AOFSRR 2015 in conjunction with User Meeting 2015

Wednesday 25 November 2015 - Friday 27 November 2015

National Centre for Synchrotron Science

Book of Abstracts

Information for Delegates

This book of abstracts is organised by presenter surname. Should you wish to produce your own customised book of abstracts more suited to your personal interests, please follow the *Abstract Index* link on the meeting website. Here, you can filter abstracts by author, keyword, track, session or presentation type, and export the results to a pdf file.

Contents

Techniques II / 9

Visualizing Au-Au bond formation in solution with femtosecond X-ray scattering

Prof. ADACHI, Shin-ichi[1]

[1] *Photon Factory, IMSS, KEK*

Corresponding Author(s): shinichi.adachi@kek.jp

Bond formation is an essential process in chemical reactions, but it is challenging to keep track of detailed atomic movements associated with bond formation because of its bimolecular nature. Bond formation in solution phase has been especially elusive because it is difficult to initiate and follow such diffusion-limited bimolecular processes with ultrafast time resolution. In this regard, a dicyanoaurate(I) oligomer complex, [Au(CN)2–]n, offers a good model system in which to study the dynamics of bond formation in solution. Using femtosecond time-resolved X-ray scattering, we successfully visualized in real time the birth of a gold trimer complex, [Au(CN)2–]3, that occurs via photoinduced formation of Au-Au covalent bonds [1]. This work showcases the possibility of tracking detailed structural changes in solution with sub-ps temporal and sub-angstrom spatial resolutions, thanks to the advent of X-ray free electron lasers and the advance of data analysis of time-resolved solution scattering data.

REFERENCE

[1] Kim, K. H., Kim, J. G., Nozawa, S., Sato, T., Oang, K. Y., Kim, T. W., Ki, H., Jo, J., Park, S., Song, C., Sato, T., Ogawa, K., Togashi, T., Tono, K., Yabashi, M., Ishikawa, T., Kim, J., Ryoo, R., Kim, J., Ihee, H. & Adachi, S., Nature, 518, 385-389 (2015).

Poster Session 1 - Board: BT-31 / **207**

Adaptive control of scanning stages

Author(s): Mr. AFSHAR, Nader[1]
Co-author(s): HOWARD, Daryl [2] ; Dr. DE JONGE, Martin [2] ; PATERSON, David [2] ; Dr. STEPHENSON, Macleay [3]

[1] *Controls Engineer*

[2] *Australian Synchrotron*

[3] *ANSTO*

Corresponding Author(s): nader.afshar@synchrotron.org.au

Scanning motion axes are increasingly becoming key components to many beamlines. The velocity control requirements raise challenges at hardware and software control levels. Tracking a velocity profile with the required precision and stability can be a challenging task for the motion systems. It is not unusual to see motion stages, motors and sensor working close to their technical limits so hardware shall be design and configured very precisely. On top of the hardware configuration, we usually require a very fine-tuned controller to achieve the tracking and disturbance rejection performance required. In addition to that, the scanner stages are usually expected to perform at the same level of precision and stability, over a very wide range of velocity and accelerations. Assuming that requirements are achievable for different conditions (velocities) with different tunings, it is usually very difficult to achieve adequate performance with one tuned controller. One approach to cover a wide dynamic velocity range is to apply an adaptive tuning to cope with changing conditions. In this poster, the problem is demonstrated with examples and test cases of wide scanning velocity range, using our modelling framework and real stages with GeoBrick pmac controllers to prove the concept and feasibility of this approach.

Energy Materials I / 37

Effects of Ag-Embedment on electronic and ionic conductivities of LiMnPO4 and performances as a cathode for lithium-ion batteries

Dr. AHN, Docheon[1]

[1] *Pohang Accelerator Laboratory*

Corresponding Author(s): adc4055@postech.ac.kr

Ag-embedded LiMnPO4 (LMP) cathode was synthesized by solid-state reaction using 1 wt% Ag precursor. Structure, morphology, and electrical conductivity studies of Ag-embedded LMP were performed by high resolution synchrotron powder X-ray diffraction, high resolution transmission electron microscopy, energy dispersive X-ray spectroscopy, and four probe measurements. An Ag nanoparticle (˜ 26 nm) surrounded by several olivine crystallites within a single particle dramatically improved overall electrical conductivity of LMP by four orders of magnitude relative to that of pristine LMP, playing roles as conducting bridges among LMP crystallites as well as particles. Rietveld analysis confirmed structural variations related to modification of atomic bond lengths of Mn-O, P-O, and Li-O coordination due to Ag-embedment and thereby leads to facile Li ion diffusion in LMP. Consequently, although small amount of Ag was included, Ag-embedded LMP cathode exhibited outstanding electrochemical performances (92 mAhg-1 at 10 C) versus lithium.

