy, albeit with some underestimation of the valley dose for larger field sizes.
Compared to the clinical megavoltage treatment plans, MRT plans demonstrated adequate target coverage whilst meeting normal tissue dose constraints when target volumes were small and relatively superficial. As expected, planning goals for deep seated tumours and target regions distal to bone could not be met using MRT.
Conclusion
There are real advantages to using the familiar environment of Eclipse with a new radiotherapy paradigm such as MRT. Although, there are limitations to our MRT calculation engine in Eclipse and further work is required, the data generated in this work are overall encouraging and indicate that the potential for this calculation engine to be implemented in the future as part of a Phase 1 clinical trial.

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X-ray Fluorescence Microscopy at the Australian Synchrotron

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The spatial distribution of metals can provide key information for a range of studies. Metals are key to virtually every aspect of life, including health, culture, society, nutrition, and technology. This poster will outline the fundamental concepts in X-ray Fluorescence Microscopy, providing points of departure for understanding the method and its application. We actively encourage prospective users to visit the poster to discuss their research and the possible use of XFM to add value to that work.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 225

Fluorinated NDI-based copolymers acceptors for efficient all-polymer solar cells: Morphology and Photo-physics

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All-polymer solar cells employ an electron deficient conjugated polymer as an acceptor in lieu of the ubiquitous fullerene acceptor. All-polymer solar cells have seen a steady rise in efficiency

over the past few years going from about 2% to 8.3% with the development of new donor and acceptor polymers. All-polymer solar cells have certain advantages over their fullerene counter parts in terms of tunability, morphological stability and possible cost benefits. It is due to these reasons that the study of various aspects like morphology, physics and chemistry of all-polymer systems is garnering more attention amongst the research community. With an aim to further the development of polymer acceptors, we have developed and studied three new candidates P(NDITPhT), P(NDITF2T) and P(NDITF4T). These polymers are analogous to the well-studied P(NDI2OD-T2), with P(NDITPhT) possessing a phenyl ring between the two thiophene units, and P(NDITF2T) and P(NDITF4T) possessing fluorinated phenyl rings with increasing degrees of fluorination. When paired with the donor polymer PTB7-Th, we find that the overall power conversion efficiency (PCE) increasing with increasing degree of fluorination despite a systematic decrease in open-circuit voltage. With further optimisation of molecular weight, an efficiency of up to 5.5% is achieved with P(NDITF4T) as the acceptor, higher than that achieved with the benchmark P(NDI2OD-T2) (4.5%). The effect of fluorination of the morphology is studied using synchrotron techniques such as GIWAXS, NEXAFS spectroscopy and RSoXs and lab based AFM and TEM. Photo-physics is employed to discuss the effect of morphology on charge generation and geminate recombination in these blend. The effects of fluorination on morphology and the subsequent charge generation is discussed.

Concurrent Session 3: Radiotherapy I / 200

Breast cancer rotational radiotherapy with synchrotron radiation

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In 2012, J. Boone proposed the external-beam kilovoltage radiotherapy of the breast cancer with a dedicated setup adopting an orthovoltage X-ray tube 1 rotating in full circles around the breast, with the woman in prone position. For comparison, conventional radiotherapy for breast cancer adopts a medical linac irradiating the breast with tangential beams, in supine position: the megavoltage X-ray beam produces a buildup effect for skin tissue sparing. We propose a new technique for image guided rotational radiotherapy of breast cancer for the pendant breast (SR-EBRT), using a synchrotron radiation (SR) collimated beam [2,3]. The use of the high-flux monoenergetic SR beam permits to obtain dose delivery times comparable to the one of conventional radiotherapy, and to select the optimal photon energy, in a parallel beam geometry. The same setup may produce breast CT scans for tumor 3D localization and beam centering. We carried out a proof-of-principle study of the SR-EBRT technique at the Imaging and Medical Beamline (IMBL) of the Australian Synchrotron (AS). The experimental plan included dose distribution measurements with TLDs, radiochromic films and ionization chambers in cylindrical PMMA and PE phantoms, at 60 keV. This study showed a 7:1 tumor-to-skin ratio and the possibility of realizing dose-painting by multiple rotations. SR-EBRT with SR beam could be adopted for partial irradiation, dose painting, and whole breast irradiation with a skin sparing effect close to that of orthovoltage EBRT at 320 kVp and the potential for high-resolution image-guided radiotherapy. A further investigative goal is SR-EBRT at low energy (60-100 keV) coupled to gold nanoparticles or iodine contrast agent for dose-enhanced breast SR-EBRT.
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Concurrent Session 1: Earth & Environment / 215

Synchrotron Tomography in Geotechnical Engineering Applications

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Synchrotron Radiation-based X-ray Micro-Computed Tomography (SR-μCT) is a leading edge technology allowing unprecedented grain-scale observations helping with a better understanding of geomaterial behavior. The higher energy level used in this technique allows rapid scanning of geomaterials under high stress levels to study the progress of crushing and crack propagation. This paper demonstrates and discusses application of synchrotron tomography of geomaterial in two different applications in field of energy geotechnics.
A new loading apparatus was developed to conduct compression tests of up to 61 MPa on geomaterials including assemblies of different particles. The equipment allows for studying particle breakage in granular assemblies under different loading sequences to be monitored and analyzed. Experiment results completed at Imaging and Medical BeamLine (IMBL) suggest particle shape as a noteworthy factor controlling degree of crushing in a granular assembly. Test results also indicate the changes in particle-scale characteristics such as morphology evolution of sand specimens due to breakage.
The apparatus was later equipped with a contact thermal conductivity sensor enabling measuring thermal conductivity properties of a range of geomaterials under different states of stress and crushing. Heat conduction is of critical importance in geotechnical engineering applications such as geothermal systems. Though largely overlooked, microstructural properties govern heat flow in geomaterials. A numerical heat flow simulation is highly desirable because it reveals the intimate relation between microstructure and the bulk macro-scale thermal (conductivity) properties used in engineering design applications. Development of such a model, however, has historically been hampered by lack of access to image data of real geomaterials and the effect of imperfect real grain contacts. The equipment developed and test results conducted at IMBL in the Australian Synchrotron addresses these shortcomings through the use of high-resolution 4D imaging and a new grain contact correction factor.
Test results suggests how synchrotron tomography can be used to study the change in micro structure of soils and aggregates and how it can help in bridging the knowledge gap between micro and macro behavior of geomaterials.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 214

Structural characterization by Small Angle Scattering suggests models for monomeric and dimeric forms of full-length ezrin

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Ezrin is member of the ERM (Ezrin-Radixin-Moesin) family of proteins that have been conserved through metazoan evolution. These proteins have dormant and active forms, where the latter links the actin cytoskeleton to membranes. ERM proteins have three domains: an N-terminal FERM (band Four-point-one ERM) domain comprising three subdomains (F1, F2 and F3); a helical domain; and a C-terminal actin-binding domain. In the dormant form, FERM and C-terminal domains form a stable complex. We have determined crystal structures of the active FERM domain and the dormant FERM:C-terminal domain complex of human ezrin. We observe bistable array of phenylalanine residues in the core of subdomain F3 that is mobile in the active form and locked in the dormant form. As subdomain F3 is pivotal in binding membrane proteins and phospholipids, these transitions may facilitate activation and signaling. Full-length ezrin forms stable monomers and dimers. We used small-angle x-ray scattering to determine the solution structures of these species. As expected, the monomer shows a globular domain with a protruding helical coiled-coil. The dimer shows an elongated dumbbell structure that is twice as long as the monomer. By aligning ERM sequences spanning metazoan evolution, we show that the central helical region is conserved, preserving the heptad repeat. Using this, we have built a dimer model where each monomer forms half of an elongated anti-parallel coiled-coil with domain-swapped FERM:C-terminal domain complexes at each end. The model suggests that ERM dimers may bind to actin in a parallel fashion.

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Coordination Polymers from Amine-Based Ligands

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By directly incorporating amine functionality into the ligand, the adsorption of CO2 into porous coordination polymers has been shown to be increased in comparison to the unfunctionalised frameworks. Using small polyamines such as diethylenetriamine and 1,4-bis(aminomethyl)benzene to synthesise the ligands N,N[U+02BA]-(4-carboxybenzyl)-N,N′,N[U+02BA]-(carboxymethyl)-diethylenetriamine (H5L1) and N,N′-di(4-carboxybenzyl)-1,4-bis(aminomethyl)benzene (H4L2), which contain tertiary amines along the core of the ligand. Both L1 and L2 ligands are able to form three-dimensional coordination polymers which contain moderate solvent free void volumes. The framework poly-[Cd3(L1)(OH2)]·2H2O contains 1D square solvent channels with 23 % void volume, a CO2 uptake of 66 cm3/g at 273 K and maintains crystallinity in water. The framework poly-[Cd2(L2)(OH2)] contains 1D hexagonal solvent channels with 37 % void volume.

Concurrent Session 2: Surfaces / 254

The new RAIRS system at the THz/Far-IR Beamline - Laboratory Astrochemistry.

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The second half of 2016 has seen the completion of a bespoke experiment installed at the THz/Far-IR Beamline. Funded by the ARC through CI Ennis' DECRA project, the apparatus has been designed for dual-purpose Matrix-Isolation and Reflection-Absorption Infrared Spectroscopy studies. A chamber sitting within the beamline's Bruker FTIR sample compartment reaches high-vacuum by differential pumping. This chamber supports the second-stage of a compressed helium cryocooler where the mounted sample surfaces (either IR transmission windows or polished metal substrates for reflection studies) can be cooled to 10 K. Low temperature chemical vapour deposition methods are used to deposit thin films of molecular ices where their morphologies can be controlled by annealing the solid. Alternatively, inert matrices of noble gases containing reactive radicals and intermediates could be produced by electric discharge or photolysis of the deposition gas stream. 270 degree rotation of the coldhead allows for sequential 'sample deposition/spectrum acquisition' for temporal film growth studies, as well as allowing for transmission and grazing angle measurements to be performed on the same instrument.
Initial experiments will interrogate the physical and optical properties of thin nitrile films. Small nitrile molecules, such as hydrogen cyanide, acetonitrile, and propionitrile have all been identified in their condensed phase within the cold atmosphere of Saturn's largest moon Titan. The product of ongoing photochemical and fast particle processing of nitrogen and methane in the ionosphere, nitrile species transport to lower altitudes. Here, they can condense as icy layers on the surfaces of haze particles, where the layer morphology is specific to the physical conditions present at the atmospheric location. The condensed-phase also act as sites where higher-order chemistry can unfold more efficiently than the gas – such as complex cyanide chemistry pathways thought to lead to amino-acid synthesis in cold, extra-terrestrial environments.
This talk will introduce our first forays into laboratory astrochemistry at the Australian Synchrotron; connecting previous aerosol experiments to our current thin-film work on nitrile ice morphology. Also highlighted will be new DFT methods (using computationally lenient code Crystal14) that have returned accurate vibrational frequencies, particularly for intermolecular translation and libration modes associated with the far-IR for molecular crystals. Finally, the capabilities of the new RAIRS system will be detailed to promote its use amongst the infrared beamline community as an additional accessory for low temperature analysis of the condensed-phases.

Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 255

Mirror, mirror in the vacuum tank; an MX2 optics upgrade

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The micro-crystallography beamline, MX2, depends on three mirror elements for conditioning and focussing the beam at the sample position. One of these, the Microfocussing Horizontally Focussing Mirror (MHFM) is showing signs of beam damage. A likely source of this damage is the high-voltage piezo bender bimorph system used to shape the mirror.
This manifests as significant structure in the beam, as well as greatly reduced transmitted flux from one of the three substrates that coat the mirror surface (Pt, the other two are Si, and Rh). All three substrates, however, are showing signs of staining and distortion.
Further damage to the Rh-stripe, or a failure of the bimorph, would render the beamline inoperable as a microfocus instrument.
The planned upgrade will greatly mitigate this risk, simplify beam conditioning and setup, and bring beam steering closer to the sample postion. Additionally, these changes will allow for a smaller and hotter beam.

Concurrent Sessions 1: Biological Systems / 280

The shape of things to come: Resolving biological and palaeontological mysteries using microCT imaging

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The shape and structure of animals is fundamental to their survival, including how they move and feed: bone shape determines how forces are transmitted from muscles during running and flying, and the microstructure of a tooth dictates whether it will break when crushing food. Our ability to adequately capture the fine-scale 3D structure of biological materials has until recently been very limited, severely restricting the questions we could ask about modern and fossil animals. With the extensive availability of synchrotron and laboratory X-ray microcomputed tomography (microCT), we can now peer inside structures with astounding fidelity, revealing not only what is inside but also how many of these components work. MicroCT has the great advantage of allowing internal imaging of unique and irreplaceable fossil specimens that would otherwise need to be examined using destructive techniques. In this talk I will give examples illustrating the importance of microCT imaging to a range of biological and palaeontological questions. As X-ray imaging relies on differences in electron density among materials, it is most effective for imaging mineralised structures, including bone and teeth, as well as fossils. MicroCT has been used to reconstruct the anatomy of Australian fossil dinosaurs, mammals and reptiles, including the Victorian fossils of the ornithopod dinosaur *Leaellynasaura* and the Cretaceous mammal *Ausktribosphenos*. We have also learned a great deal about some of the earliest multicellular life and the earliest vertebrates (conodonts) from microCT imaging. Demonstration and exhibition of the tiniest fossils is now immensely easier with high-resolution 3D printing based on the microCT data. New advances in microCT allow high-resolution imaging of soft tissues using contrast agents that differentiate tissues, and we can use this to investigate development and evolution in embryos and juvenile animals. The data from quantitative 3D imaging can be the basis of new shape analyses, including the evolution of complexity in animals and predicting the shape of undiscovered fossils.

Concurrent Session 3: Imaging - Sponsored by MASSIVE / 161

Quantified, multi-scale element mapping of geological samples using the Maia detector array

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Studies of ore systems require microanalysis of samples to gather information on mineral chemistry. Information from in-situ microcharacterisation studies can be used both to recognise mineral zonations and chemical relationships among mineral phases that provide a record of hydrothermal activity, fluid chemistry and fluid-rock reactions. Such information is vital in constraining the physio-chemical conditions during ore genesis and mineral alteration.

The Maia large solid-angle detector array on the X-ray Fluorescence Microscopy (XFM) beamline at the Australian Synchrotron is capable of collecting high-resolution images of up to ∼100 M pixels in size with dwell times of less than 0.2ms per pixel. Thus it is possible to document variation in mineral textures associated with trace element chemistry by collecting quantified elemental maps of geological samples on the scale of entire thin sections (5x2.5 cm) in a short time frame (6-8 hours). The analysis is non-destructive and allows variation to be recognised on centimetre scale while also recognising zonations at the micron scale.

The large area scanning capability and the geometry of the Maia Detector array have also led to this technique becoming an effective tool for rare phase detection; a result of the penetrating

power of synchrotron X-ray radiation and the consequent ability to image small grains within a sample volume (Ryan et al. 2014). The use of synchrotron radiation increases by ˜70 times the chance of intersecting rare phases compared to conventional 2D techniques such as SEM (Godel 2013).
Two case studies show-casing these different applications of the Maia imaging approach to geological materials are presented: (1) an investigation of the microstructural and microchemical changes characteristic of large-scale fluid pressure cycling in vein-hosted high grade gold mineralisation; (2) a study of primary cumulus platinum minerals to understand magmatic microenvironments.

Concurrent Session 3: Imaging - Sponsored by MASSIVE / 272

Quantified, multi-scale element mapping of geological samples using the Maia Detector array

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Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 283

Structural Insights into the Assembly and Regulation of Distinct Viral Capsid Particles

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The assembly and regulation of viral capsid proteins into highly ordered macromolecular complexes is essential for viral replication. Recent reports have elucidated the ability of capsids to switch between T1 and T3 symmetry, however little is known regarding how capsid proteins can switch between smaller, non-icosahedral macromolecular complexes. Here we utilize crystal structures of the capsid protein from the smallest and simplest of all known viruses capable of autonomously replicating in animal cells, circoviruses, to establish structural and mechanistic insights into capsid morphogenesis and regulation. The beak and feather disease virus is responsible for infecting critically endangered parrots, and remarkably, like many circoviruses, these viruses encode only two genes, a capsid protein, and a replication initiation protein. The capsid protein forms distinct macromolecular assemblies during replication and here we elucidate these structures at high resolution, showing that these complexes reverse the exposure of the N-terminal arginine rich domain responsible for DNA-binding and nuclear localization. We show that assembly of these complexes is regulated by single-stranded DNA (ssDNA), and provide a structural basis of capsid assembly around single stranded DNA, highlighting novel binding interfaces distinct from the highly positively charged N-terminal ARM domain. These structures of the world's smallest viral capsid assemblies serve as an important basis for enhancing our understanding viral capsid assembly and regulation.
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Concurrent Session 3: Industry & Innovation / 284

FACTORY OF THE FUTURE: COMPOSITE AUTOMATION AND GRAPHENE CERTIFICATION FACILITY

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Swinburne's Factory of the Future is located in the recently opened $100 million Advanced Manufacturing and Design Centre at the university's main campus in Melbourne, Australia. The Factory of the Future is one of three pillars of Swinburne's newly launched Innovation Precinct which emphasises design and digital technologies to tackle manufacturing challenges, and pilot production and fabrication processes developed in collaboration with industryThis facility is an intentionally designed platform to demonstrate to Australian manufacturers the principles and benefits of Industry 4.0 concepts and will exploit Swinburne's emerging strengths in composite materials and existing strengths in design, visualisation, robotics, automation and big data.
This presentation will describe the current capabilities of the Factory of the Future and will highlight the future directions for the development of the first Graphene Certification Facility to connect Australian industry into global advanced manufacturing supply chains that use graphene. There are currently several hundred companies producing or using graphene in their products. Industrial consumers of graphene require material produced at scale that is of replicable quality that meets their specific application needs. There is an urgent need for collaboration across the supply chain to develop standard certification processes that are end user centric, ensuring advanced materials containing graphene are sufficiently well characterized to enable proven supply chain management processes to be followed. The facility will conduct the foundation research required to identify the analytical tools that can be routinely applied to certify graphene products, enabling companies to validate their supply chains.
The facility will utilise significant infrastructure and expertise at the Australian Synchrotron with special focus on SAXS/WAXS and XFM techniques. These techniques are critical for informing different stages of graphene manufacturing such as isolation of graphene from the starting material, to intermediates, and the final product. X-rays can quantitatively inform the success of exfoliation or intercalation of graphene and is particularly useful to demonstrate functionalization. The Swinburne/Synchrotron partnership will play a key role in building unique insight into the translation of research-based characterisation into the manufacturing sector, which in turn will be able to impact the wider advanced materials industry.