Poster Session 2 - Board: AM-08 / **54**

The Thermal Expansion of Li and Na intercalated ZrW2O8

Author(s): Mr. AL BAHRI, Othman[1]
Co-author(s): Ms. JEFFRESS, Laura [1] ; Mr. CHRISTIAN, James [1] ; SHARMA, Neeraj [2]

[1] *The University of New South Wales*

[2] *UNSW*

Corresponding Author(s): z3435486@zmail.unsw.edu.au

Thermal expansion has been associated with many factors limiting the functionality and lifetime of various devices. Zirconium Tungsten Oxide, ZrW2O8, is known for its isotropic Negative Thermal Expansion (NTE) from 0.3 to 1050 K. In this study we report a novel approach to controlling the thermal expansion of this material. Li- and Na-ion batteries were constructed with ZrW2O8 used as an anode into which Li and Na intercalates. The main advantage of using batteries is the ability to precisely control the amount of Li and Na that is inserted. Electrochemical analysis shows that ZrW2O8 exhibits higher first discharge capacity of 463 mAh/g as an anode for Li-ion batteries compared to 114 mAh/g in Na-ion batteries. In principle, this suggests that more Li can intercalate into ZrW2O8 than Na. In situ synchrotron powder X-ray diffraction (XRD) data shows that Li and Na intercalates into ZrW2O8 as the batteries are discharged. While ZrW2O8 maintains its stability as Na was inserted to the maximum capacity, it breaks down into an amorphous phase as Li is inserted. Interestingly, in both cases no shifts were observed in the ZrW2O8 reflection positions as Li and Na are inserted which may suggest that ZrW2O8 is a zero-strain material for Li and Na insertion.
Synchrotron VT-XRD will be used to quantify the effect of the amount of intercalated Li and Na into ZrW2O8 on its thermal expansion and whether that may result in zero thermal expansion.

Poster Session 1 - Board: AM-05 / **40**

Activation energies for phase transformations in electrospun titania nanofibers: comparing the influence of argon and air atmospheres

Author(s): Mr. ALBETRAN, HANI[1]
Co-author(s): Prof. O'CONNOR, B. H. [2] ; Prof. LOW, I. M. [2]

[1] *Curtin University & University of Dammam*

[2] *Curtin University*

Corresponding Author(s): hani.albatran@postgrad.curtin.edu.au

The paper reports the way in which titania absolute phase levels (amorphous, anatase and rutile forms) in electrospun amorphous titania nanofibers change with temperature over the range 25–900 °C according to the controlling environment for calcination as the material is heated non-isothermally. The environments chosen for study were air and argon. A novel method was developed to extract the absolute levels of amorphous titania and crystalline anatase and rutile from the synchrotron radiation diffraction (SRD) data. Determination of absolute phase levels facilitated estimation of the activation energies for the amorphous-to-anatase transformation, 45(9) kJ/mol in argon and 69(17) in air; and for the anatase-to-rutile transformation energies, 97(7) kJ/mol for argon and 129(5) for air. An activation energy estimate for amorphous-to-crystalline titania in argon, 142(21) kJ/mol using differential scanning calorimetry (DSC) is consistent with the SRD results. The differences between the activation energies for heating in air and argon are attributed to the presence of substantial oxygen vacancies when the material is heated in argon. Estimates of anatase and rutile oxygen site occupancies from the SRD data show that (i) anatase has discernible oxygen vacancies in argon between 700–900 °C corresponding to the stoichiometry TiO2-x with x < 0.4; (ii) the anatase stoichiometry in air at these temperatures is TiO2; and (iii) rutile does not have significant oxygen vacancies in either argon or air between 800–900 °C.