Concurrent Session 4: Radiotherapy II / 209

Microbeam Dosimetric Verification using Presage® Dosimeters

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Dosimetric properties of synchrotron microbeams are extremely difficult to measure due to the small field sizes employed (typically 50 um width with 200 – 400 um peak-to-peak spacing) and must undergo rigorous validation before patient treatments can be performed on the IMBL.
The radiochromic PRESAGE® dosimeter offers a unique opportunity to validate dosimetry models in 3D with similar radiological responses to water over a wide energy range that includes synchrotron energies for SSRT and MRT treatments.
Our previous work on the IMBL verified the dosimetric properties of synchrotron beams with ion chamber measurements, radiosensitive film and Monte Carlo simulations for SSRT beams using 3D optical CT on water-equivalent PRESAGE® dosimeters.

In this work Laser Fluorescence Confocal Microscopy (LFCM) has been utilised to investigate the dosimetric properties of MRT beams with water-equivalent PRESAGE® dosimeters.

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Crystallography for soft matter – can a crystal be soft and alive?

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Diffraction is a standard technique to study crystal structure, alignment, texture and grain structure in hard matter. The important role of neutron diffraction in (hard) materials has been cemented by the penetrative and non-ionising nature of neutrons allowing non-destructive measurements in quite unusual sample environments, the sensitivity of neutrons to thermal motions, and the opportunities for isotopic studies. Similar issues arise in soft matter, where material properties (e.g. mechanical functioning, transport properties, internal surface, optical properties etc) are highly influenced by analogues to these quantities formed by the arrangements of ensembles of molecules, often in a solvent, such as amphilipilic molecules or polymers rather than atoms. The structures formed consequentially occur at longer length-scales, and the role of thermal motions is quite different.

Concurrent Sessions 1: Biological Systems / 250

Structural changes in an elastin hydrogel during extension and drying by small angle neutron and x-ray scattering

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Èlastin is a highly elastic protein found in connective tissue of vertebrates. It has an important mechanical physiological function by virtue of its highly elastic nature, namely to provide recoil in tissue such as skin and vasculature. The structure is extremely stable being produced mainly early in life where it persists and is not replaced during a lifetime. The structure and mechanical properties of elastin is important in many pathologies. In this study we examine the structural changes in a cross-lined elastin hydrogel during stretching and drying with small angle x-ray scattering (SAXS), and with uniaxial deformation by compression in a specially designed cell, by small angle neutron scattering (SANS).
SAXS measurements from the hydrogel at rest consisted of a broad isotropic correlation peak superimposed upon an isotropic decay in intensity. We attribute the correlation peak to the interaction between monomers and the decay in intensity to the fibres formed by linking of monomers. As the free standing film is stretched the scattering pattern becomes increasingly anisotropic. For subsequent stretches the induced anisotropy becomes increasingly irreversible as the sample dries out. The position of the correlation peak moves to higher q and the different anisotropies exhibit varying degrees of reversibility during the extensional cycles. We attribute this loss of reversibility to the drying of the sample with water acting as a plasticiser. To decouple the effects of drying from extension we have measured the SANS pattern for the elastin hydrogel during many cycles. Again the isotropic scattering pattern consisting of a correlation peaks superimposed on decay. In this case, while the anisotropic scattering pattern is entirely reversible, with a small anisotropic shift in the position of the correlation peak. The role of water in the plasticisation of tropoelastin is discussed.

Concurrent Session 3: Industry & Innovation / 160

Synchrotron Industry Case Studies over 20+ years

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This presentation will provide an overview of industrial studies using synchrotron-based techniques undertaken over the past 20+ years by the presenter. The objective is to provide perspective on the wide scope of possible applications and motivations for industry participation. These applications focus mainly on minerals and materials studies and have included: • wax crystallisation from diesel fuels using in situ energy dispersive diffraction and powder diffraction at Daresbury Laboratory; • doping of titania pigments using XAS at Daresbury Laboratory and Hasylab; • gibbsite precipitation using in situ diffraction at the Photon Factory, • Cu activation of sulfide minerals using XAS at the Photon Factory, • analysis of glass lenses at the Photon Factory, • Pt speciation during refining using XAS at Anka, • Ni and U mineralogy using microprobe analyses at the Advanced Light Source and Advanced Photon Source, • Ni laterite leach residues using XAS at Anka, • analysis of Ni alloys using microdiffraction at the Advanced Photon Source; • cryogenic treatments of steels using microdiffraction at the Advanced Photon Source, • chalcopyrite and pyrite leaching using SPEM at Electra and the Advanced Light Source, • scaling in Bayer refineries using XAS at the Australian Synchrotron, A wide range of companies have provided support of these studies including Exxon, QAL, Comalco, Alcoa, Worsley, Nabalco, Biliton, Rio Tinto, BHP Billiton, Amplats, Anglo America, Cytec, State Governments and Tiwest. Examples from these studies will be presented. How to involve companies in projects involving synchrotron studies will also be discussed as will the issues limiting greater industry participation.

Concurrent Session 4: Technique Development / 155

Micro Materials Characterisation (MMC) Beamline: Scope and Focus

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Crystalline phase determination, polycrystallinity, strain, grain orientation as well as defect structure, migration and organisation are fundamental to the understanding of materials' properties. The MMC beamline is the only facility planned for the Australian Synchrotron that will enable these properties to be spatially resolved at the micron scale.
We present the current design and capabilities of the MMC beamline. In particular we highlight its extensive potential application to both the scientific and to the industrial R&D communities and to the contributions that can be made to Australia's strategic scientific and research priorities. The MMC beamline has enormous potential to provide a highly sophisticated tool that brings together industry and research.
The MMC beamline will be able to be used to address critical issues with respect to solar, high-temperature and nuclear energy materials, can enable novel studies of pollutants in the environment, can help understand geological processes, mining and mineral recovery and can even provide new information on biological materials. The reality is that the world is heterogeneous and that the micron scale is an important length scale where heterogeneities start to resolve themselves into homogeneous crystals and structures.
Synchrotron X-ray microprobes have commonly used a monochromatic X-ray beam. When the crystallite size is smaller than the incident beam size, monochromatic diffraction measurements yield either complete or fragmented Debye-Scherrer diffraction rings. These rings can provide

considerable information. However, monochromatic radiation has the important disadvantage that where the crystallite size is of the order of or larger than the beam size, few or no diffraction peaks may be measurable for a given sample and detector geometry, and hence vital information may be simply overlooked. To overcome this increasingly common circumstance a broad bandpass incident X-ray beam may be used.
The MMC beamline's key capability will be the provision of both monochromatic and Laue microdiffraction (< 1 micron) with rapid interchange between the two. This will be coupled to subsidiary capabilities of X-ray fluorescence mapping and selected area XAS. The breadth of potential application of this facility, as well as its world-class capabilities, have already been acknowledged by its international Specialist Design Committee and its very significant potential user base.

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Synthesis of Multinuclear Lanthanoid Complexes with 2-Methyl-8-hydroxyquinoline

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Lanthanoid-8-quinolinolates and its derivatives have attracted a lot of interest due to their structures and behaviour as single molecular magnets [1-3]. A few multinuclear of lanthanoid complexes with 2-methyl-8-hydroxyquinoline (HMQ) were successfully synthesized at elevated temperature using a Teflon Sealed autoclave. It was observed that heating the mixture above the boiling point of the solvent produces dinuclear, trinuclear and tetranuclear compunds as products. 1 Deacon,G. B., Dierkes, T., Hubner, M., Junk ,P. C., Lorenz., Y., and Urbatsch, A., Eur. J. Inorg. Chem., 4338–4348, 2011. [2] Deacon, G. B., Forsyth, C. M., Junk, P. C., and Urbatsch, A., Eur. J. Inorg. Chem., vol. 2010, 18, 2787–2797, 2010. [3] Chilton, N. F., Deacon, G. B., Gazukin,O., Junk,P.C, Berthold, K.,Langley,S.K., Moubaraki,B., Keith S. M.,Frederik ,S., Shome, M., Turner,D.R. ," Inorg. Chem, 53, 2528–2534, 2014
[enter link description here]https://www.dropbox.com/s/g122j9lxa9kx84s/SYNCHROTRON.docx?dl=0

Concurrent Sessions 1: Biological Systems / 173

Role of the solvophobic effect in protein-ionic liquid interactions

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Biological applications which utilise enzymes, or other proteins, require the tertiary structure of the protein to be retained. However, many proteins readily undergo aggregation or denaturation when outside their native environment, and/or over longer timescales. The stability of proteins in solvents other than water is usually considered unappealing due to an assumption that the protein will be insoluble or denatured. However, a few solvents, such as glycerol and dilute alcohols have been shown to have protein stabilising properties, such as in cryopreservation.

Previously we have developed extensive structure-property relationships between the chemical structures and mesostructures of non-aqueous solvents and the solvophobic effect experienced by amphiphiles for molecular solvents 1 and protic ionic liquids [2]. Here we have extended this to develop a greater understanding of what solvent features are important for protein stability. We have utilised a series of small polar non-aqueous molecular solvents and protic ionic liquids consisting of the four acid-base combinations of ethyl- and ethanolammonium cations paired with formate or nitrate. Solutions were prepared of these solvents combined with water, and with added formate or nitrate for the ionic liquids to explore a broad range of pH effects. For this initial work egg white lysozyme (HEWL) was used. These solvent systems enabled us to explore the effect of pH, solvent concentration, solvent cohesive energy density and polarity towards protein stability [3]. The activity of the lysozyme was assessed based on its lytic activity towards Micrococcus lysodiekticusce using UV-Vis spectroscopy. The secondary and tertiary structures of the lysozyme were determined using Small angle X-Ray scattering (SAXS) and IR spectroscopy. Protein crystallisation studies have been successfully conducted for many of these protic ionic liquid solvent systems, with significant differences in the crystal structures formed.
This work extends our understanding of protein stability in a wide variety of solvent environments, and has enabled structure-property relationships to be developed for a protein in concentrated molecular solvent and protic ionic liquid solvent systems. This work has the potential to lead to the development of tailored solvent systems to optimise protein stability.
1 E. C. Wijaya, T. L. Greaves and C. J. Drummond, Faraday Discuss., 2013, 167, 191-215.
[2] T. L. Greaves, C. J. Drummond, Chem. Soc. Rev., 2013, 42, 1096-1120
[3] Emmy C. Wijaya, Frances Separovic, Calum J. Drummond, Tamar L. Greaves, Phys. Chem. Chem., Phys. 2016, DOI: 10.1039/c6cp03334b.

Radiotherapy Workshop: Should we MRT Treat Canines / 299

What would canine MRT data bring on our way to human MRT trials?

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Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 253

Structural basis of Plasmodium vivax specificity towards reticulocytes

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Understanding the process of invasion is essential for developing strategies to stop blood stage infection. An important feature of *Plasmodium* invasion is the host cell selectivity that the different species have for cells of the erythroid lineage. Indeed, *Plasmodium vivax* preferentially invades reticulocytes which are immature red blood cells. Several members of *P. vivax* Reticulocyte Binding Protein (PvRBP) family have been shown to bind specifically to reticulocytes. One of the major unanswered questions in *P. vivax* biology is the identity of the reticulocyte specific receptor required for invasion.
We report the first crystal structures of the erythrocyte-binding domain from two members of the PvRBP family, PvRBP2a and PvRBP2b, which were solved at 2.12 and 1.71 angstrom resolution

respectively. Both structures share a strikingly similar fold with PfRh5, an essential invasion ligand in *P. falciparum* and a leading vaccine candidate for blood stage infection.
While PvRBP2a binds both mature and immature erythrocytes, PvRBP2b exhibits strong specificity towards reticulocytes. We have identified the reticulocyte-specific receptor for PvRBP2b. We characterized the ligand-receptor complex in solution using small angle X-ray scattering and analytical ultracentrifugation. We generated monoclonal antibodies toward PvRBP2b that inhibit the interaction with its receptor and solved crystal structure of reticulocyte-binding domain in complex with three different Fab fragments.
This study provides the fundamental characterization of the structural features that govern *P. vivax* red blood cell binding as a framework for generating new therapeutics and answers the long standing question of the reticulocyte-specific receptor for *P. vivax* invasion.

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Investigation of metal-organic framework materials and zeolites for advanced gas absorption mechanism

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Combining synchrotron radiation with various sample environment setups, such as capillary flow cell, we are able to understand the mechanism of gas absorption properties from MOFs and zeolites. In-situ powder X-ray diffraction (PXRD) measurements have been conducted to discover a “molecular trapdoor” mechanism for exclusive gas discrimination, which is demonstrated as an unusual operating regime for a chabazite zeolite in which the adsorption selectivity for N2 over CH4 inverts from being more selective for N2 at 253 K, to becoming less selective with increasing temperature and eventually becoming selective for CH4 over N2 above 293 K 1. PXRD also demonstrates it as an outstanding tool to reveal the novel metal organic framework (MOF) structures and monitor the progress of a new acid solvent synergistic ligand exchange (ASSLE) synthesis method. PXRD shows the case of Zn(BPDC)(BPP) (BPDC = 4,4’-biphenyldicarboxylate, BPP = 1,3-Bis(4-pyridyl)propane) incorporated an exotic flexible-ligand into a rigid pillar-layered MOF structure via structural rearrangement during ligand exchange, creating structural flexibility in the daughter material [2]. The adsorption properties of the daughter material suggest a superior gas separation performance to the parent material.
1 Shang J., Li G., Gu Q., et al. Chem. Commun., 50, 4544, (2014) [2] He Y., Shang J., Gu Q., et al. Chem. Commun. 51, 14716, (2015)

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Synthesis of lanthanoid pyrazolates by redox transmetallation utilising trispentafluorophenylbismuth

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Syntheses of high reactivity lanthanoid organometallics (Ln-C), organoamides (Ln-NR2), and aryloxides (Ln-OAr) by redox transmetallation (RT) and redox transmetallation protolysis (RTP)

reactions have been widely and successfully studied by using mercury compounds. 1 This report describes a new method to synthesize metal-organic lanthanoid derivatives by using trispentafluorophenylbismuth replacing more toxic mercury reagents. This approach is more environmentally friendly. Lanthanoid pyrazolates were successfully synthesized from lanthanoid metal, pyrazoles and trispentafluorophenylbismuth.
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Concurrent Sessions 1: Biological Systems / 242

New Secrets Unveiled from the 'Rosetta Stone' of Neuroscience: Using Synchrotron Light to Study Fundamental Neurochemistry within the Hippocampus during Health and Disease

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The hippocampus is a key anatomical brain structure required for spatial learning and memory in all mammals. The structure of the hippocampus is highly conserved between mammalian species, which highlights a fundamental importance to higher order brain function. As such, the hippocampus is one of the most studied anatomical structures in the field of neuroscience. However, much remains unknown about the underlying neurochemistry driving hippocampal function, and many refer to this brain structure as the 'Rosetta Stone' of neuroscience. Unfortunately, the hippocampus is vulnerable to neurodegenerative conditions and disorders, with selective neuron damage occurring during Alzheimer's disease, and after epileptic seizures, traumatic brain injury and stroke. Techniques available at synchrotron light sources offer the ability to study at cellular and sub-cellular resolution the distribution of important biochemical and elemental markers of normal and abnormal brain function. Specifically, Fourier transform infrared (FTIR) spectroscopy can be used to study markers of oxidative stress, such as aggregated proteins and oxidised lipids, within individual neurons of the hippocampus. Complementary elemental information is provided by X-ray fluorescence microscopy, which is invaluable for providing a wealth of information at the cellular level on ion homeostasis (Cl-, K+, Ca2+) and metal homeostasis (Fe, Mn, Cu, Zn). A multi-modal approach incorporating FTIR and XFM, in combination with histology and light microscopy enables investigation of the mechanistic pathways through which excitotoxicty and disturbed brain metal homeostasis contribute to oxidative stress and neuronal injury during disease. Specifically, this presentation will discuss recent findings regarding the underlying neurochemistry of the hippocampus during health and disease in rodent models of Alzheimer's disease, stroke, and schizophrenia.