Soft Matter / **100**

Water and organic solvent behavior of thin and long cellulose nanofibrils easily deconstructed from Australian arid grass T. pungens

Author(s): Dr. ANNAMALAI, Pratheep Kumar[1]
Co-author(s): Dr. GARVEY, Chris [2] ; Dr. AMIRALIAN, Nasim [1] ; Prof. MARTIN, Darren [1]

[1] *The University of Queensland*

[2] *ANSTO*

Corresponding Author(s): p.annamalai@uq.edu.au, n.amiralian@uq.edu.au

The utilisation of lignocellulosic plant biomass has gained revived interest due to the increased awareness fuel economy and sustainable materials. Many teams around the world are producing nanocellulose by the careful removal of some or the entire matrix to produce nanocellulose. Recently we have discovered and patented a unique, very high quality grade of nanofibrillated cellulose (NFC) or cellulose nanofibrils which can be isolated from Australian native spinifex grass, with no aggressive chemical pre-treatment, and with the lowest reported mechanical energy [1]. When benchmarked against any known NFC in both academic and commercial materials, this nanocellulose has the highest aspect ratio (length-to-thickness) achieved at very low energy consumption. In order to understand and correlate the low-energy processing of nanofibrils with structural morphology of grass, we have studied the structural changes at length scales of fibrils and their bundles, upon those mild chemical and mechanical treatments using small angle neutron and X-ray scattering technique. Here we have made the simplification that all polymers while chemically distinct are homeogenous to the perspective of small angle x-ray / and neutron scattering.[2] Our preliminary investigation using X-ray diffraction, SAXS and SANS under dry and swelling conditions of the raw and isolated cellulose nanofibrils indicated that the cellulose nanocrystals are embedded in a water-responsive (swellable) polysaccharide matrix. The presentation will be made on the water and organic solvent behaviour of native and isolated cellulose nanofibrils and their relationship with low-energy homogenisation.

Poster Session 1 - Board: IM-11 / **156**

Design and Implementation of an Optical Ptychographic Microscope for quantitative bio-imaging at La Trobe University

Author(s): Mr. ANTHONY, Nicholas[1]
Co-author(s): Dr. BRIAN, Abbey [1] ; Mr. CADENAZZI, Guido [1]

[1] *La Trobe University, ARC Centre of Excellence for Advanced Molecular Imaging*

Corresponding Author(s): n.anthony@latrobe.edu.au

Ptychography is a method for quantitatively determining the phase of a samples' complex transmission function. The technique relies upon the collection of multiple overlapping coherent diffraction patterns from laterally displaced points on the sample. The overlap of measurement points provides complementary information that significantly aids in the reconstruction of the complex wavefield exiting the sample. Moreover the method is sufficiently robust to simultaneously recover both the sample and probe functions from a single dataset.
Ptychography was initially realised for applications involving electron microscopy (Hoppe et al., Acta Cryst. A, 1969) but has been widely adopted by the x-ray lensless imaging community. More recently, it has found application in the optical regime (e.g. Godden et al. Optics Express, 2014) where it can be applied to 2D and 3D quantitative phase contrast imaging of weakly interacting specimens.
Here we describe and demonstrate the realisation of a high-quality optical ptychographic microscope at La Trobe University comprising 'off the shelf' components. Our microscope provides quantitative sample information with extreme sensitivity opening up a range of applications including bio-mechanical measurements on cellular samples. Some recent results using this microscope are showcased here.

Poster Session 1 - Board: BT-09 / **86**

Condensed Phase applications at the THz beamline

Author(s): APPADOO, Dominique[1]
Co-author(s): PLATHE, Ruth [1]

[1] *Australian Synchrotron*

Corresponding Author(s): dom.appadoo@synchrotron.org.au

Spectroscopic studies of condensed phase matter have been successfully conducted at the THz/Far-IR beamline of Australian Synchrotron for a few years and applications range from nanotechnology, geology, renewable energy sources, forensics, biology, engineering and the environment. 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 in studying liquids in the THz spectral region.

Poster Session 1 - Board: BT-21 / **177**

yaIBEX - Yet Another Integrated Beamline Environment for (X)-ray Crystallography

Author(s): Dr. ARAGAO, David[1]
Co-author(s): Dr. JONG, Lenneke [1] ; Mr. CLARKEN, Robbie [1] ; MUDIE, Nathan [1] ; Dr. PRICE, Jason [1] ; ERIKSSON, Daniel [1] ; MOLL, Andreas [1] ; FELZMANN, Uli [1] ; CARADOC-DAVIES, Tom [2]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron.*

Corresponding Author(s): david.aragao@synchrotron.org.au, lenneke.jong@synchrotron.org.au