Concurrent Session 3: Industry & Innovation / 177

New Detectors for IMBL

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IMBL Users have a range of demands for x-ray imaging detectors which cannot be met by one single instrument. For the past four years of operation we have kept a suite of six detectors to

match the foreseeable needs. As the beamline has developed in capability over time, the demands on detection have also changed. Furthermore, some of the original detectors are now getting to the end of their useful life. A recent review has highlighted the need for new and altered specifications. As a result two new detectors have been added to the IMBL imaging instrument list. One is a large field of view high aspect ratio device, designed to make better use of the wide beams in our hutch 3B. The other is a smaller field-of view photon counting detector aimed at ultra-low dose imaging. This second device also has some spectroscopic capability. Both have been tested on the beamline and are now being integrated into the IMBL control systems. Important aspects of the detectors and some test results are shown here.

Concurrent Session 3: Industry & Innovation / 207

IMBL facilities for in-vivo research

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The Imaging and Medical Beamline (IMBL) has extensive facilities for holding, preparing and performing imaging and radiotherapy experiments with animals.
Animal held and/or prepared to date

- Mice, rats, rabbits, sheep and a piglets.

Animal care

- The IMBL team includes a veterinary surgeon and we can provide excellent support to our users with anesthetics, surgery and animal care practices.

Technical - Radiotherapy

- A high-throughput dynamic micro-beam radiation therapy (DynMRT) setup for rodents is available for users.
- Image guidance and dose delivery through standard or custom conformal masks are available.
- The DynMRT setup includes a validated Patient Safety System (PaSS), an important step in our programme towards human trials.

Technical - Imaging

- Convenient and modular positioning stages are available for mice and rats.
- For animals up to 100kg the positioning is done using the robotic Large Animal Positioning System (LAPS).
- Software triggering of shutter and detector is implemented, with limited (slow) physiological triggering.
- Full physiological triggering (hardware, fast) of shutter and detector will be available in 2017. This will include dose reduction shuttering.
- *Ex vivo* Computed Tomography (CT) is available during imaging experiments if requested in advance.
- *In vivo* CT will be trialed in 2017 and developed if successful and in demand.

Technical - General

- Radiotherapy and imaging enclosures include laser beam guidance and live monitoring.
- We provide a large range of surgery, anesthetic, ventilation and monitoring (off-line and remote on-line) equipment, as well as all the drugs required for preparation and experiments.

- 2 surgeries and three laboratories are available for our users.

User training

- We recently ran a 4 days training session for potential users. It focused on small animal cannulation for contrast agent injection in micro-angiography. Targets were lung and heart, brain, rear limbs. EOIs for future training will be recorded at the poster sessions.

Our poster will describe our facilities and equipment, and present the technical side of recent *in vivo* experiments.

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Naturally Better Digestion at the AS SAXS Beamline

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Observing time resolved changes to weak signals has always been a challenge that the Australian Synchrotron SAXS beamline has been well placed to address. Recent work at the beamline has aimed to find the optimum sample environment and beamline setup for picking out weak signals from in-situ digestion experiments. Aided by some knowledge gained from the i22 beamline at the Diamond synchrotron in the UK these tests were very successful. Weak signals from dilute crystalline drug additives could be clearly seen above a significant water background signal during in-situ digestion. The results and sample environment shown here show the results that can be achieved and the straightforward considerations that need be kept in mind when planning experiments that will require the observation of weak signals.

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Rare Earth Corrosion Inhibitors using 4-(4'-Methylphenyl)-4-oxo-butanoic acid

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Rare earth 4-(4'-methylpenyl)-4-oxo-butanoate, (L) complexes [RE(L)3(H2O)] (RE = Y, La, Ce, Nd, Ho, Er) have been prepared by metathesis reactions between the corresponding rare earth chloride and NaL to assess the potentiality as new corrosion inhibitors. The products were analysed by IR- and NMR-spectroscopy, elemental- and metal analysis and TGA measurements. The single crystal X-ray diffraction studies of [RE(L)3(H2O)] (RE = Ce, Nd) and [Ce(L)3(dmso)] revealed a 1D carboxylate bridged polymeric structure in the solid state, featuring nine coordinate rare earth ions. Upon comparison with x-ray powder diffraction patterns of the bulk materials, all of the [RE(L)3(H2O)] complexes with the exception of RE = La are isomorphous, implying that no fundamental structural changes were detected from RE = Ce to RE = Er despite the lanthanoid contraction.

Plenary 2 / 166

Tuneable Materials and Material Dynamics

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Characterisation of tuneable and adaptive materials at the Australian Synchrotron has enabled an understanding of non-equilibrium processes such as solute partitioning and phase competition in alloys [1-6], architecturing of free volume in polymers [7-9], and biomineralisation of metal-organic-frameworks (MOFs) [10-16]. In situ small angle X-ray scattering (SAXS) and in-situ powder X-ray diffraction (PXRD) have been used to gain insight into the dynamic processes that lead to superior performance of materials for use as structural alloys, corrosion resistant alloys, gas separation membranes, and for use in encapsulation of biomolecules and biological units.
The talk will highlight the work of CSIRO and collaborators (all work has been advanced by Australian Synchrotron results).
Acknowledgements: The work has been supported by funding from a number of programs including CSIRO OCE Science, ARC, AS and ISAP. All of the co-authors on the publications listed below and their funding agencies are valued contributors to, and enablers of, this work. Paolo Falcaro and Raffaele Ricco are now located at Institute of Physical and Theoretical Chemistry, Technical University Graz, Stremayrgasse 9, 8010 Graz, Austria.

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Concurrent Session 1: Advanced Materials I / 262

Engineering "Disorder" : From Designing New Catalysts to Reactivity in Natural Systems

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One of the greatest challenges of the 21st century will be securing cheap and renewable sources of energy. One of the most promising approaches to this challenge is to design catalysts from earth abundant materials capable of implementing key chemical reactions including the splitting water into hydrogen and oxygen (H2O $\rightarrow$ H2 + $\frac{1}{2}$O2); the oxidation of hydrogen (H2$\rightarrow$ 2H+) and reduction (2H+$\rightarrow$ H2) of protons as well as the reduction of molecules like CO2 and N2.
Some of the most promising catalyst materials for these reactions are metal oxides and metal sulfides which commonly exist in nature. Despite the ubiquity of these materials their structures and the relationship to reactivity is often poorly understood. This may be because materials that are most reactive are often "disordered" or nano-crystalline. In our work we have been able to engineer series of metal oxides that systematically differ in their degrees of disorder. By careful correlations between XAS, TEM and reactivity we can begin to understand the effects of crystalline "order" on "reactivity". Our results point to important correlations between "sacrificial" and "catalytic chemistry" that have implications to both catalyst design and clues to a possible role these materials may have played in the evolution of metallo-protein type catalysis.

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GeoPIXE update at XFM

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GeoPIXE is the primary X-ray fluorescence analysis software used at the XFM beamline. Several new developments in GeoPIXE will be outlined, such as fitting for multiple sample matrix phases. Information will be given regarding a GeoPIXE workshop planned for 2017. User input for workshop topics is welcomed.

Concurrent Sessions 1: Biological Systems / 158

Element-specific small-angle X-ray scattering studies of mineral nanoparticles in iron-fortified milk

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Most of the dietary calcium in milk is contained within casein micelles as so-called 'colloidal calcium phosphate' (CCP) nanoclusters around 2-3 nm in size. Small-angle X-ray and neutron scattering (SAXS and SANS) have been used for several decades to study the internal structure of bovine casein micelles, but there is lingering controversy over the interpretation of the scattering data 1.
Recent synchrotron scattering experiments have shed new light on this long-standing problem. Resonant soft X-ray scattering (RSoXS) of bovine milk at the Ca L2,3-edges using beamline 11.0.1.2 at the Advanced Light Source, Lawrence Berkeley National Laboratory conclusively identified features arising from the CCP particles [2]. These measurements were supported

by experiments conducted using the SAXS beamline at the Australian Synchrotron where the milk chemistry was modified [3]. We have extended these techniques to investigate the mineral structures in iron-fortified milk, using SAXS, RSoXS (at both the Ca and Fe L2,3 edges) and anomalous SAXS (at the Fe K-edge). The results will be presented and the implications discussed in terms of developing new food ingredients; the benefits and challenges of the RSoXS and anomalous SAXS techniques will also be discussed.

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Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 282

The role of protein dynamics in the evolution of new enzyme function

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Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 264

The role of protein dynamics in the evolution of new enzyme function

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Enzymes must be ordered to allow the stabilization of transition states by their active sites, yet dynamic enough to adopt alternative conformations suited to other steps in their catalytic cycles. The biophysical principles that determine how specific protein dynamics evolve and how remote mutations affect catalytic activity are poorly understood. Here we examine a 'molecular fossil record' that was recently obtained during the laboratory evolution of a phosphotriesterase from Pseudomonas diminuta to an arylesterase. Analysis of the structures and dynamics of nine protein variants along this trajectory, and three rationally designed variants, reveals cycles of structural destabilization and repair, evolutionary pressure to 'freeze out' unproductive motions and sampling of distinct conformations with specific catalytic properties in bi-functional intermediates. This work establishes that changes to the conformational landscapes of proteins are an essential aspect of molecular evolution and that change in function can be achieved through enrichment of preexisting conformational sub-states.

Concurrent Session 3: Industry & Innovation / 258

micro-CT analysis of metallurgical coke

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Coal is a highly complex and heterogeneous material. Certain coals will convert to coke when heated in the absence of oxygen. Coke, which is a high strength reducing agent, is required for conversion of iron ore into molten iron in a blast furnace. As such, it is a key element in the steelmaking process. Annual exports of Australian coking coals amount to around A$20b. Our research has extensively utilised the Imaging and Medical Beamline at the Australian Synchrotron to obtain micro-CT images which accurately map the microstructure of different coke samples. We use these images to relate the coke microstructure to its strength and reactivity properties, which account for its quality. Insights from the work assist in identifying new ways to improve the quality of coke made from a particular coal, or blend of coals, as well as identifying ways that

models used to predict coke strength can be improved. Our research demonstrates the value of micro-CT imaging at the Australian Synchrotron as a research tool in cokemaking, helping to keep Australia at the forefront of innovation in this field as well as to maintain and extend the value of Australia's metallurgical coal resources.

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Synchrotron SAXS of Collagen Biomaterials for Industrial Applications

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The Haverkamp research group at Massey University (NZ), scientists at the Australian Synchrotron, and a number of international companies are collaborating on several research projects into collagen materials using small angle X-ray scattering (SAXS). The research advances basic knowledge by revealing the structural basis of physical properties, boosts understanding which improves industrial processes control, and then informs the development of improved new materials. This poster gives a snapshot of current projects supported by collaborating companies.

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Artificially induced collagen fibril orientation affects tear propagation in leather

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Ovine leather has around half the strength of bovine leather and is therefore not suitable for high value applications such as shoes. For leather from a variety of animals it has been found that the extent of collagen fibril alignment (orientation index) is closely correlated with the strength of the leather. We tested whether biaxial stretching for the duration of tanning or compressing pickled pelts prior to tanning the ovine skins could increase the orientation index of the collagen fibrils and the strength of the final product. Control and test ovine skins were tanned using conventional chrome tanning methods. After the pickling and bating the test skins were compressed between rollers before tanning or stretched biaxially during the tanning process. The stretch was applied was between 2.3%, 10% and 15% of the pickled pelts original length; either uniformly (10% and 10%) in both directions or with 2.3% in one direction and 7.5% in the other. Tear strengths were measured by standard methods in two directions, normal to one another relative to the backbone of the skin. Collagen fibril orientation was measured using synchrotron based small angle X-ray scattering, both edge on to the leather and flat on to the leather. The in-plane collagen fibril orientation index rose from ca. 0.45 to ca. 0.70 both with compression with rollers and biaxial stretching. With non-uniform biaxial stretching there was an increase in the flat-on orientation index. Tear strengths are affected by both the in-plane fibril orientation. Tear propagation is resisted by collagen fibrils arranged at right angles to the tear front but propagates more readily along the direction of fibril. While it was possible to increase the collagen fibril orientation, this lead to direction specific tear strength increase rather than an overall increase in the skins tear strength, which has a more complex but rational behaviour.

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Engineering disorder into heterogenite-like cobalt oxides by phosphate doping: Implications for the design of water oxidation catalysts

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Metal oxides are amongst the best known and most extensively studied water oxidation catalysts. Many metal oxide materials function best in a proton accepting electrolyte such as a borate or phosphate buffer. The inclusion of these electrolyte anions in the bulk material (in small amounts) is recognized to result in amorphous metal oxides with "molecular-like" structure. The importance of these disordered "molecular-like" metal oxides in water oxidation catalysis has been difficult to deconvolute from the effects of the electrolyte used for deposition. In this study we have synthesized as series of heterogenite-like cobalt oxides with different levels of phosphate doping (0 - 9%) and carefully characterized the materials using a range of analytical techniques including, XAS, TEM and XRD. It was found that phosphate doping systematically altered the nano-scale and molecular-level structure of the materials, with the materials changing from nano-crystalline to amorphous as the level of phosphate doping increased. The changes were correlated with reactivity for water oxidation catalysis and as sacrificial oxidants. It was found that the most disordered materials were most reactive in sacrificial reactions, however, less effective for water oxidation catalysis. The result demonstrate how subtle structural ordering effects can significantly impact on reactivity.

Concurrent Session 4: Technique Development / 249

Coflow and Fast-SEC Improvements on the SAXS/WAXS Beamline

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Small angle X-ray scattering (SAXS) is an extremely useful tool for analysing protein structures that is becoming increasingly popular. SAXS displays a number of advantages over other techniques, but radiation damage and sample consumption limit the utility of the technique to the wider protein community. Of the various avenues being pursued to circumvent radiation damage, we have focused on the dynamics of laminar flow inside capillaries because of the well-known zero flow velocity at the edge of the capillary that causes elevated radiation damage. We have modelled the dose-distribution under laminar flow in the x-ray beam profile, showing the edges receive severe over-dosing if the sample fills the capillary, which requires overall under-dosing of the sample to manage radiation damage.
We have developed a new method for SAXS which avoids this problem by limiting the sample flow to the centre of a sheath fluid which avoids the boundary condition for the radiation sensitive protein component, and acts as a barrier between the sample and the capillary wall. In practice, this approach is very effective in reducing radiation damage, allowing sensitive protein solutions to be exposed to at least 10 fold greater flux despite much lower sample flow rates. Up until this development, protein experiments had to be run at a low flux, but now the full flux of the beamline is a key limitation. There are a number of other advantages, including that biomolecule

samples do not come into contact with the capillary at all, and hence do not stick, and less samples is needed for the same degree of sensitivity, improving the efficiency of measurements. At the same time, significant improvements have been made to the size elution chromatography (SEC) setup that push the capability essentially to the limitation of SEC columns themselves. For routine samples, this can halve the measurement time, reduces the dilution in the system to that of the column itself, removes peak broadening of the SAXS measurement, allows quantitative UV measurement for normalising SEC traces by concentration during SAXS, and reduces the delay between elution off the column to SAXS to only a few seconds reducing the potential for post-column recombination to a minimum. These developments represent a major advance for the current and future solution scattering beamlines that unlocks the full capability of current beamline technology for challenging and high throughput applications for solution samples.

Concurrent Session 1: Advanced Materials I / 238

Simultaneous orientation and strain determination in polycrystals using the Maia detector

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X-ray micro-beam Laue diffraction is a powerful tool for mapping the orientation and elastic strain within polycrystalline materials. Interactions between neighbouring grains influence the macroscale characteristics of a material, particularly its deformation behaviour, damage initiation and propagation mechanisms. Here we report on recent experiments using energy scanning diffraction of a polycrystalline nickel foil at the XFM beamline using the Maia energy dispersive area detector. Using the elastic back scatter measured by the pixelated Maia detector we are able to determine local crystallographic orientation within the polycrystalline foil. Knowledge of the photon energy of specific Bragg peaks also makes it possible to determine the strain state within the sample. Here the elastic strain was mapped across the sample and the full elastic strain tensor determined. These results thus demonstrate the first steps towards simultaneous elemental, crystallographic orientation and strain imaging at the microscale.

Plenary 3 / 150

With the synchrotron and beyond the synchrotron towards the structure of the TIR-domain signallosome

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TIR (Toll/interleukin-1 receptor, resistance protein) domains are key components of innate immunity signaling pathways. They are found in animals, plants and bacteria, for example in TLRs (Toll-like receptors) and TLR adaptors in animals, NLRs (nucleotide binding, leucine-rich repeat receptors) in plants, and virulence factors interfering with immune responses in bacteria. While it has been well established that signaling depends on regulated self-association and homotypic association of TIR domains, every single TIR domain structure has revealed a different association mode 1. In the search for common features, we have targeted a number of TIR domains from mammals, plants and bacteria to characterize structurally. We used the Australian Synchrotron to determine a number of TIR-domain crystal structures and study association using SAXS, including those from the human TLR adaptor proteins MAL [2] and SARM (unpublished),

the bacterial protein TcpB from Brucella melitensis [3] and the plant immune proteins L6 from flax [4], RPS4 and RRS1 from Arabidopsis [5], SNC1 and RPP1 from Arabidopsis and MrRPV1 from grapevine (unpublished). These crystal structures have started revealing common trends in the TIR-domain association modes, in particular for bacterial and plant TIR domains. Furthermore, for the TLR adaptors MAL and MyD88, we have been able to reconstitute large assemblies and determine the structure for the former by cryo-electron microscopy (unpublished), while we are characterizing the structure of the latter by synchrotron and X-FEL-based serial crystallography. Jointly, these studies suggest a general mechanism of function of TIR domains, which involves "signalling by cooperative assembly formation (SCAF)" with prion-like features that is consistent with signaling in other innate immunity pathways.