The MX1 and MX2 beamlines at the Australian Synchrotron are single crystal diffraction beamlines, servicing the needs of protein and chemical crystallography communities. We have developed a web-based user interface for driving data collections, called YAIBEX (Yet Another Integrated Beamline Environment for Crystallography). This system is designed to replace the collect tab on the SSRL BluICE system which is written in TCL language and was forked at deployment from the original code making it difficult to take advantage of bug fixes and improvements from the upstream. Our system utilises Flask, a minimalist Python web application framework, chosen to leverage the existing Python-based infrastructure existing at the beamline, the language's widespread use in the scientific community including existing libraries, and better support from the local Controls and Scientific Computing groups. Improvements on the existing system include integration with custom beamline libraries, user portal integration for pre-filling information and an easy, tabular layout to view a history of data collections for the current session and remote access directly in the user internet browser. Current developments include interaction with the robotic sample changer to allow mounting samples autonomously.

Poster Session 2 - Board: AM-06 / **42**

Structural damage evaluation of a ceramic matrix composite

Author(s): Dr. ARHATARI, Benedicta[1]
Co-author(s): Mr. ZONNEVELDT, Matthew [2] ; Dr. THORNTON, John [2] ; Dr. ABBEY, Brian [1]

[1] *La Trobe University*

[2] *Defence Science and Technology Organisation*

Corresponding Author(s): b.arhatari@latrobe.edu.au

We studied Ceramic Matrix Composites (CMC) as a new class of structural materials that combine high strength at high temperatures with moderate toughness. Mapping the failure of CMC under mechanical load explains the mechanisms responsible for their toughness. In this study, the correlation of the x-ray radiographs of CMC samples to critical points in the load/displacement curve show that the fibre bundles slowed crack propagation due to strain energy being expended in breaking these fibres and in pulling bundles out of the surrounding matrix material. The results were also complemented with micro X-ray Computed Tomography after failure. Finally, mapping the strain evolution at length scales of micrometres during bending were done using Digital Image Correlation.

Poster Session 2 - Board: EM-04 / **87**

Altering the UV-Vis spectra of photoactive molecules using small fragments

Author(s): Ms. AROOJ, Qudsia[1]
Co-author(s): Prof. WANG, Feng [1] ; Mr. CHENG, Yibing [2] ; Mr. ZHAO, Zhixin [3] ; Mr. LIU, zonghao [3]

[1] *1Molecular Model Discovery Labortary, Department of Chemistry and Biotechnology, School of science, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Melbourne, Victoria 3122, Australia.*

[2] *3Department of Materials Engineering, Monash University, Melbourne, Victoria, 3800, Australia*

[3] *2Michael Grätzel Center for Mesoscopic Solar Cells, National Laboratory for Optoelectronics and College of Optoelectronic Science and Engineering, Huazhong University of Science and Technology, Wuhan 430074, P. R. China.*

Corresponding Author(s): qarooj@swin.edu.au

Qudsia Arooj1, Feng Wang1*, Zonghao Liu2, Zhixin Zhao2, Yi-Bing Cheng3
The energy provided by the sun in one hour is larger than the energy consumption globally each year thus it has been a challenge to convert solar energy to electricity cost-effectively in organic dye sensitized solar cells (DSSC). In recent years photoactive molecules such as the most recently available zzx-op dyes have gained attention due to their potential to construct high efficiency tandem cells with conventional n-DSSCs. A number of high performing p-type push and pull dyes, i.e., zzx-op dyes which consist of a perylenemonoimide (PMID) as an electron acceptor (A) and a di(p-carboxyphenyl)amine (DCPA) as an electron donor (D) and a pi-conjugated linker for the D-pi-A dyes are recently synthesized. In this presentation, we focus on the expansion of the UV-Vis spectra of these photoactive molecules through rationally change the pi-linkers through molecular modelling by combining their optimal combinations which best enhance the UV-Vis spectra of the new photoactive molecules (Fig. 1). Time-dependent Density functional theory (TD-DFT) simulation using DFT based PBE0/6-311G(d) model are employed to simulate the UV-Vis spectra. The results have shown in the improvement of the UV-Vis absorption and preliminary results will be presented.

Earth and Environment / 96

Mid-infrared and far-infrared synchrotron sourced spectroscopy of Titan's cyanide haze

Author(s): Ms. AUCHETTL, Rebecca[1]
Co-author(s): Dr. ENNIS, Courtney [1] ; Mr. RUZI, Mahmut [2] ; Dr. ROBERTSON, Evan [1]

[1] *La Trobe University*

[2] *Latrobe University*

Corresponding Author(s): rebecca.auchettl@gmail.com

Saturn's largest moon Titan has a chemically diverse atmosphere, an icy surface and is the only other planetary-body with comparable molecular complexity to Earth. Thus, analysis of Titan's atmosphere can give new insight towards prebiotic Earth chemistry. In Titan's atmosphere, ongoing photolytic and radiolytic interactions with N2 and CH4 precursor molecules yield a suite of nitrile species. Polymeric nitriles (tholins) condense and form suspended aerosols which contribute to the distinctive orange haze of Titan's atmosphere. These unidentified species are seasonally reactive as seen via suspected aerosol far-infrared absorption bands at 220cm-1. However, to complicate assigning these features, there have been no infrared analyses on the morphology of nitrile aerosols under Titan conditions. Researchers have also not yet determined the importance of temperature, pressure and particle size on the spectra of pure nitrile aerosols over IR wavelengths. Yet without such an understanding, the fundamental morphology of nitrile aerosols will remain unresolved and the unidentified emission features of Titan's stratosphere cannot be identified. In this talk we present mid-infrared and far-infrared studies of select nitrile aerosols under conditions replicating the Titan atmosphere. The laboratory study was completed at the Australian Synchrotron Terahertz/Far-Infrared beamline using a specialised enclosive flow cooling cell to generate nitrile aerosols. Our research provides the astrochemistry community complete infrared signatures of pure nitrile aerosols in mid-infrared and far-infrared over a range of astrochemical conditions.

Poster Session 2 - Board: AM-12 / **91**

Study of the precipitation strengthening in Mg-Sn-Zn alloy using synchrotron radiation

Author(s): Mr. BAHRAMI MOTLAGH, Ehsan[1]
Co-author(s): Prof. BARNETT, Matthew [2] ; Dr. GHADERI, Alireza [2] ; Dr. KADA, Sitarama Raju [2] ; Dr. LYNCH, Peter [2] ; Dr. DORIN, Thomas [2]

[1] *Institute for Frontier Materials, Deakin University*

[2] *Institute for Frontier Materials, Deakin University,*

Corresponding Author(s): ebahrami@deakin.edu.au

In this work, SAXS/WAXS and powder diffraction beamlines at the Australian synchrotron were employed to study the mechanical response of an Mg-Sn-Zn alloy. First, volume fraction and particle size of [U+3016]Mg[U+3017]_2 Sn precipitates as a function of aging time (0h, 2h, 4h, 10h, 24h) at [U+3016]200[U+3017]^oC was evaluated using small angle x-ray scattering (SAXS). Then the corresponding samples were deformed in-situ using the powder diffraction beamline to determine internal strains and deformation mode activity. [U+3016]Mg[U+3017]_2 Sn precipitates were found to provide a strong electronic density contrast and thus act as strong X-Ray scatterers, which is ideal for SAXS. The SAXS data were analysed assuming spherical precipitate morphology to yield the size distribution and volume fraction. Elastic strains were determined to an accuracy of $\pm 2 \times$ [U+3016]10[U+3017]^(-4). Relaxation of internal stresses (indicated by internal strain measurements) were used to determine the onset of basal slip. Intensity changes were used to mark the onset of twinning. The results show a good correlation between precipitate volume fractions and onset of plasticity. Internal stresses within the precipitates reveal negligible influences of back-stresses. These findings provide important insight into the mechanism of strengthening

Poster Session 2 - Board: AM-14 / **97**

Photoemission study on local phase transition of MoTe2

Author(s): Prof. YANG, Heejun[1] ; Prof. LEE, Young Hee[1] ; Prof. KIM, Sung Wng[1] ; Dr. CHO, Suyeon[1]

Co-author(s): Dr. BAIK, Jaeyoon [2] ; Ms. KIM, Sera [1] ; Mr. KIM, Jung Ho [1] ; Mr. KEUM, Donghoon [1] ; Mr. SEOK, Jinbong [1]

[1] *IBS Center for Intergrated Nanostructure Physics(CINAP), Institute for Basic Science, Sungkyunkwan Univertsity, Suwon 440-746, Korea*