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Concurrent Session 3: Imaging - Sponsored by MASSIVE / 148

Aluminum (Al) accumulates within the root apoplast in an Al-tolerant wheat cultivar

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Acid soils comprise ca. 4 billion ha of the global ice-free land or ca. 40 % of the world's arable land. In these acid soils, the elevated solubility of Al-containing minerals results in increased concentrations of Al in the soil solution. Soluble Al is highly toxic to root growth, reducing elongation of roots in as little as 5 min due to an inhibition of wall loosening as required for cell elongation. Some plant species tolerate high levels of Al by releasing simple organic ligands (such as malate) to complex Al and reduce its toxicity. It is known that the secretion of malate from wheat roots occurs rapidly (within 15 min), increases with increasing Al concentration, and occurs largely from the apical 3-5 mm of the root. However, it remains unclear whether complexation of Al actually occurs within the rhizosphere or whether it occurs within the root tissue itself. We utilized low energy X-ray fluorescence (LEXRF) to examine the distribution of Al within root apices of two near-isogenic lines (NILs) of wheat (ET8 and ES8, being tolerant and sensitive, respectively) that differ ca. 15-fold in their tolerance to Al. When grown in solutions containing Al at concentrations resulting in a 50 % reduction in RER over 48 h (i.e. 3.5 μM Al for ES8 and 50 μM for ET8), concentrations of Al in the root apical tissues were ca. 4- to 6-times higher for ET8 than for ES8 despite the magnitude of the reduction in RER being the same. Of particular interest, we compared ES8 and ET8 at Al concentrations causing similar reduction in growth, and it was noted that the distribution of Al within the rhizodermis and outer cortex was similar – most Al was located within the cell wall in all instances. In the present study, we have shown that the ability of the Al-tolerant wheat NIL, ET8, to grow at elevated Al concentrations results not only from a reduction in Al concentrations within the root tissue due to the complexation of Al by malate external to the root (i.e. within the rhizosphere).

Improving Beam Stability with a Fast Orbit Feedback System

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The fast orbit feedback system in development at the Australian Synchrotron aims to improve the stability of the electron beam by reducing the impact of moving insertion devices and targeting orbit perturbations at the mains frequency (50 Hz, 100 Hz and 300 Hz). The feedback system is designed to have a unity gain at a frequency greater than 300 Hz using a PI controller with harmonic suppressors in parallel to specifically target perturbations at the mains frequency and its harmonics. In the lead up to the project completion at the end of 2016, a prototype system based on standard PCs running CentOS 7 with the PREEMPT patch was used. The effectiveness of a fast orbit feedback system is demonstrated by the prototype system where the integrated RMS motion up to 300 Hz was reduced by 75% to 90%.

Concurrent Session 3: Radiotherapy I / 277

Optimizing Microbeam Radiation Therapy with High-Z Nano-structured Ceramic Particles

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Microbeam radiation therapy (MRT) implements spatially-fractionated kilovoltage x-rays for deep-seated tumour treatment [1,2] to provide better normal tissue sparing [3]. However, tumour treatment with MRT can be further optimized with high-Z nanoparticles (NPs), which have been shown to enhance the dose delivered by conventional radiotherapies [4]. Tantalum pentoxide (Ta2O5) NPs are novel nano-structured ceramic particles that are non-toxic [4] and show optimal x-ray absorption in kilovoltage energies [5,6]. This research assesses the ability of ceramic NPs, including Ta2O5 NPs, to selectively raise the tumour valley dose in MRT. This multi-modal approach is named: Synchrotron Microbeam Activated Radiation Therapy (SMART).
Geant4 [7,8] simulations investigated the physical dose enhancement of Ta2O5 NPs to a population of cells due to monoenergetic broad-beams and microbeams (50-200 keV).
Simulation results were correlated to in-vitro experiments obtained in hutch 1B and 2B at the Imaging and Medical Beamline (IMBL), Australian Synchrotron, using tumorous 9L gliosarcoma and normal Madin Darby Canine Kidney cells. NPs were added to cells in T12.5cm2 flasks 24hrs before 90-100% confluence. Cells were irradiated using a 1.4T or 3T wiggler field to produce 50μm/400μm or 50μm/200μm microbeams with weighted average energies of 42 keV and 95 keV respectively. Cell survival following treatment was evaluated with clonogenic assays after 15 doubling times.
Ta2O5 NPs improved the MRT and broad-beam selectivity towards tumour cells, due to the NPs clustering about the nucleus of 9L tumour cells. Other ceramic NPs such as bismuth oxide, with more homogeneous NP distributions, also saw improvement to the MRT treatment efficiency.
Simulations confirmed that NP clusters produced the most selective dose enhancement to MRT. Modelling micro- and broad-beams showed that NP dose enhancement is energy dependent.

For Ta2O5 NPs, 40 keV x-rays are optimum for dose enhancement in broad-beam cases, and microbeam energies greater than 100 keV produce better NP dose enhancement with more secondary electrons that raise the valley dose (>100 μm from the microbeam).
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Concurrent Session 1: Earth & Environment / 190

XAS and XFM investigations of arsenic uptake in hydrothermal apatite

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Element substitution that occurs during fluid-rock interaction permits assessment of fluid composition and interaction conditions in ancient geological systems, and provides a way to fix contaminants from aqueous solutions. We conducted a series of hydrothermal mineral replacement experiments to determine whether a relationship can be established between arsenic (As) distribution in apatite and fluid chemistry. Calcite crystals were reacted with phosphate solutions spiked with As(V), As(III), and mixed As(III)/As(V) species at 250 $^\circ$C and water-saturated pressure. Arsenic-bearing apatite rims formed in several hours, and within 48 hours the calcite grains were fully replaced. X-ray Absorption Near-edge Spectroscopy (XANES) data show that As retained the trivalent oxidation state in the fully-reacted apatite grown from solutions containing only As(III). Extended X-ray Fine Spectroscopy (EXAFS) data reveal that these As(III) ions are surrounded by about three oxygen atoms at an As-O bond length close to that of an arsenate group (AsO43-), indicating that they occupy tetrahedral phosphate sites. The three-coordinated As(III)-O3 structure, with three oxygen atoms and one lone electron pair around As(III), was confirmed by geometry optimization using ab initio molecular simulations. The micro-XANES imaging data show that apatite formed from solutions spiked with mixed As(III) and As(V) retained only As(V) after completion of the replacement reaction; in contrast, partially reacted samples revealed a complex distribution of As(V)/As(III) ratios, with As(V) concentrated in the center of the grain and As(III) towards the rim. Most natural apatites from the Ernest Henry Iron Oxide Copper Gold deposit, Australia, show predominantly As(V), but two grains retained some As(III) in their core. The As-anomalous amphibolite-facies gneiss from Binntal, Switzerland, only revealed As(V), despite the fact that these apatites in both cases formed under conditions where As(III) is expected to be the dominant As form in hydrothermal fluids. Our study shows for the first time that As(III) can be incorporated into the apatite structure, although not as efficiently as As(V). Uptake of As(III) is probably highly dependent on the reaction mechanism. These results show that incorporation of As in apatite is a complicated process, and sensitive to the local fluid composition and kinetic effects during crystallization.

Concurrent Session 4: Radiotherapy II / 261

Progress report on the European MRT program: What can the Australian MRT community learn from the European experience?

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There are currently two biomedical synchrotron beamlines in the world with an MRT program and an active MRT user base: ID17 at the European Synchrotron Radiation Facility (ESRF), France, and the Australian Synchrotron's Imaging and Medical Beamline (IMBL). The European program has been ongoing since the 1990s and has identified radioresistant brain tumours as a clinical target for MRT. Indeed, much of the radiobiological data available in the literature relates to MRT irradiation of healthy and tumour inoculated brains of mice and rats. The Australian program has a different focus, instead proposing to target naturally occurring osteosarcomas in domestic dogs. Despite the different directions of the two programs, both communities share a common goal: to begin human clinical trials within 5 years. The past 5 years have seen many critical developments in this direction: the emergence of protocols and techniques for accurate dosimetry in broadbeams and microbeams, treatment planning systems dedicated to keV photons, and beamline specific image guidance protocols. In a "make or break" attempt to prove the safety of MRT for human patients, the European MRT collaboration have proposed a long term study on both healthy and brain tumour bearing pigs, where MRT is delivered as a dose "boost" to conventional stereotactic radiotherapy. The first steps of this project – end-to-end quality assurance (dosimetry and treatment plan verification) on a phantom and a dry-run on a pig carcass – were recently performed. The results from these experiments will be presented, as well as a discussion of what the Australian MRT community can learn from this.

Concurrent Session 3: Imaging - Sponsored by MASSIVE / 212

Extreme imaging on Imaging and Medical Beamline

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The Imaging and Medical Beamline (IMBL) of the Australian Synchrotron is recognised as one of the most advanced facility for the Computed Tomography (CT) experiment. It was designed for the macro-imaging, just touching the microscopy ranges in the highest magnification configuration. This design assumes that the beamline must be capable of imaging large objects up to 50cm wide. The monochromatic beam available on the IMBL can penetrate through the large object only if it consists of softer materials usually met in the biological tissues, while the samples of higher densities are not transparent enough to form the contrast of sufficient quality. In order to overcome this limitation we have been testing the pink-beam imaging modality. In this mode we are not using the monochromator which extracts a very narrow band from the wide spectrum produced by the superconducting multipole wiggler of the IMBL, but instead applied extensive filtration which suppresses the low-energy component of the beam allowing only the highest energy fraction to pass through. This approach is optimally implemented when the high magnetic field (4T) is applied to the wiggler magnet, what shifts the spectrum toward the high-energy end. In the last year we have tested this technique in two major beamline configurations: the near-source imaging in the enclosure 2B and the far-end in the enclosure 3B. The first of these configurations is optimal for the highest energy beam due to the high flux which is achieved for the price of the relatively small beam - up to 70(w) x 7(h) mm. Combination of this beamline configuration with the most sensitive of our detector (Hamamatsu flat panel, 200μm pixel size) defines the most extreme imaging conditions available on the IMBL. The pink beam produced under these

conditions has the peak energy above 360keV and allows to perform a successful CT scan of a 4cm led sample in less than one hour. In the far-end configuration of the IMBL the beam reaches 45(w) x 4(h) cm in size, what reduces the flux and dictates softer filtration with the peak energy of the pink beam being slightly above 300keV. The beam was tested with various objects which included a soil sample more than 35cm in width, metal tools of various sizes and large fossils. This presentation describes the method in details and presents some of the results obtained.

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Dynamic micro-CT of gas uptake in coal

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The behaviour of gases in coal is critical to processes affecting both coal seam gas extraction and carbon sequestration. These depend on the affinity of different gases for coal and the effect they have on the coal itself when adsorbed, such as causing the coal to swell.
Dynamic micro-CT offers the possibility of observing these processes on the microscopic scale as they are happening. Here we use krypton and xenon gas to explore gas uptake in five different types of coal. these gases are readily visible in micro-CT scans making quantitative analysis feasible. Krypton in particular is thought to be a close analogue for methane.
A time-series of tomographic scans of samples in containers pressurised with krypton or xenon were made over a period of three days resulting in many hundreds of tomographic datasets. Batch reconstruction and data analyses using the MASSIVE cluster enabled this large amount of data to be analysed in 3D.
This analysis has enabled us to quantify the gas uptake over time in different coal types, and to compare the behaviour of two gases with different affinities for coal. Diffusion profiles over time have also been obtained which will be used for comparison with gas diffusion models.

Figure 1: Tomographic cross section showing xenon gas diffusing into coal with insert displaying diffusion profile

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Structural insights into enolase-enhanced activation of plasminogen

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Plasmin is essential for a number of physiological functions including fibrinolysis, tissue remodelling and wound healing. The conversion of the zymogenic plasminogen to its active, serine protease form, is an important molecular event that regulates the timely delivery of active plasmin at the critical locations as required. Furthermore, binding of plasminogen to cell surface receptors promotes conformational change of plasminogen and enhances its processing by its activators, tissue plasminogen activator and urokinase plasminogen activator. α-enolase is a specific plasminogen receptor expressed on the surface of a variety of cell types, in addition to its main roles in the cytoplasm as a key glycolytic enzyme. Moreover, a number of pathogenic species of bacteria and parasites are capable of expressing enolase on their surface as a means of hijacking the plasminogen activation system and assisting their own migration through the host. Here, we

have attempted to use x-ray crystallography and activity assays to structurally and functionally characterize enolase from parasitic origins and their interaction with the host plasminogen. We have successfully expressed active, recombinant enolase originating from Leishmania mexicana (lmEno), Fasciola hepatica (fhEno) and Schistosoma japonicum (sjEno), with high yield and purity, and solved the structure of fhEno to 2.0 Å. We believe that continued research in this area will reveal the structural features of enolase that mediate its association with plasminogen and its ability to induce conformational change.

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Beachrock: A microbial mechanism for maintaining sand cay stability in the Great Barrier Reef

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Beachrock is produced through the lithification of sediments in the intertidal zone of tropical beaches on both continental coastlines and sand cays in reef environments. Beachrock formation through carbonate cement precipitation has the capacity to slow sea-level rise induced erosion of sand cays, islands that host vulnerable habitats, including inhabited cays and sea turtle rookeries. Beachrock formation has been linked to a number of interconnected physicochemical and biological processes, making it difficult to discern the key mechanism responsible for this geological process. This investigation employed synchrotron-based, X-ray fluorescence microscopy (XFM) to characterise beachrock specimens from Heron Island in the southern Great Barrier Reef. High-resolution elemental mapping of beachrock indicated that cementation in part occurs through the internal cycling of cations through microbial dissolution and re-precipitation of carbonate minerals. Boring of endolithic cyanobacteria in carbonate sand grains in the intertidal zone generates elevated concentrations of soluble calcium, magnesium, and strontium in the pore spaces of the sediment. Cyanobacterial photosynthesis produces microenvironments enriched in alkalinity, which, when combined with the high cation concentrations, induces supersaturating conditions with respect to carbonate minerals. Cement precipitation is also aided by the production of nucleation sites in the form of microbial exopolymer. This biogeochemical pathway for beachrock production was verified by synthesising new beachrock in the laboratory. Samples of beach sand and microbial communities from Heron Island were used in aquarium experiments that simulated the conditions typical of the intertidal zone with respect to tidal activity, light, temperature, and water chemistry. The seawater was doped with a strontium enrichment that enabled the identification of new cement precipitates using XFM. When observed using scanning electron microscopy (SEM), the new cements were shown to contain abundant microfossils. Linking high-resolution characterisation of the chemistry (XFM) and structure (SEM) of these cements has elucidated the biogeochemical mechanism that controls the progression from unconsolidated beach sand to lithified rock. Understanding this process, which may be encouraged by stimulating microbial activity, may be critical to maintaining island stability in the face of global sea-level rise.

Concurrent Session 3: Imaging - Sponsored by MASSIVE / 222

Elevated airway liquid volumes at birth: a potential cause of transient tachypnea of the newborn

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Before birth the fetal lungs are filled with liquid, which must be cleared at birth to allow entry of air and onset of gas exchange. The rate of preterm birth and non-labour caesarean delivery has substantially increased, which delays lung liquid clearance and increases the risk of neonatal respiratory complications. Retention of liquid in airways and/or lung tissue is thought to underpin the respiratory morbidity associated with transient tachypnea of the newborn (TTN). TTN results in rapid and laboured breathing immediately after birth or in the hours following delivery, that often requires respiratory support. We examined the effects of elevated airway liquid volumes on respiratory function in the immediate newborn period. Pregnant New Zealand white rabbits underwent caesarian surgery and fetal rabbits (kittens) were delivered at 30 days of gestation (term, ˜32 days). Following delivery, kittens were surgically intubated, and either had lung liquid drained to mimic the natural clearance at birth (Control, n=7) or had liquid added to the lungs (30ml/kg; 0.9% sodium chloride) to mimic delayed liquid clearance (TTN, n=7). Kittens were positioned inside a plethysmograph and were mechanically ventilated. Phase contrast X-ray images were obtained (24keV; 10Hz framerate; 20ms exposures; 2m propagation distance; at the SPring-8 synchrotron in Japan), and imaging analysis was undertaken to determine regional lung gas volumes, airway dimensions and chest and lung shape and size. Data were analysed using a two-way repeated measures ANOVA with Sidak's multiple comparisons test ($P<0.05$). Following ventilation onset, TTN kittens exhibited differences in the temporal and spatial pattern of lung aeration. TTN kittens required a greater time to achieve lung aeration and exhibited regional differences in aeration pattern. Delayed lung liquid clearance in the TTN group resulted in differences in the size of alveoli and uniformity of lung aeration. The average airway size was greater in TTN kittens, particularly in the upper lung quadrants. The excess liquid in the TTN group resulted in an increase in the radius of the diaphragm, increased lung height and total chest area. We have provided evidence for adverse effects of delayed lung liquid clearance on lung structure and function in the immediate neonatal period. This reduced ability of the lung to aerate efficiently provides evidence for increased respiratory morbidity in these neonates following birth. Overall, tailoring respiratory management strategies may lead to improved outcomes for these babies in clinical practice.

Concurrent Session 2: Surfaces / 202

Controlling the Edge-on vs. Face-on Stacking of Semicodundcting Polymers Using Diffusive Noncovalent Interactions

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In thin films of semiconductor polymers, the polymer chains often exhibit distinct orientation with respect to the substrate. The planar -face of the backbone typically orients either in an edge-on or face-on manner. Generally, an edge-on alignment is thought to be favourable for transport in thin film transistors, whereas face-on alignment is considered to improve vertical transport as desired in solar cells. However, molecular orientation is among the very few parameters that usually cannot be controlled when tailoring new semiconducting polymers. Here we show for an important class of semiconducting polymer that both the mode of orientation as well as the degree of alignment can be well controlled by exploiting diffusive non-covalent interactions along the backbone. Studying polydiketopyrrolopyrroles (PDPPs) as a case study, by strategically varying chemical structure we demonstrate systematic variation in molecular orientation with degree of chain planarization resulting from different degrees of diffusive non-covalent interactions. This observation opens the possibility of controlling and optimizing the orientation of semiconducting polymer chains in thin films by rational design.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 239

Investigation of protein stability and activity in Ionic liquids (IL) to control 3D Structure and Function of Simple and Complex Biomolecules in a quantitative and systematic manner.

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Ionic liquids (ILs) can have a stabilizing or destabilizing effect on proteins, which is strongly dependent on the cation and anion of the IL (1). Consequently ILs have potential to be tailored as beneficial solvents for enzymatic reactions and protein storage. The aim here is to develop detailed structure-property relationships between protic ionic liquid cations and anions and their ability to stabilize proteins. This will advance our understanding of specific solvent properties on protein stability, such as cation, anion, ionic strength, salt concentration and pH. The understanding of protein stability and function in ionic liquids will be advanced through employing an approach which builds molecular complexity from simple amino acids to multiple amino acids connected by peptide (bonds) to proteins (2). The proteins of primary interest to this project are water soluble proteins, which are also enzymes, whose functionality is dependent on their 3-D structure. The quantitative approach will enable direct comparison of protein properties between these IL and IL-water solvents in conventional aqueous systems.

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Concurrent Session 2: Advanced Materials II / 230

Effects of Solvents on Organic Field Effect Transistor (OFET) Charge Transport and Thin-Film Morphology of a High Mobility n-type Semiconducting Copolymer P(NDI2OD-T2)

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The interaction between a solvent and semiconducting polymer plays a fundamental role in the formation of thin-films that are used to fabricate solution processed organic electronic devices. Depending on this interaction, polymer chains form different aggregates in a solvent that affects film morphology and in turn, charge transport properties. To realise efficient charge transport in an organic field effect transistor (OFET), understanding the effects of solvents on film morphology is thus crucial. This study explores the effects of solvents on OFET performance and morphology of a high mobility naphthalene-diimide-thiophene based n-type semiconducting copolymer P(NDI2OD-T2) with Mn = 31.2 kDa and Đ = 2.1. In particular, six solvents have been used ranging from tolerably-good solvents such as o-dichlorobenzene to tolerably-poor solvents such as chloroform and chlorobenzene and poor solvents such as p-xylene and toluene. A direct correlation between OFET mobility with the change in solvent quality is observed where average mobility increases from less than 0.30 cmˆ2/Vs for samples prepared from tolerably-good solvents to ˜0.55 cmˆ2/Vs for samples prepared from poor solvents with a maximum mobility of ˜1.5 cmˆ2/Vs, thanks to an

intermediate aggregate formation. Interestingly, when molecular orientation is probed at the top interface by Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy, this increase in mobility is found directly proportional with increase in backbone tilt angles with poor solvents showing more edge-on orientation, resulting an efficient intra-chain charge hopping. Atomic Force Microscopy (AFM) and Resonant Soft X-Ray Scattering (R-SoXS) were used to investigate inter-and intra-chain connectivity of polymer chains and their orientational correlations across the samples. With fibrillar microstructures ranging a few hundred nm, samples prepared from poor solvents show correlations in the order of a few microns forming an efficient interconnected microstructure. Moreover, probing local order crystallinity of thin-films with Grazing Incidence Wide Angle X-Ray Scattering (GIWAXS) experiment indicates that samples prepared from poor solvents predominantly form longer order and closely packed edge-on components compared to face-on crystallites. Taken together, improvement in the saturation mobility of P(NDI2OD-T2) samples prepared from poor solvents such as p-xylene and toluene is attributed to intermediate aggregate formation in solutions, that in turn orients polymer backbones in a predominantly edge-on registry and forms micron-long orientationally correlated microstructures.

Concurrent Session 1: Advanced Materials I / 257

Exploiting Pressure to Induce "Guest-Blocked" Spin Crossover

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Spin Crossover (SCO) is a phenomenon where a 3d4-7 metal ion reversibly switches between two electronic states, namely high spin (HS) and low spin (LS), under an external perturbation, such as temperature, pressure or light irradiation.1 SCO behaviour is driven by short- and long-range lattice interactions which enables spin state cooperative propagation throughout the material, resulting in hysteretic and multi-step spin transitions.[2] Hofmann-type framework materials, in particular, are of interest as their robust lattice structure allows direct correlation of magnetic and structural effects in terms of both guest steric (i.e., internal pressure) and electronic effects.[3] This study focuses on a 2D Hofmann-type framework incorporating a 1,2,4-triazole functionalised ligand where the application of hydrostatic pressure uncovers "hidden" SCO properties as well as the range of host–host and host–guest interactions associated with these features.[4]
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Concurrent Session 4: Technique Development / 256

Optimising sample preparation for solids, pellets, liquids and solutions for Far-IR and IR analysis at the Australian Synchrotron

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This presentation gives an overview of the development and comparison of different sample preparation techniques for presenting samples to the Far-IR and IR beam line at the Australian Synchrotron.
We have investigated using polyethylene (PE), polytetrafluoroethylene (PTFE), polyvinylacetate (PVA), paraffin, and mixtures, as matrixes for pellets. We have also trialled pressing pure compounds without an added matrix. Most recently we have investigated using specially constructed liquid cells for liquid samples and those compounds that can be in solution.
Not surprisingly, there is not one 'solution' to all sample preparations and there are compromises to be made. Samples that do not bind into stable pellets as pure compounds need a matrix to support them and compounds that are strong absorbers may need matrix to dilute them.
For solutions the choice of solvent is also critical (especially for compounds that are poorly soluble in convenient solvents) as there needs to be enough material to give a signal without being swamped by the signal form the solvent.
Presenting results from those samples that produced good spectra from a range of applications - riboflavin (fluorescence of semen), ninhydrin (from fingerprint developing reagents) and bilirubin and biliverdin (from studying breakdown of blood and ageing of bruises) and those that didn't - this presentation draws conclusions about the process of optimising the preparation of varied samples to obtain the best results from your time at the Australian Synchrotron.

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Thermochemical conversion of low-rank fuels to bio-based products

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Low-rank fuels such as biomass and mixed municipal solid waste (MSW) can be valorised into useful products ranging from chemicals to bio-oil through thermochemical treatment. However, disparate physical and chemical properties of these fuels entail usage of different heating rates for isolating the product of interest. Rapid thermal degradation of biomass is conducive for producing chemicals whereas slow thermal degradation of MSW would facilitate simultaneous investigation of thermochemical breakdown and associated kinetics for bio-oil production. In this study, two different heating rates of 30°C/min and 150°C/min are employed to examine thermal degradation of MSW and biomass respectively through synchrotron infra-red (IR) microscopy. Eight different constituents of MSW namely, yard waste, food waste, paper, rubber, low-density polyethylene (LDPE), polypropylene (PP), poly-(ethylene terephthalate) (PET) and poly-styrene (PS); and biomass (softwood-Pinus radiata), impregnated with five different acid concentration of 0.01M, 0.05M, 0.1M, 0.2M, and 0.5M are considered in this study. Thermal degradation of each constituent of MSW and acid impregnated biomass is performed at 30°C/min and 150°C/min to assess their suitability for producing bio-oil and chemicals respectively. The various aliphatic and aromatic functional groups identified in this study during thermal degradation of MSW prove its suitability for bio-oil production. For biomass, the synchrotron IR analysis shows that acid-impregnation does not alter the surface functional groups but induces catalytic effect during thermal degradation. This information can help in enhancing the yield of bio-oil and chemicals from low-rank fuels through thermochemical treatment.

Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 269

The role of protein dynamics in the evolution of new enzyme function

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Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 169

Observing proteins at play: structural techniques to probe function

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We have used protein crystallography and small angle X-ray scattering to understand the way that enzymes respond to remote signals – a process known as allostery (from the Greek *allos* meaning "other" and *stereos* meaning "solid"). Allostery is critical to the control of metabolism, and although allostery has been known for many years, it is only more recently that the molecular networks that govern this communication in proteins have begun to be unravelled in detail. We have used a combination of structural, computational and biophysical approaches to examine the allosteric function of several enzymes that operate at important control points in key metabolic pathways. We have used crystallography and small angle X-ray scattering to demonstrate significant changes in structure and dynamics are part of the allosteric response. Our studies have revealed the details of the molecular events that are associated with the allosteric response and shed light on the evolution of allosteric properties by enzymes.

Concurrent Session 4: Technique Development / 205

How to get the most from your XFM data: GeoPIXE analysis on MASSIVE

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Richly detailed high definition elemental images are routinely collected during experiments at the X-ray Fluorescence Microscopy (XFM) beamline 1. In addition, complex 3D data sets may be collected - X-ray fluorescence tomography and/or XANES image stacks. For many experiments there can be up to $\frac{1}{4}$ TB of raw data to process from a 3 to 4 day visit.
This presentation will describe the latest workflow now available to all AS users for GeoPIXE analysis [2,3] on MASSIVE. Users can take advantage of the powerful combination of GeoPIXE software and parallel computing on MASSIVE. An account is automatically created for new users and a dedicated project created on MASSIVE for each experiment.
Users can continue data analysis with GeoPIXE in the same remote desktop environment they employed during their experiment and easily collaborate and share data amongst experiment participants. The local computing requirements to run a MASSIVE desktop are modest, a laptop is sufficient, although connection to a high definition display is useful.
Continued investigation and reprocessing of elemental images (potentially with new two-pass multiphase method [4]) along with extraction of integrated spectra from regions of interest to verify rare and dilute elements can be accomplished quickly and efficiently. Users can now get the most from their rich data sets by continuing to deeply interrogate and explore their samples using GeoPIXE analysis on MASSIVE.
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Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 167

Comparison of the microstructure of Mozzarella cheese using synchrotron-based transmission and ATR-FTIR microspectroscopic techniques.

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Fourier transform infrared (FTIR) spectroscopy is a well-established technique for the analysis of dairy products due to its ability to rapidly provide molecular information related to chemical composition. Despite the widespread use of FTIR spectroscopy, FTIR microspectroscopy has only had limited applications in dairy products to date. Current methods of analysis of the microstructure of dairy products involve fluorescent stains and time-consuming sample preparation. In contrast, FTIR microspectroscopy is label-free, non-destructive and requires minimal sample preparation.

In this study, synchrotron-based FTIR (S-FTIR) microspectroscopy was used to acquire spatially-resolved chemical images of the microstructure of Mozzarella cheese in both transmission and surface-specific attenuated total reflection (ATR) modes. Fixed cheese sections were used for transmission measurements, whilst a small piece of fresh cheese was measured directly at 4 C in ATR mode without any further preparation. This was achieved using an in-house developed macro-ATR device coupled with a cooling stage at the IR Microspectroscopy (IRM) beamline (Australian Synchrotron). S-FTIR spectra obtained from the two modes were subsequently compared to identify differences in molecular structure and distribution patterns of major components, particularly proteins and lipids, between fixed and fresh cheese. These results have been used to determine the optimal methods of analysis for cheese.

High-resolution S-FTIR chemical maps of *pasta filata* Mozzarella cheese were obtained, clearly showing the characteristic parallel alignment of proteins. Areas high in protein or lipid were separated using hierarchical cluster analysis (HCA). Principal component analysis (PCA) was subsequently applied, using spectra with the same protein/lipid ratio previously identified by HCA, to distinguish differences in molecular structures of cheese with different treatments. This study demonstrates the potential of the S-FTIR microspectroscopy technique, together with chemometric approaches, to analyse cheese microstructure. Insights into molecular structures of proteins and lipids present in Mozzarella cheese not available through other microscopic methods were gained. This information provides a better understanding of the impact of processing on cheese structure and will assist efforts to support Australian dairy manufacturers to improve shelf life, texture or the functionality of dairy products.

Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 285

UNRAVELLING THE STRUCTURAL AND MECHANISTIC DIVERSITY OF BACTERIAL AUTOTRANSPORTER VIRULENCE FACTORS

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Autotransporter proteins are the largest group of outer membrane and secreted virulence factors from important bacterial pathogens such as Salmonella enterica, Shigella flexneri, Neisseria meningitidis and pathogenic E. coli strains. They are important contributors to bacterial pathogenesis, functioning as toxins, adhesins and facilitators of biofilm formation. Their importance to human health has generated great interest. However, we are still struggling to understand their mechanisms of action. There are currently only 12 structures of autotransporters in the protein data bank.
Our research centres on the AIDA-I-type autotransporters which are the largest family of autotransporters. We were the first to determine the structure and mechanism of action for one of these family members Antigen 43a from uropathogenic E. coli (UPEC)1. Our work showed how Antigen 43 causes aggregation and biofilm formation, which are important for UPEC colonisation and persistence within the urinary tract. Since this time we have been using the MX beamlines at the Australian Synchrotron to determine the crystal structures of two new autotransporters. Our findings have revealed a surprising structural diversity amongst the autotransporters, which has allowed us to elucidate their distinct mechanisms of action and roles in bacterial pathogenesis. Interestingly, the structures have also revealed how bacteria use post-translational modifications to change the virulence functions of their proteins.
This research is also helping us to understand how we can target these autotransporters for therapeutic intervention. To this end we are again using X-ray crystallography to help aid us in the development of specific inhibitors of key autotransporters.

Plenary 1 / 153

Cryo Soft X-ray Tomography of Cells

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In Structural Cell Biology detailed structural and functional descriptions of the different cellular components must be correlated with a topological map of these components at the whole cellular level. Cryo soft X-ray nanotomography (cryo-SXT) is a new complementary approach in this field that can provide information at 50 nm (full-pitch) 3D resolution of the organelle organization in whole, unstained, un-sectioned cells [1, 2]. An overview of the technique as well as examples of applications in the field of pathogen-host interaction will be presented [3, 4, 5].
1 Schneider G et al. Nature Methods 7, 985-987 (2010). [2] Carrascosa JL et al. J. Struct. Biol. 168, 234-239 (2009). [3] Chichón FJ et al. J. Struct. Biol. 177, 202-211 (2012). [4] Kapishnikov S et al. PNAS 109, no.28, 11188-11193 (2012). [5] Pérez-Berná AJ et al. ACS Nano 10, 6597-6611 (2016).

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Substitution Effects on N2O Schiff Base Ligands in Unprecedented Abrupt Fe(II) Spin Crossover Complexes with Symmetry Breaking

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A family of Fe(II) spin crossover complexes with halogen substituted 5-X-N-(8-quinolyl)salicylaldimines (HqsalX, X = F 1, Cl 2, Br 3 and I 4) has been investigated. With N4O2 octahedral environments, a somewhat unusual donor system for Fe(II) spin crossover 1, this is the first time that [Fe(II)(qsal-X)2] complexes have been studied [2]. Compounds 2, 3 and 4 unexpectedly show completed abrupt spin transition at or above RT. Importantly, compound 4 also exhibits the photoconversion efficiency, above 90 % with a T(LIESST) temperature estimated at 54 K. Variable temperature single crystal structures are performed in both LS and HS states for complexes 2 and 3. The influence on spin crossover properties are discussed of intermolecular interactions and structural packing effects in various halogen substitution complexes.
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Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 198

Chemical Crystallography at the Australian Synchrotron MX Beamlines

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The macromolecular (MX) beamlines at the Australian synchrotron are mixed use between the structural biology and chemical crystallography (CX) communities. Since commissioning the high throughput MX1 bending magnet and the MX2 microfocus undulator beamlines have proven very successful for both communities.
With the transfer of the Australian Synchrotron under ANSTO as recognition as its importance as landmark infrastructure for Australia and the federal government has committed to the future funding of the synchrotron for an addition 10 years. MX2 is in the process of completing the purchase, delivery and implementation of a state of the art Eiger detector (Structural Biology laboratories and Australian Cancer Research Foundation) and is well situated to continue to benefit both communities.
It is fair to say that transitioning MX2 to the new generation of single photon counting detectors is going to be a game changer with data collection speeds increased at least ten fold. As such, the ability to handle an increase in sample numbers sample tracking through to automated methods of data analysis are currently under development.
What is the future for chemical crystallography at the MX beamlines? A review of the current developments that are underway and some discussion of what may lie in the future will be presented.