[2] *Pohang Accelerator Laboratory, South Korea*

Corresponding Author(s): cla100@postech.ac.kr

We investigate local phase transition of MoTe2 using scanning photoemission electron spectroscopy. In spite of many effort of realizing ohmic-contacted heterostuctures between 2-dimensional atomic materials, inherent limitation in the transfer method or chemical doping method, such as impurities, inhomogeneous junction and so on, has not allowed true ohmic contact due to a large interface resistance. In this work, phase transition from the 2H to 1T' phase in MoTe2 was driven by laser-irradiation, where this system allow us clean homogeneous homojunction ohmic contact between semiconducting 2H- and metallic 1T'-MoTe2 with low interface resistance. Here we verified the laser irradiation induced the phase transition by analyzing the Mo and Te 3d core-level spectrum on each micron-domain area.

Biological Systems / 80

Synchrotron FTIR microspectroscopy coupled with Principal Component Analysis shows evidence for the cellular bystander effect

Author(s): Dr. LIPIEC, Ewelina[1] ; Dr. BAMBERY, Keith R[2]
Co-author(s): Dr. LEKKI, Janusz [1] ; Dr. TOBIN, Mark J [2] ; Dr. VOGEL, Christian [3] ; Dr. WHELAN, Donna [4] ; Dr. WOOD, Bayden R [4] ; Prof. KWIATEK, Wojciech M [1]

[1] *The Henryk Niewodniczanski Institute of Nuclear Physics, PAN, Kraków, Poland*

[2] *Infrared Microscopy Beamline, Australian Synchrotron*

[3] *BAM Federal Institute for Materials Research and Testing, Berlin, Germany*

[4] *Centre for Biospectroscopy, Monash University*

Corresponding Author(s): keith.bambery@synchrotron.org.au

Synchrotron Radiation - Fourier Transform Infrared (SR-FTIR) microscopy coupled with multivariate data analysis was used to monitor the radiation induced cellular bystander effect. Living prostate cancer PC-3 cells were singly irradiated with various numbers of protons, ranging from 50-2000, with an energy of either 1 or 2 MeV using a proton microprobe. SR-FTIR spectra of cells, fixed after exposure to protons and non-irradiated neighboring cells (bystander cells) were recorded. Principal Component Analysis (PCA) was applied to analyse the data set. Spectral differences associated with changes in the nucleic acids and with changes in protein secondary structure were observed in both the directly targeted and the bystander cells. The percentage of affected bystander cells versus the applied number of protons at the two different energies was calculated. It was found that, of all the applied doses, 400 protons at 2 MeV was the most significant in causing macromolecular perturbation in PC-3 bystander cells.

Techniques II / 123

Porous coordination polymers of alkyl amine ligands for carbon dioxide capture

Author(s): Prof. BATTEN, Stuart[1]
Co-author(s): Dr. TURNER, David [1] ; Dr. HAWES, Chris [1] ; Dr. HICKS, Jamie [1] ; Mr. EMERSON, Adrian [1] ; Ms. BEECHING, Lianna [1]

[1] *Monash University*

Corresponding Author(s): stuart.batten@monash.edu

We have been investigating the use of alkyl amine ligands in the synthesis of porous coordination polymers. The amine groups form part of the ligand backbones, and are designed to improve

the selectivity of carbon dioxide capture over other gases. More than 50 new ligands have been made, and more than a dozen porous frameworks identified and tested. The ligands investigated fall into three different categories: (i) azamacrocycles, (ii) piperazines, and (iii) linear alkyl amines. Good carbon dioxide capacities and selectivities have been observed, as well as unusual structural transformations and interesting structural features. Related work has also looked at the use of these materials for the separation of complex aromatic hydrocarbon mixtures, and the incorporation of metal carbonyl species into the ligand backbones, with a view to creating new heterogeneous catalysts.

Poster Session 1 - Board: AM-13 / **93**

Chemistry and Single Molecule Magnetism of Halogenated 8-Quinolinolatodysprosium(III) Complexes

Author(s): Mr. BEAUMONT, Owen[1]
Co-author(s): Prof. DEACON, Glen [1] ; Dr. MOUBARAKI, Boujemaa [1] ; Dr. LANGLEY, Stuart [2] ; Prof. MURRAY, Keith [1] ; Dr. TURNER, David [1] ; Prof. JUNK, Peter [3]

[1] *Monash University*

[2] *London Metropolitan University*

[3] *James Cook University*

Corresponding Author(s): owen.beaumont@monash.edu

Long term data storage devices, such as computer hard drive disks, utilize magnetic field orientations of ferromagnet arrays to encode and store information.The size of these devices is therefore contingent upon the size of the magnets used. Molecules capable of magnetic hysteresis, termed single molecule magnets, are of interest then as a means to miniaturize data storage devices. Realization of this application however requires single molecule magnets capable of magnetic hysteresis above the temperature of liquid nitrogen. Effort to increase single molecule magnet thermal stability is therefore twofold. The first is the discovery of new single molecule magnets. The second is the elucidation of how chemical structure influences the thermal stability of single molecule magnet magnetic hysteresis. Details on the discovery of three new single molecule magnets along with ongoing efforts to elucidate the influence of structure upon thermal stability of magnetic hysteresis will therefore be covered.

Poster Session 1 - Board: BT-33 / **214**

Low-volume electrochemical cell for in-situ measurement of XAS spectra of reactive metal compounds and biomolecules

Author(s): Dr. BEST, Stephen[1]
Co-author(s): Prof. LAY, Peter [2] ; Dr. LEVINA, Aviva [2]

[1] *University of Melbourne*

[2] *Sydney University*

Corresponding Author(s): spbest@unimelb.edu.au

The design and operation of a low volume spectroelectrochemical (SEC) cell for the measurement of X-ray absorption spectra (XAS) of solutions at room temperature will be described. The XAS-SEC cell is suitable for operation with fluorescence detection where the 2×2×12 mm working electrode chamber doubles as the solution cell for XAS measurements. A key element of the design of the experiment is the control of the flow properties of the solution under electrochemical/XAS interrogation where a continuous pulsing of the solution with a small nett flow rate ensures both rapid electrosynthesis and that photoreduction can be controlled. The operation of the XAS-SEC cell is demonstrated by the X-ray absorption near edge spectra (XANES) of solutions of K3[Fe(C2O4)3] under static and dynamic flow conditions and the XANES of [Fe(C2O4)3]4- obtained by electrochemical reduction. The suitability of the approach for the study of protein samples is demonstrated by preliminary measurement of the ubiquitous electron transport protein cytochrome c.

Poster Session 1 - Board: EM-03 / **83**

Low temperature IR spectra of frozen solutions of Ferrocene – The meeting place of experiment and theory?"

Author(s): Dr. BEST, Stephen[1]
Co-author(s): Prof. WANG, Feng [2] ; Prof. CHANTLER, Christopher Thomas [1] ; Mr. ISLAM, Shawkat [3] ; Mr. ISLAM, Taulid [4] ; Mr. TREVORAH, Roy [4] ; Dr. APPADOO, Dominique [5]

[1] *University of Melbourne*

[2] *Swinburne University of Technology*

[3] *PhD Candidate*

[4] *The University of Melbourne*

[5] *The Australian Synchrotron*

Corresponding Author(s): spbest@unimelb.edu.au

While the measurement of low-temperature spectra of "isolated molecules" can achieved by the use of noble-gas matrices, a simpler method using paraffin wax has been applied to the preparation of samples of ferrocene (Fc) for cryogenic IR spectroscopy. By control of the solute concentration it has been possible to achieve spectra characteristic of those obtained from RT solutions in non-coordinating solvents where the wax samples have the advantage of being suitable for low temperature measurements, avoiding further crystallisation during cooling.
The key IR bands sensitive to the conformational form of Fc are found to have a complicated temperature dependence that provides information on the conformational distribution of the species and the shape of the potential energy surface. Importantly, the low temperature spectra give a pattern of IR bands in excellent agreement with calculation (band splitting and intensities). The study has implications both in terms of the conformational analysis of the archetypal organometallic arene, Fc, but also the relationship between the calculated and observed IR spectra of molecules with low energy conformational barriers.