Concurrent Session 1: Advanced Materials I / 165

Investigation of microstructural variations in cold sprayed titanium after heat treatment

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Titanium alloys are widely used in aerospace applications due to their unique superiority of low density and high strength. In order to optimize the performance of Ti alloy, prior knowledge of the microstructure-property relationships and microstructural evolution as a result of processing should be studied. Synchrotron radiation-based X-ray micro-computed tomography (SR μ-CT) has been developed and become a powerful tool for investigating metallic materials, due to its unique capability of non-destructive 3D characterization over various techniques such as optical microscopy, SEM and TEM. However, it is difficult to quantitatively identify compositional distribution in some fine structures that are smaller than the pixel size. In this article, data-constrained modelling (DCM) 1 based on SR has been applied for the purpose of resolving the partial distribution of multiple compositions in single voxel more accurately of a cold sprayed Ti sample before and after heat treatment. SR μ-CT experiments were performed on imaging and medical beamline (IMBL) at Australian Synchrotron (AS). Projections with effective pixel size of 0.65μm were processed by X-Tract [2] for background correction, image normalization, phase retrieval, ring artefact correction and CT reconstruction. A cubic grid of N = 580 × 590 × 150 voxels was imported into DCM software for compositional analysis, cluster computation, quantitative characterization, and 3D visualization [3]. Although the porosity is 5.1% before annealing and 4.5% after annealing, the total number of voids cluster has decreased slightly after annealing compared with that before annealing. Quantitative information such as surface area and volume was obtained according to the cluster analysis. The surface area and the volume both have a trend of reduction, however, with an equivalent variation percentage. As a result, the value of surface area-to-volume ratio of void clusters almost keep as the same level as the environment changed. The results reveal a smaller dimension and similar shape profile of void clusters after heat treatment.
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Radiotherapy Workshop: Should we MRT Treat Canines / 298

Dog cancers - Why the interest for an MRT programme

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Concurrent Session 4: Radiotherapy II / 218

Curing Cancer with the Synchrotron

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Microbeam radiotherapy (MRT) was proposed as a novel RT paradigm for treating cancer some time ago. However, progress has been slow and it is unclear when or if human cancers will be treated with synchrotron radiation. There are numerous biological, medical, technical, regulatory and ethical issues to consider before a human is subjected to synchrotron MRT. This talk will give an overview of the issues that are being, and still need to be, addressed. Latest data from the current AS/IMBL MRT program will also be presented.

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Status of MRT research – What we have done and what is still to do

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Pulmonary computed tomography using a laboratory-based X-ray source in murine asthma models.

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Rodent models of allergic airways disease largely replicate the pathophysiology of asthma and are widely used in basic science and in preclinical drug evaluation.The phenotype of allergic airways disease rodents with a genetic deficiency or their response to pharmacological treatment can be assessed according to clinically relevant endpoints including lung function tests.This often takes the form of invasive plethysmography where airway resistance and dynamic compliance are determined from flow and pressure measurements in anesthetised tracheostomized mice with a bronchoconstrictor challenge.However, as in human medicine, the technology is advancing, and techniques such as X-ray imaging with computed tomography (CT) 4D reconstruction and X-ray velocimetry (XV) may allow further insights, particularly with regard to spatial localization of responses in the regions of the lung.
The aim of the current study was to compare normal and allergic airways disease mice using four dimensional x-ray velocimetry(4DXV).
Adult female Balb/c mice(n=12)were subject to a model of allergic airways disease. In-vivo 4DCT was performed on the live anaesthetized mice under mechanical ventilation using a 70 kV Excillum laboratory-based X-ray source, without need for a contrast agent. Images were acquired 30 frames per second, and image acquisition was gated to the breath cycle. XV was then performed on the 4DCT dataset to obtain 4DXV data. Baseline measurements and measurements at four ascending concentrations of methacholine bronchoconstrictor were taken on each mouse. Analysis of the functional data using particle-image velocimetry allowed us to observe and quantify preferential damage of airways and restriction of airflow in affected mice. These alterations in flow and airway size were most pronounced in the allergic airways disease mice during the highest dose of methacholine. Imaging shows the extent and longevity of response and its regional location across lung lobes and throughout the respiratory tree with excellent resolution to the small airways.
4DXV allows regional lung function to be observed in asthma model mice with a similar data collection throughput to invasive plethysmography.. Data analysis was much more complex and ongoing but we were able to perturb clear differences between the mice groups in airway calibre and flow even in smaller airways. If uniform protocols can be adopted, these temporal-spatial analyses may have many applications in measurement of anti-inflammatory, anti-remodelling and epithelial repair drug response and live monitoring of bronchodilator response in vivo.

Concurrent Session 3: Industry & Innovation / 228

Pulmonary computed tomography using a laboratory-based X-ray source in murine asthma models.

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Rodent models of allergic airways disease largely replicate the pathophysiology of asthma and are widely used in basic science and in preclinical drug evaluation. The phenotype of allergic airways disease rodents with a genetic deficiency or their response to pharmacological treatment can be assessed according to clinically relevant endpoints including lung function tests. This often takes the form invasive plethysmography where airway resistance and dynamic compliance are determined from flow and pressure measurements in anesthetised tracheostomized mice with a bronchoconstrictor challenge. However, as in human medicine, the technology is advancing, and techniques such as X-ray imaging with computed tomography 4D reconstruction may allow further insights, particularly with regard to sptatial localization of responses in the regions of the lung.
The aim of the current study was to compare normal and allergic airways disease mice using the 4D X-ray technique.
Adult female Balb/c mice (n=12) were subject to an ovalbumin sensitization / challenge model of allergic airways disease or saline control protocol. Computed tomography was performed on the anaesthetized mice under mechanical ventilation using a laboratory-based X-ray source, without need for a contrast agent. Baseline measurements and measurements at four ascending concentrations of methacholine bronchoconstrictor were taken on each mouse. Mice were then euthanized and lung tissue taken for histology – H&E, Masson trichrome, and Alcian blue periodic acid Schiff stains.
Histological analysis showed airway inflammation, and goblet cell metaplasia in the diseased mice. Analysis of the functional data using particle-image velocimetry allowed us to observe and quantify preferential damage of airways and restriction of airflow in affected mice. These alterations in flow and airway size were most pronounced in the allergic airways disease mice during the highest dose of methacholine. Imaging shows the extent and longevity of response and its location across lung lobes and throughout the respiratory tree to the small airways with excellent resolution.
The 4D instrument allowed us to perform lung function in asthma model mice with a similar data collection throughput to invasive plethysmography and without additional animal welfare burden. Data analysis is ongoing but we were able to perturb clear differences between the mice groups in airway calibre and flow even in smaller airways. Is uniform protocols can be adopted, these temporo-spatial analyses may have many applications in measurement of anti-inflammatory, anti-remodelling and epithelial repair drug response and live monitoring of bronchodilator response in vivo.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 221

Naphthalene diimide-based molecular acceptors for organic solar cells

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Organic photovoltaics (OPV) have received much attention due to the promise of low-cost, efficient processing of solar cells onto flexible substrates. Typically, OPVs consist of a polymeric donor and a fullerene acceptor material, however, fullerene shortcomings such as poor light harvesting ability and high synthesis costs have resulted in the exploration of alternative acceptor materials. Small

molecule acceptors have recently gained attention due to their favourable absorption profile and inexpensive synthesis. While polymeric naphthalene diimide (NDI)-based materials have shown promise as alternatives for fullerenes – showing power conversion efficiencies (PCE) over 8% in some devices – their molecular counterparts have been less successful, with low initial performance resulting in their limited exploration as the highest reported device exhibits only 2.4% PCE. The lower efficiencies of NDI-based small molecules are attributed to weaker absorption in the visible wavelength range as well as susceptibility to forming large domain sizes. We report a series of NDI-based small molecule acceptors with different architectures and substitutional atoms with one material achieving the highest PCE to-date for any NDI-based molecular acceptor at 2.8%. A range of synchrotron-based techniques including grazing incidence wide-angle x-ray scattering (GIWAXS), resonant-soft x-ray scattering (R-SoXS), and near edge x-ray absorption fine structure (NEXAFS) have been used to characterize the active layer morphology for these devices. NDI-based small molecule acceptors are an attractive alternative to typical fullerene acceptors because their absorption profile can be favourably tuned to include visible wavelengths and their synthesis is both less tedious and less expensive than that of fullerene acceptors.

Concurrent Session 1: Earth & Environment / 192

Temperature Dependent Refractive Indices of Formic Acid Aerosols

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Formic acid (HCOOH) is the most abundant trace gas organic acid in the atmosphere, resulting from oxidation or photochemical processing of alkanes from biogenic and anthropogenic sources.1 Formic acid dissolves well in water and thus contributes significantly to rain acidity in remote regions. Due to its good solubility it is believed that formic acid contributes to cloud condensation.[2] It is also considered to be a source of OH radical which is one of the most active oxidising agent in the atmosphere. Temperature dependent refractive indices of formic acid are needed for composition analysis of aerosols and interstellar ices.[3]

In this work, we present mid-infrared (IR) spectra of formic acid aerosols recorded at atmospherically relevant temperatures of 80 – 210 K, and demonstrate an efficient method to extract refractive indices from measured spectra. The spectra indicate that the spectral bands below 1800 cm-1, especially around the C=O stretch region, show strong temperature dependence. The C=O stretch band profile show interesting temperature and particle size dependence. Initial analysis indicate that the band profile may be used to characterise the phase (crystalline vs amorphous) and particle size. We will discuss possible mechanisms that produce the C=O stretch band profile.

We also present the refractive indices retrieved from IR spectra using classical damped harmonic oscillator (CDHO) model. In this model, we input the CDHO band and particle size distribution parameters to simulate the Mie scattering spectra of spherical particles, and optimise the parameters to minimise the difference between the simulated and measured spectra. We evaluate the accuracy of the method with respect to particle size and CDHO band parameters, and the errors associated with assuming the spherical shape of the formic acid aerosol particles. At the end, we compare the IR spectra of formic acid thin films to our aerosol spectra and demonstrate the advantages of using aerosols to extract refractive indices from IR spectra.

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[3]. Takahama, S.; Johnson, A.; Russell, L. M. Quantification of Carboxylic and Carbonyl Functional Groups in Organic Aerosol Infrared Absorbance Spectra, Aerosol Sci. Tech. 2013, 47, 310-325.

Radiotherapy Workshop: Should we MRT Treat Canines / 297

Experience with radiotherapy treatment on dogs

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The Relevance of Sacrificial Redox Chemistry to Catalyst Design: A Study of How Disorder Changes Reaction Selectivity in Three Classes of Reactions Catalysed by Manganese (III/IV) oxides

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Birnessites and closely related phases of manganese oxides are catalysts for a range of chemical reactions. These include the classical chemical demonstration of the disproportionation of hydrogen peroxide, decarboxylation reactions, the oxidation of amines to imines and water oidation. Because these reactions are so different we seldom think about the selectivity of one reaction and what it means for the others. In this research we have studied a series of manganese oxides with different degrees of disorder. Destabilization of the manganese oxides increases the reactivity of the oxides to sacrificial reactions. Interestingly our results indicate a relationship between the sacrificial chemistry and the catalytic chemistry. We can use disorder to destabilize manganese oxides converting what are catalytic reaction through to sacrificial reactions. Our results demonstrate a relationship between the sacrificial chemistry of these systems and the catalytic chemistry that has not previously been recognized. The relationship is discussed in the context of optimizing catalysis across all classes of materials. Optimization of materials for water oxidation seems to fall between the catalytic and sacrificial limits of the materials consistent with the self-healing mechanism proposed in these families of materials.

Concurrent Sessions 1: Biological Systems / 210

Liquid crystal self-assembly during in vitro lipolysis of milk and infant formula

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Milk provides an important source of energy for children, and is one of the staple foods for adults with Western diet. The World Health Organization and the Australian government have recommended exclusive human milk feeding for infants below 6 months, although commercial infant formulas (IF) can be used as human milk substitute in circumstances where human milk is not adequate.[1,2] IF is generally manufactured from blends of vegetable oils (such as coconut, palm, palm kernel, safflower, soybean, sunflower, and recently FDA-approved canola) and/or bovine milk fat to match the required fatty acid compositions.[3] As such, there exists variation in the composition of triglycerides between IF and bovine milk, in addition to the different brands of IF. Our group has recently demonstrated, using the Australian Synchrotron time-resolved small angle X-ray scattering (SAXS), formation of different lipid nanostructures during lipase-catalysed milk digestion where transition from lipid emulsion to L2, $Fd3m$, H2, Q2, and lamellar vesicles occurred.[4,5] In this study, changes in the lipid self-assembly during the intestinal digestion process of various infant formulas were investigated. The effects of milk fat globule (MFG) sizes on the extent of digestion, and the particle size distribution of the MFG in both milk and IF were analysed. We also characterised the partitioning of the liquid crystalline structures in the milk lipolytic products using SAXS and cryo-TEM.

Radiotherapy Workshop: Should we MRT Treat Canines / 300

Do we need late toxicity data before the first human clinical trial?

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Systematic characterisation of normal tissue toxicity using Synchrotron Radiotherapy

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Background: Synchrotron Radiotherapy is characterised by high intensity beams which are capable of delivering dose-rates that are up to 10,000 times faster than conventional radiotherapy dose rates. Systematic normal tissue toxicity data is required in order to progress towards human clinical trials. Aim: To assess the safety profile of both Synchrotron broad-beam radiotherapy (SBBR) and Microbeam radiotherapy (MRT) compared to conventional radiotherapy (CRT). Method: A dose-escalation study using SBBR, MRT and CRT was performed on C57BL/6 mice (male and female, 8-10 weeks old). Mice received either Total Body Irradiation (TBI) or Partial Body Irradiation to their entire abdomen (PBI). Five mice were irradiated per group. Mice were monitored for signs of weight loss and other gastro-intestinal toxicities such as diarrhoea, and were euthanized according to strict intervention criteria. Results: For TBI, all mice survived with no signs of diarrhoea up to peak MRT doses of 144 Gy. There was a dose-dependent increase in the incidence of sustained weight loss, with four out of five mice in the 144 Gy group showing at least 10% weight loss two weeks following irradiation. In the SBBR groups, 8 Gy led to irreversible weight loss and euthanasia for all mice within three weeks of irradiation. For PBI, all mice receiving 450 Gy MRT and 15 Gy SBBR experienced 20% weight loss, severe diarrhoea and dehydration within six days of irradiation, consistent with gastrointestinal syndrome, and were euthanized. All mice receiving less than 270 Gy MRT groups and 9 Gy SBBR groups survived, experiencing reversible weight loss and showing no signs of diarrhoea. Conclusion: These are the first systematic dose-escalation toxicity data for MRT and high dose-rate SBBR using TBI and abdominal PBI. The threshold for irreversible gastro-intestinal toxicity lies between 270 and 360 Gy for MRT and between 12 and 15 Gy for high dose-rate SBBR. A comparison with toxicity data for conventional dose-rate broad beam radiotherapy is ongoing and will determine if ultra-high dose-rates provide a normal tissue sparing effect.
Lloyd. M. L. Smyth, Jessica. A. Ventura, Jacqueline Donoghue, Jeffrey. C. Crosbie & Peter A. W. Rogers

Concurrent Session 3: Radiotherapy I / 175

Differential response of Diffuse Intrinsic Pontine Glioma cell lines to microbeam versus conventional radiotherapy

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Background: Diffuse Intrinsic Pontine Glioma (DIPG) is a devastating paediatric brainstem tumour with extremely poor prognosis and limited treatment options. Radiotherapy is the mainstay treatment but is limited to palliative use. Microbeam Radiotherapy (MRT) is a promising pre-clinical synchrotron radiotherapy modality which could improve the therapeutic ratio between normal tissue toxicity and tumour control through radiobiological mechanisms that are a radical departure from those of conventional radiotherapy (CRT).
Objectives: The aim of this study was to compare the cellular response of two human DIPG cell lines to MRT and conventional broad-beam radiotherapy and compute dose equivalence between the two modalities. We hypothesised that MRT would elicit a different cellular response to CRT, and that different DIPG cell lines would have different intrinsic radio-sensitivities.
Methods: Two human DIPG cell lines, SF7761 and JHH-1, were exposed to MRT (112 to 560 Gy) or CRT (2 to 8 Gy) in vitro to produce clonogenic cell-survival curves. Equivalent CRT doses were interpolated for each MRT dose. Apoptosis induction and cell-cycle response assays were performed five days after irradiation via flow cytometry to assess differences in cellular response between the cell lines and radiotherapy modalities at equivalent doses.
Results: The SF7761 cell line, which originated from a patient with no prior history of radiation treatment, was significantly more radiosensitive to both CRT and MRT compared to the JHH-1 cell line, which originated from a six year old male who had previously undergone combined chemotherapy and radiotherapy (Figure 1). JHH-1 formed polyploid cells and exhibited delayed G2/M arrest following both CRT and MRT. Furthermore, apoptosis and cell cycle assays demonstrated that at equivalent doses, MRT induced more unrepaired DNA damage that was detrimental to the cell-cycle and cell viability for both cell lines five days following irradiation.
Conclusion: This is the first study to compare the response of DIPG cell lines to MRT and CRT. Although MRT caused more DNA damage that was detrimental to the cell cycle compared to CRT, the JHH-1 cell demonstrated radio-resistance regardless of the radiation modality used. The findings of this study support the use of MRT as a potential alternative to CRT for patients with radiosensitive tumours and also contribute to our understanding of the differential response of cancer cells to MRT and CRT.

Concurrent Session 1: Earth & Environment / 172

Microstructure Evolution of Saturated Fine-Grained Soil Consolidation Based on Data-Constrained Modelling

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The Saturated Fine-Grained (SFG) soil, as one type of important materials of dredger mud, is related closely to bearing capacity of foundation in consolidation progress of reclamation engineering. It is necessary to research the quantitative mechanism between micro and macro mechanics by microstructure evolution of SFG soil consolidation. However, it is difficult to obtain the 3D microstructure characterisation in Micro-Nano scales by image segmentation approach. The Data-Constrained Modelling (DCM) method incorporates Multispectral Energy in Synchrotron Radiation of X-ray micro-Computed Tomography (ME-SR-μCT) was applied to the 3D distribution of SFG soil in Micro-Nano scales. Based on DCM technology, quantitative parameters were obtained. With the increasing of loading pressures, 3D data was shown as follows. The correlation indexes between 3 groups changed. Especially the pores which were saturated with water migrated with organics significantly. The quantity and volume percentage of clusters of pores and minerals were varied with mechanics in 3 phases including obvious consolidation, aggregation yield consolidation and particle yield consolidation. Combined with e-p curves of macroscopic mechanical characteristics, it was found that particle yield as 400 kPa of SFG soil was smaller than conventional particle yield 800kPa in soft soil. It consolidated the importance of creep mechanics in the process of bearing capacity increasing. And an effective 3D structures

characteristics method was illustrated, which included 3 groups of SFG. It revealed that the distributions and evolutions of porosity and the minerals were in different consolidation phases which combined with micro and macro mechanical properties. Furthermore, loading velocity could be controlled by the mechanics result combined with engineering theory and engineering significance.

Concurrent Session 2: Surfaces / 227

Diamond Surfaces for Quantum Applications

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Diamonds exhibit remarkable properties at the confluence of biological and quantum sciences. The crystalline carbon lattice of this material acts as both a quantum vacuum, allowing long lived coherent states at room temperature, while also presenting a bio-friendly interface. Point defects in this material are now being used for an ever expanding array of quantum information and sensing applications, including live intra-cellular biosensing. However the diamond surface, including its typical termination structure, is to date poorly controlled or understood. This seriously compromises the quantum properties of near-surface point defects (qubits), limiting the applicability of this system. I will present our use of the full capabilities of the soft x-ray spectroscopy beamline, in conjunction with DFT-driven simulations and CVD-based diamond synthesis, to create, modify and probe diamond surfaces. This has allowed us to begin understanding and eliminating surface states and structures, which interfere with diamond's otherwise superlative materials properties. In doing so we have created novel surface chemistries, found unexpected surface crystalline defects (including air-stable dangling bonds) and optimized the production and processing steps required to create high-performance diamond devices for a variety of applications. I will also give an overview of the various associated diamond defect applications we are pursuing, including wide-field magnetic and thermal imaging, bio-sensing and 2-D materials characterization.

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The Structure of PaeDAH7PS: a Potentially Promiscuous Protein

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Pseudomonas aeruginosa is an opportunistic human pathogen associated with the chronic infection of the lungs of Cystic Fibrosis patients – New Zealand's most common lethal genetic disease. *P. aeruginosa* has an innate resistance to antibiotics and concerns exist around the appearance of multi-drug resistant strains 1.

The shikimate pathway is responsible for the biosynthesis of key aromatic metabolites including the aromatic amino acids phenylalanine, tyrosine, and tryptophan; folic acid; and, in the case of *P. aeruginosa*, the toxic secondary metabolite pyocyanin [2].

The determination of the crystal structure of a key enzyme in the shikimate pathway from *P. aeruginosa* reveals a distinct regulatory mechanism and provides only the second example of a crystal structure of this type of enzyme.

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Estimating the flux distribution for a synchrotron X-ray beam using absolute ionisation-chamber measurements with various filters

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It is shown that an extensive set of absolute ionisation-chamber (IC) measurements with a primary polychromatic synchrotron X-ray beam and various filter combinations/ thicknesses can be used to quite effectively estimate the flux distribution. The basic technique is simple but the "inversion" of the raw data to extract the flux distribution is fundamentally ill-posed. We demonstrate, using data collected at the Imaging & Medical Beamline (IMBL) of the Australian Synchrotron, that the absolute flux can be quickly and reliably estimated if a suitable choice of filters is made. Results are presented as a function of the magnetic field (from 1.40 to 4.00 T) in the superconducting multi-pole wiggler (SCMPW) insertion device installed at IMBL. A non-linear least squares refinement of the data is used to estimate the incident flux distribution and then comparison is made with calculations from the programs "SPECTRA" (Tanaka & Kitamura, 2001, 2007), "XOP" (Sánchez del Río & Dejus, 2011) and "spec.exe" (Stevenson et al., 2016).
The technique described is important not only in estimating flux itself, but also for a variety of other X-ray properties such beam quality, power density and absorbed-dose rate.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 213

Hybrid Protein-lipid materials for drug delivery into the cellular environment

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Hybrid protein-lipid materials such as cubosomes are a novel way to encapsulate and protect proteins for a range of nanobiotechnological applications. Peptides and proteins used in new and exciting drug applications may degrade when introduced to the human blood stream, or undergo attack by the immune system. Therefor a biologically stable and safe compound such as a lipid based cubosomes are needed to transport these peptides to the cellular environment. To discover the loading potential of these lipid cubic phase(LCP) bulk and Cubosomes SAXS/WAXS was used to look at the lattice parameter of the LCP at a range of protein concentrations to analysis cubic phase swelling. This showed that the uptake and swelling of the LCP was dependent on the lipid used as well as layer stiffness. Synchrotron CD in Aarhus was used to determine the protein stability when incorporated into the cubic phase which showed no change in secondary structure when a protein is incorporated into the cubic phase.

Concurrent Session 3: Imaging - Sponsored by MASSIVE / 163

Synchrotron radiation imaging of aortic stent grafting: An in vitro phantom study

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This study was conducted on a human aorta phantom with a commercially available stent graft placed in the aorta with the aim of investigating visualization of aortic stent graft by synchrotron radiation. Synchrotron tomography experiments were performed on imaging and medical beamline at the Australian Synchrotron facility, with beam energy ranging from 40 to 100 keV, with spatial resolution of 19.88 μm per pixel. Computed tomography (CT) scans were performed on a 64-slice CT scanner with slice thickness of 1.0, 1.5 and 2.0 mm. Maximal transverse diameter of stent wires was measured on synchrotron radiation and 64-slice CT images at suprarenal stent struts and main body of aortic stent graft. The stent wire diameter measured on synchrotron images was between 0.4 and 0.5 mm, representing the actual diameter of wire thickness, while overestimated wire thickness was seen in 64-slice CT images with measured wire diameter ranging from 1.0 to 1.6 mm. There were no significant differences in stent wire diameter between suprarenal stent struts and main body stent graft by comparing two-dimensional (2D) axial (p=0.93) and three-dimensional (3D) synchrotron image measurements (p=0.07). Significant difference was found between 2D and 3D synchrotron measurements of stent wire diameter in the main body of stent graft (p=0.001). In contrast, significant differences were found in stent wire diameter at the levels of suprarenal stent struts and the main body of stent graft by comparing 2D axial and 3D CT image measurements (p=0.03 and 0.001 respectively). Also, significant differences were reached by comparing measurements taken at the suprarenal stent struts and main body of stent graft with use of 2D axial (p=0.04) and 3D CT images (p=0.001). Synchrotron radiation provides superior advantages over multislice CT for visualization of aortic stent wire structure with measurements representing the actual diameter, thus allowing accurate assessment of endovascular stent graft repair.

Concurrent Session 3: Industry & Innovation / 208

A comparison of collagen fibre orientations in articular cartilage measured using SAXS and DTI

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Background: Diffusion Tensor Imaging (DTI) is a popular technique used to study collagen fibre architecture in articular cartilage. Interpretation of DTI images, however, is limited to the predominant alignment of fibres only1. Dispersion of fibre orientations can be measured using Small angle X-ray scattering (SAXS). Here, we present a comparison of SAXS and DTI measurements in cartilage. We propose that the SAXS measurements be used to refine DTI-based studies of cartilage microstructure.
Methods: Sixteen matched pairs of articular cartilage samples and eight ligament samples were excised from bovine knee joints. Three cartilage and two ligament samples were treated with trypsin to remove proteoglycans. The diffusion tensor was reconstructed from DTI images and Fractional Anisotropy (FA) was calculated1. The remaining cartilage samples for SAXS measurements were halved depth-wise to represent the transitional zone (top half- with fibres having no particular alignment) and radial zone (bottom half- with fibres predominantly aligned perpendicular to the articular surface)[2]. Ten cartilage (both halves) and four ligament samples were dehydrated before SAXS data acquisition. 2D SAXS patterns were processed to extract azimuthal intensity distributions of scattered X-rays. Intensity distributions obtained from each cartilage sample of interest and a reference ligament sample were deconvolved to obtain the distribution of fibre orientations within the cartilage sample[3].
Results: Fractional anisotropy increases with depth from the articular surface and collagen fiber orientation distributions obtained from SAXS are narrower in the radial zone, corresponding to greater alignment of collagen fibres in the radial zone. This direct correspondence between DTI and SAXS measurements varied from sample to sample, indicating the need for further analysis. <img src="https://www.dropbox.com/s/lflcm63wrw2xb6v/Sample4$_F$*AandODF.pdf?dl* = 0"*alt* = "*FractionalAnisotropyandCollagenFibreOrientation*"/ >
Conclusion: SAXS shows promise as a complementary tool to DTI for the study of cartilage microstructure. Follow-up studies using SAXS patterns obtained at different locations of the

cartilage sample can provide a spatial view of the collagen fibre orientation distributions, making comparisons with spatially varying fractional anisotropies more straightforward.
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Optimization of in-line X-ray phase-contrast tomographic imaging for breast cancer screening

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The problem of optimising the experimental protocol and data analysis for in-vivo breast cancer screening was investigated using synchrotron-based in-line X-ray phase-contrast tomography. Results are presented of experiments conducted at the IMBL and SYRMEP beamlines of Australian and Elettra Synchrotrons using the propagation-based phase-contrast mammographic tomography method, which incorporates both absorption and X-ray phase information. The study aims to obtain images of full-size human breast tissue samples, with radiologically acceptable X-ray dose, in order to investigate the degree of improvement of the diagnostic image quality achievable using in-line phase-contrast image acquisition protocols via the incorporation of X-ray phase retrieval into the reconstruction pipeline. Parameters such as the X-ray energy, sample-to-detector distance and data processing methods were tested, evaluated and optimized (with respect to the estimated diagnostic value) using a mastectomy sample with a malignant lesion. The results of quantitative evaluation of images were obtained by means of radiological assessment carried out by experienced specialists. A comparative analysis was performed between corresponding X-ray and histological images of the specimen. The outcomes of this study provide the practical imaging conditions and the CT reconstruction procedures appropriate for low-dose phase-contrast mammographic screening of live patients at specially designed synchrotron beamlines.

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Automated NEXAFS collection on the Soft X-Ray beamline – towards remote access on the High Vacuum Automated NEXAFS chamber.

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The Soft X-Ray beamline is in the process of developing a High Vacuum Automated NEXAFS chamber. To this end we have started developing automated methods for collecting NXAFS data on our existing end station. This presentation will describe the latest automated procedures that we have implemented and tested as well as what is yet to come. It is envisioned that many of the automated procedures that we are currently developing will be directly transferable to the new

High Vacuum Automated NEXAFS chamber. An overview of how we foresee the new chamber can run will be presented.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 149

infrared mapping as a predictive tool in wound care

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Aberrant wound healing, as observed in the presence of co-morbidities such as diabetes, represents a major clinical problem. To improve wound care, a better understanding of the cellular and molecular details of healing processes is required. Our aim was to utilize Synchrotron- and focal plane array (PFA)-based Fourier-transform infrared (FTIR) chemical mapping for further characterizing the wound healing process. Skin tissue samples were obtained from therapeutic debridement procedures over several weeks, from a chronic diabetic venous ulcer and a full-thickness burn with fully-informed patient consent. Normal tissue was obtained from murine skin samples. Sections (4μm) were mounted onto calcium fluoride windows and analysed at the Infrared beamline (Australian Synchrotron) by both Synchrotron- and FPA-based FTIR mapping. Microscopic analysis and visualization of heat maps generated by infrared imaging provide a distinctive view of the wound matrix. Analysis of intensities at appropriate wavelengths, highlight discrete patterns of lipid and protein composition in control and wound tissue in distinct cellular layers. Together, FPA-based imaging allows for a relatively large overview and Synchrotron-FTIR enables detailed spectral analysis at the single-cell level providing a clear illustration of the dynamic wound environment. Normal wound healing requires a well-organized and orchestrated series of molecular events involving numerous cell types. For example, haemostasis is mediated by platelets, endothelial cells form new blood vessels and fibroblasts deposit collagen. Overall, cell type analysis using Synchrotron- and FPA-based FTIR and correlation with conventional immunofluorescence studies, highlight the potential use of these technologies as diagnostic tools in wound care.

Concurrent Session 2: Surfaces / 240

Investigation of fungal infestation on metallic and polymer surfaces using synchrotron-based macro ATR-FTIR microspectroscopy

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Fungi possess the ability to colonize a wide array of surfaces, including metallic surfaces; the product of colonization is the proliferation and formation of a fungal biofilm followed by the degradation and alteration of the metallic surface. In particular, microbially-induced corrosion on the surface of metals occurs due to changes in the local acidity, creating galvanic and differential aeration cells, with the galvanic corrosion rate being shown to be a function of temperature. Three common fungi (*Aspergillus niger* ATCC 9642, *Aureobasidium pullulans* ATCC 9348 and *Epicoccum nigrum* ATCC 42773) were utilised to study the fungal spores adhesion, hyphae development followed by the biofilm formation on different types of metallic surfaces (stainless steel SL316, titanium commercial grade 2, polyester-coated steel and anti-fungal paints (Microban®). Growth behaviour and molecular characteristics of fungal infestation on these surfaces were monitored using scanning electron microscopy and synchrotron-macro ATR-FTIR microspectroscopy. It was found that three fungal species studied were able to attach and colonise the metallic surfaces after 18 h incubation. Hyphae development was observed after 3 days of fungal interactions with metallic surfaces except anti-fungal paints surfaces. The latter were colonized by fungi after 7 days. ATR-IR microscopy revealed that only *E. nigrum* and *Aspergillus niger* were found to deposit pigments on these surfaces.

Concurrent Session 2: Advanced Materials II / 201

Chiral Coordination Polymers and Cages

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Chiral metal-organic materials, either infinite coordination polymers or discrete cages/capsules, are areas of considerable research interest due to their potential to act as catalysts for enantioselective reactions or agents to separate and purify racemic mixtures. Towards these ends, we have recently been investigating a series of enantiopure dicarboxylate ligands, built using diimide scaffolds, their inclusion into both infinite and discrete complexes and the properties of these compounds towards a variety of guest species. Naphthalenediimides have been investigated for their ability to give rise to interpenetrated networks some of which have shown activity in the resolution of racemates by liquid chromatographic methods. Coordination cages have been prepared in which the coordination of four amino acids around a copper paddlewheel induces helicity into the resulting M4L4 species. The direction of the helicity is a direct consequence of the handedness of the ligand that is used.

Concurrent Sessions 1: Biological Systems / 236

Multi-technique investigations of nickel hyperaccumulator plant ecophysiology

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Our team, together with international collaborators, has been studying plants that hyperaccumulator trace elements, especially nickel, from various ecosystems around the world. The aim of these investigations has been to advance our understanding of the ecophysiology of these unusual plants.
We have employed a range of micro-analytical methods to reveal the in situ distribution, biogeochemical pathways and chemical speciation of nickel and other elements. Elucidating the cellular and tissue-level distribution of trace element ions is inherently challenging due to the limitations of all analytical techniques. Therefore, we have combined the strengths of different techniques to interpret physiological processes in hyperaccumulator plants. Synchrotron X-ray Fluorescence Microscopy (XFM), micro Proton-Induced X-ray Emission (PIXE) and Scanning Electron Microscopy- Energy Dispersive X-ray Spectroscopy (SEM-EDS) have been used to map elemental distribution at the tissue-level and also at the sub-cellular level. X-ray Absorption Spectroscopy (XAS) has been used to reveal the chemical speciation of nickel and cobalt in intact plant tissues. The use of bright-field microscopy as well as SEM is essential for visualizing underlying anatomical features of the plant material being studied. Optionally, laser confocal microscopy in combination with selective fluorescent probes can assist to map trace element ions. Critical to the use of all aforementioned methods is appropriate sample preparation. The use of samples in frozen-hydrated state is preferred to minimize the effects of radiation-damage and movement of the sample during measurement. Therefore samples for XFM, PIXE and cryoSEM are rapidly frozen either using liquid propane or a metal mirror technique to affect water in vitreous state (direct freezing in LN2 is not suitable due to the Leidenfrost Effect). The use of a small LN2 cryoshipper enables collection of samples directly in the native habitat in the field. If not measured in frozen-hydrated state, then freeze- drying is suitable for measuring/mapping elemental concentrations providing the freeze-drying protocol is undertaken at a low temperature (starting <100°C) and with a long duration to limit sample shrinkage and morphological variations.
This presentation will demonstrate how combining multiple analytical techniques has shed light on the ecophysiology of nickel hyperaccumulator plans.

Concurrent Session 3: Radiotherapy I / 224

Synchrotron MRT radiation induces DNA damage and inflammatory response in normal mouse tissues distant from the irradiated volume

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Discovery of the radiation-induced bystander effect (RIBE) demonstrates that cell death and genomic instability are not restricted to cells that are directly exposed to ionising radiation. The RIBE refers to a situation where cells that have not been directly exposed to IR behave as though they have been exposed. This phenomenon presents real clinical consequences such as increased risk of secondary malignancies and inflammatory diseases after localised radiotherapy. Past reports indicate pronounced increase of DNA damage in bystander cells, especially in those of highly proliferative tissues. The fluctuations of the host's immunological response elicited by localised radiation exposure are a proposed mechanism of the bystander effect. Our aim was to establish the contributions of DNA damage response and the immunological components in the propagation of the RIBE, by using synchrotron-generated irradiation of immune-compromised mice. The Imaging and Medical Beamline (IMBL) at the Australian Synchrotron made it possible to investigate a new pre-clinical modality, microbeam radiation therapy (MRT), which yields superior therapeutic benefit while also preserving neighbouring healthy tissues in animal models, contrary to the broad beam modality currently used in hospitals. The MRT beam is generated when a single X-ray beam is split by a collimator, producing a lattice of planar microbeams. Wild-type C56BL/6 and Balb/c mice and immune-compromised mice (macrophage-depleted, CCL2 K/O and NSG) were irradiated with 10 Gy peak dose of MRT in an 8x8 mmˆ2 area on the right hind leg, with a dose rate of 49 Gy/sec. At 3 and 6 days post-irradiation, irradiated skin and unirradiated tissue samples were collected and probed for DNA damage using the γ-H2AX assay, apoptotic cell death and local immune response. Pronounced and robust DNA damage, apoptotic cells and immunological response were discovered in intestinal crypt cells of wild-type mice; these events were compromised in immune-deficient mice. The role of immune system components in propagation and persistence of systemic genome destabilisation after localised irradiation will be discussed.

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Recent Advances in Macro ATR-FTIR Microspectroscopic Technique for High Resolution Surface Characterisation at Australian Synchrotron IR Beamline

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Highly collimated synchrotron-IR beam offers 100-1000 times higher brightness than that of internal IR source used in laboratory-based FTIR instruments, enabling acquisition of high-quality FTIR spectra at diffraction-limited spatial resolution. Such properties make synchrotron-IR an excellent analytical platform for acquiring spatially resolved chemical "mapping" of materials at lateral resolution between 3-10μm.

Attenuated total reflection (ATR) FTIR technique is widely used for probing surface-specific molecular information of materials. Coupling synchrotron-IR beam to an ATR element further enhances the lateral resolution greater than those in transmission/reflectance, by a factor of refractive index (n) of the ATR element. For mapping measurements using Ge element (n=4), this has the effect of not only reducing the beam focus size (improving the lateral resolution) by

a factor of 4, but also reducing the mapping step size by 4 times relative to the stage step motion. As a result, ATR-FTIR measurement at Australian Synchrotron IR Beamline can be performed at minimum beam size of 1.9μm/1.2μm (with 20x/32x objective), and at minimum mapping step size of 250 nm.
Unlike microscopic-ATR (micro-ATR) technique, macro-ATR approach requires only a single contact between the ATR element and the sample throughout the measurement minimising potential of sample damage and also providing a faster scanning speed.
This work presents recent advances in macro-ATR devices developed at Australian Synchrotron. Two macro ATR devices have been made available for the users since February 2016. The first model, "hybrid macro-ATR", was developed by modifying the cantilever arm of the standard macro-ATR unit to accept Ge ATR elements with different facet sizes (1mm, 250μm and 100μm in diameter) normally used with micro-ATR objective. While the larger tip works well with softer materials that do not require high pressure, the small tips can provide higher pressure and allow measurements inside smaller regions with limited access suitable for hard/rough surfaces. The other macro-ATR device, "soft-contact piezo-controlled macro-ATR", was designed specifically for analysis of delicate and soft materials, by using a unique combination of piezo-controlled linear translation stages to achieve precise positioning and gentle approach of the sample towards the ATR facet. The capabilities of the technique have been demonstrated through a diverse range of research from material and food science to biology and single fibres.

Concurrent Session 2: Surfaces / 231

The Evolution of Surface Silica Nanoparticles on Coated Steel Surfaces under High UV and High Humidity Environments Observed Using Synchrotron Macro ATR-FTIR Microspectroscopy

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Corrosion of metallic surfaces is prevalent and of great concern in a wide range of industries, particularly those in transport, aviation, building and food sectors, reportedly responsible for a direct cost of $276 billion per annum(1). Galvanization has been widely used as a corrosion preventative method by coating the metallic surfaces with zinc that serves as a physical barrier to prevent corrosive substances from reaching the underlying metal. In tropical and sub-tropical climates with prolonged exposure to high UV and high humidity, thermosetting polymer coatings based on polyesters have also been used to provide an additional protection to the galvanized metal. This prevents the build-up of moisture within the pits present on the metallic surface where the zinc oxide passive film is weak, leading to localized corrosion(2). Recent advances in surface engineering using silica nanoparticles (SiO2NPs) have allowed the development of innovative and highly functional surface coatings with enhanced corrosion resistance and durability(3). Nevertheless, long-term effect of environmental factors upon these materials remains unknown.
In this study, chemical evolution of SiO2NPs-embedded polyester coatings on steel substrata was analysed after 5 years of exposure to tropical/sub-tropical environments in Singapore and Australia using synchrotron-based macro ATR-FTIR microspectroscopy and surface topographic techniques. Principal component analysis (PCA) based on FTIR spectral data observed at 9% SiO2NPs shows differences in their response to environmental factors between the control group and the surfaces subjected to 3-year exposure. The clustering feature suggests changes in molecular structure of the coating resulted from the exposure, which principally involved triazine ring vibration in the melamine resins. Such molecular evidence corroborates well with the fact

that the triazine ring is very sensitive to hydrolysis, particularly under high humidity conditions in tropical environments.

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Concurrent Session 4: Structural Biology II - Sponosred by DECTRIS / 204

Combating multidrug resistance. Structure of an endotoxin modifying enzyme

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Multiple drug resistance (MDR) in Gram-negative bacteria represents one of the most intractable problems facing modern medicine. Colistin and polymyxin are cationic antimicrobial peptide antibiotics which permeabilise the bacterial outer membrane and have been used to treat infections. Resistance to these antibiotics is conferred by the modification of the lipid A headgroups with phosphoethanolamine (PEA) moieties resulting in a reduced negative charge of the bacterial surface and exclusion of the drug. This modification is carried out by the enzyme, lipid A PEA transferase (LptA). Recently a mobile colistin resistance determinant, mcr-1, encoding an LptA homologue was identified in MDR Escherichia coli. We have determined the crystal structure of a full-length LptA from Neisseria sp. to 2.75Å resolution. The structure reveals a previously uncharacterized helical membrane domain and a periplasmic facing soluble domain. The domains are linked by a single helix that runs along the membrane surface interacting with the phospholipid head groups. Two helical insertions containing conserved charged residues lie between two transmembrane helices and are implicated in substrate binding. Intrinsic fluorescence, limited proteolysis and molecular dynamics studies suggest that the protein may sample different conformational states to enable the binding of two very different sized lipid substrates. These results provide novel insights into the mechanism of endotoxin modification and will aid a structure-guided rational drug design approach to treat multidrug resistant bacterial infections.

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EDOT-diketopyrrolopyrrole copolymers for polymer solar cells

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The photovoltaic properties of a series of diketopyrrolo[3,4-c]pyrrole (DPP) copolymers containing 3,4-ethylenedioxythiophene (EDOT) as a comonomer are reported. With use of different aryl

flanking units on the DPP core, namely thiophene, pyridine or phenyl, optical gaps ranging from 1.91 eV to 1.13 eV are achieved. When blended with the fullerene derivative [6,6]-phenyl C71- butyric acid methyl ester (PC71BM), the thiophene-flanked copolymer PDPP[T]2-EDOT with an optical gap of 1.13 eV was found to have the best photovoltaic performance, with an efficiency of 2.5% in an inverted device architecture. Despite having the lowest open circuit voltage of the three polymers studied, PDPP[T]2-EDOT-based devices were able to achieve superior efficiencies due to the high short circuit current of up to ˜ 15 mA/cm2. PDPP[T]2-EDOT-based devices also exhibit higher external quantum efficiencies which are associated with a superior microstructure as revealed by transmission electron microscopy (TEM) and grazing incidence wide-angle X-ray scattering (GIWAXS), which are associated with the enhanced aggregation tendency of PDPP[T]2- EDOT chains. In particular PDPP[T]2-EDOT:PC71BM blends were found to have a finer phase separated morphology with superior thin-film crystallinity. Surface morphology was also investigated with atomic force microscopy and near-edge X-ray absorption fine-structure spectroscopy.

Concurrent Session 1: Advanced Materials I / 286

Development of Efficient Semiconductor Photocatalysts for Solar Energy Capture

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Global energy concerns motivate the development of new and improved technologies for solar energy capture, with semiconductor photocatalysis expected to make an important contribution towards satisfying the energy needs of future societies. This talk will overview some of our recent research aimed at photocatalyst development for H2 production in alcohol-water mixtures, focussing primarily on transition metal oxide (TiO2), oxynitride (LaTiO2N, TaON) and nitride (Ta3N5) systems. The potential of 2D nanosheet photocatalysts made from earth-abundant elements, especially layered double hydroxides (M2+M3+-LDH, where M2+ = Ca2+, Mg2+, Mn2+, Fe2+, Co2+, Ni2+ or Zn2+ and M3+ = Al3+, Ga3+ or Fe3+) and graphitic carbon nitride (g-C3N4), for future solar energy harvesting and fuel production will also be explored. Strong emphasis here will be placed on the importance high resolution transmission electron microscopy (HRTEM), synchrotron-based X-ray spectroscopies (XPS, NEXAFS, EXAFS) and supporting DFT calculations to the understanding of photocatalyst function and ultimately performance optimization via exploitation of structure-activity relationships.

Concurrent Session 2: Advanced Materials II / 244

Investigation of electronic and morphological changes from thionation of naphthalene diimide (NDI)

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Organic semiconductors (OSCs) possess many inherent advantages that allow them to be used effectively as organic field effect transistors (OFETs). Solution processablility allows rapid, large area fabrication on low cost flexible substrate that make them ideal for specialized applications such as flexible displays and radio frequency identification (RFID).
Small molecule OSCs provide chemical specificity that allows changes to be mapped and examined more effectively than polymer based OSCs. Naphthalene diimide (NDI) provides a versatile framework with which to build upon and explore the effects of chemical functionalization. Recent work 1 on a small molecule framework from the same chemical family has shown that substitution of oxygen for sulphur, known as thionation, leads to an increase in crystallinity and an electron mobility. A thionated series of NDI OSCs has been synthesized to examine the effects of increased

degrees of thionation on optical, electronic and morphological properties. Investigation via the complimentary synchrotron based techniques of near edge x-ray absorption fine structure (NEXAFS) spectroscopy and grazing incidence wide angle xray scattering (GIWAXS) combine with atomic force microscopy (AFM) and top gate bottom contact (TGBC) transistors to help illuminate the resulting changes of the top interface with increasing degrees of thionation.
1 Tilley, A. J., Guo, C., Miltenburg, M. B., Schon, T. B., Yan, H., Li, Y. and Seferos, D. S. (2015), Thionation Enhances the Electron Mobility of Perylene Diimide for High Performance n-Channel Organic Field Effect Transistors. Adv. Funct. Mater., 25: 3321–3329. doi:10.1002/adfm.201500837

Concurrent Session 2: Advanced Materials II / 185

Behaviour and Strength of Collagen Materials

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Collagen is the main structural component of many natural materials including leather and surgical scaffold materials derived from skin, and heart valve leaflets derived from pericardium. Strength is one of the key characteristics required for the application of these materials however the basis for strength in these materials is not fully understood. We have used small angle X-ray scattering in combination with electron microscopy and atomic force microscopy to study the collagen structure in materials and better understand the behaviour of collagen fibrils during stress. Leather, pericardium and surgical scaffold materials were investigated, and a relationship was uncovered between material strength and collagen fibril orientation, fibril diameter and d-spacing. While there is still many unanswered questions, we are making progress on understanding the relationship between collagen structure and material strength in collagen based materials. This information could be used to optimize these natural materials for application and assist in the development of synthetic analogues of these natural tissues.

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Fe K-edge XANES of silicate glasses: A comparison between XAS and XFM

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Fe K-edge XANES was conducted on a suite of synthetic basaltic glasses on both the XAS beamline and the XFM beamline using the Maia detector. The results will be compared.

Concurrent Session 4: Technique Development / 171

First experiments with D-DIA apparatus on XAS

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The Macquarie University-Australian Synchrotron D-DIA apparatus is a large-volume solid-media apparatus for high pressure, high temperature in-situ x-ray experiments. The apparatus can subject a sample volume of up to 5 mmˆ3 to pressures to 6 GPa and temperatures to 1500 °C. During 2016/2 initial experiments were conducted on the XAS beamline. Uranium and Thorium L3-edge transmission XANES spectra were successfully collected from silicate liquid at ˜2 GPa, 1350 °C. Further tests with the sample assembly under ambient conditions indicate the lowest energy edge accessible in the apparatus with the present sample assembly is Ge K (11.1 keV). XAS was run in mirrorless mode at 38 keV for a proof-of-concept falling-sphere viscometry experiment. Soda-lime glass was rapidly melted by heating from ˜800 °C to ˜1400 °C at ˜2 GPa, and a falling platinum sphere was imaged with a CCD via YAG-mirror-lens setup.
Prospects for future applications of the D-DIA apparatus at the Australian Synchrotron will be discussed.

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Synchrotron Fourier Transform Infrared Mapping: A Novel Approach for Membrane Fouling Characterization

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We described a synchrotron Fourier transform infrared (IR) microscope method to characterize fouling layer. Combined fouling with organic foulant and colloidal silica in membrane distillation (MD) was used as an example. The synchrotron IR mapping was capable of revealing the spatial distribution of foulants as well as chemical information of foulant-membrane interface. Our results showed that synchrotron IR mapping was able to resolve the foulant spatial distribution in combined fouling in MD. Synchrotron IR mapping showed the spatial distribution of binary foulant (i.e., colloidal silica with alginate, bovine serum albumin (BSA) and humic acid, respectively) of the cross-section of MD fouling layer. The well-resolved synchrotron IR mapping is also able to quantify the foulant distribution along the cross-section of the fouled MD membrane, providing detailed description regarding the transport and accumulation of specific foulant, which is of paramount importance to elucidate fouling mechanisms. Our results indicate that the synchrotron IR mapping method has considerable potential for both qualitative and quantitative characterization of membrane fouling layer.

Concurrent Session 2: Structural Biology I - Sponsored by DECTRIS / 178

Investigation of Structure-Property Relationship Between Protic Ionic Liquids (PILs) and Biomolecules

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Protic ionic liquids (PILs) are increasingly being used as solvents for biological molecules due to their desirable properties. Biomolecules such as amino acids, peptides and proteins can be easily destabilized by small changes in their molecular interactions with solvents or solutes. In this study, the structure-property relationship between all 20 amino acids and 7 different peptides will be investigated in a broad range of PILs.

The PILs will comprise of alkyl ammonium cations combined with organic or inorganic anions. They will be synthesized based on an acid-base reaction by using conventional and high throughput methodology. The resulting PILs will then be characterized in terms of their key physicochemical and solvent properties by a number of experimental and instrumental analysis such as density, viscosity, conductivity measurements, thermal properties and spectrophotometry using NMR, SAXS/WAXS and DSC. Next, a detail solubility studies will be conducted for all amino acids and peptides in all of those PIL combinations. These biological molecules in PIL solvents will also be characterized via instrumental analysis such as SAXS/WAXS, DSC, FTIR and CD, respectively. This will enable the role of changing PIL cations and anions on amino acid and peptide stability to be quantified.

As a more general outcome of this study, design rules for stabilising functional biomolecules in PIL based solvents will be developed.

Concurrent Session 1: Advanced Materials I / 194

Probing Long- and Short-Range Disorder in Y2Ti2-xHfxO7 by Diffraction and Spectroscopy

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We have studied the long-range average and short-range local structures in Y2Ti2-xHfxO7 (x = 0-2.0) using diffraction and spectroscopy techniques respectively. Both neutron and synchrotron X-ray powder diffraction data show a clear phase transition of the average structure from ordered pyrochlore to disordered defect-fluorite at x ˜ 1.6; the long-range anion disorder appears to develop gradually throughout the entire pyrochlore region in contrast to the rapid loss of cation ordering from x = 1.4 to 1.6. The commonly observed two-phase region around the pyrochlore / defect-fluorite phase boundary is absent in this system demonstrating high sample quality. X-ray absorption near-edge structure (XANES) results at the Y L2-, Ti K- and L3,2-, Hf L3- and O K-edges indicate a gradual local structural evolution across the whole compositional range; the Y coordination number (CN) decreases and the CN around Ti and Hf increases with increasing Hf content (x). The spectroscopic results suggest that the local disorder occurs long before the pyrochlore to defect-fluorite phase boundary as determined by diffraction, and this disorder evolves continuously from short- to medium- and eventually to long-range detectable by diffraction. This study highlights the complex disordering process in pyrochlore oxides, and the importance of a multi-technique approach to tackle disorder over different length scales and in the anion and cation sublattices respectively. The results are important in the context of potential applications of these oxides such as ionic conductors and radiation-resistant nuclear waste forms.

Concurrent Session 3: Industry & Innovation / 292

Discussion Panel