Poster Session 1 - Board: SB-03 / **94**

Structural and functional investigation of CprB, a member of the TetR-family of proteins from Streptomyces coelicolor A3(2)

Author(s): Mr. BHUKYA, Hussain[1]
Co-author(s): Dr. YANG, Yuanzhong [2] ; Dr. ZHANG, Chunfang [2] ; Prof. HEARN, Milton [2] ; Prof. ANAND, Ruchi [3] ; Dr. MITRI, Khosse [2] ; Dr. BOYSEN, Reinhard [2]

[1] *1. IITB-Monash Research Academy, IIT Bombay, Powai, Mumbai 400076, India. 2. Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India. 3. Australian Centre for Research on Separation Science (ACROSS), School of Chemistry, Monash University, Melbourne, Victoria 3800, Australia*

[2] *Australian Centre for Research on Separation Science (ACROSS), School of Chemistry, Monash University, Melbourne, Victoria 3800, Australia*

[3] *Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India*

Corresponding Author(s): hussaingps@gmail.com

Metabolic pathways activated by small chemical signaling molecules in the soil-dwelling, filamentous Gram-positive bacterial genus *Streptomyces* regulate antibiotics production, morphogenesis and resistance mechanisms. These species produce a wide spectrum of biologically active secondary metabolites contributing to $> 70\%$ of the known naturally occurring antibiotics. Small diffusible molecules, γ-butyrolactones (GBLs) are signaling molecules in *Streptomyces* and interact with transcriptional regulatory proteins that trigger downstream responses. Their identity and mode of action in *Streptomyces coelicolor* is hitherto unknown. In this investigation, purified CprB, a GBL receptor, was used as an affinity matrix to enrich and identify the target molecule(s) from an extracellular extract of *S. coelicolor*. Results from LC-ESI-MS/MS studies of compounds bound to CprB suggest that there is more than one signaling molecule that controls its DNA binding activity. Furthermore, in order to decipher the structural basis and associated conformational

changes during CprB-DNA interaction, we here present a CprB-DNA complex crystal structure at 3.25 Å resolution. CprB binds to the DNA as dimer of dimers via the helix-turn-helix (HTH) motif with the mode of DNA binding analogous to the broad spectrum multidrug resistance regulator QacR from *Staphylococcus aureus*. Binding of the DNA induces restructuring of the CprB dimeric interface, thereby triggering a pendulum-like motion of the HTH motif. Our studies suggest that CprB serves as an autoregulator and is a part of a regulatory network for antibiotic production and resistance pathways responding to signalling molecules in *S. coelicolor*.

Poster Session 2 - Board: SB-12 / **135**

Structural studies of the Moraxella catarrhalis DOXP reductoisomerase

Author(s): Dr. BIRKINSHAW, Richard[1]
Co-author(s): Prof. BRADY, Leo [2]

[1] *Walter and Eliza Hall Institute*

[2] *University of Bristol*

Corresponding Author(s): birkinshaw.r@wehi.edu.au

Emerging resistance to current therapeutics and the inadequacies of current treatments for human diseases have led to a strong demand for the development of novel therapeutics. Moraxella catarrhalis is a human mucosal pathogen frequently associated with opportunistic respiratory and middle ear infections. As with other gram-negative bacteria, it relies on the methylerythritol (MEP) pathway for biosynthesis of terpenes, essential secondary metabolites. The MEP pathway is absent in humans providing an attractive target for novel therapeutic design.
The first committed step in the MEP pathway is performed by the 1-deoxy-D-xylulose 5-phosphate (DOXP) reductoisomerase enzyme. We have expressed, purified, performed preliminary kinetic analysis and solved crystal structures of the DOXP reductoisomerase determined in three different forms related to its catalytic cycle. These include a catalytically relevant inhibitory complex with fosmidomycin (a DOXP analogue), which help to delineate features of the active site that could be selectively targeted in the development of inhibitor-based therapeutics. This study provides a strong foundation for the rational design of novel DOXP reductoisomerase inhibitors in the future and provides a new target to alleviate the burden on established anti-bacterial treatments.

Poster Session 2 - Board: AM-04 / **28**

Self-Selecting Homochiral Quadruple-Stranded Helicates and Mesocates

Author(s): Ms. BOER, Stephanie[1]
Co-author(s): Dr. TURNER, David [1]

[1] *Monash University*

Corresponding Author(s): stephanie.boer@monash.edu

A series of quadruple-stranded Cu4L4 cages have been synthesised using ligands containing a biphenylsulfonediimide core substituted with two amino acid groups. Analogous chiral complexes (helicates) and achiral complexes (mesocates) can be formed by controlling or removing the stereocentres within the ligands. Helicates, complexes which have supramolecular chirality generated by a helical sense within the complex, are formed using leucine-substituted ligands. These quadruple stranded Cu4L4 helicates contain copper paddlewheels at either end with the four ligands twisting between the Cu2 units. Changing the isomer of the amino acid changes the handedness of the helicate, with L-leucine forming the Λ helicate and the D-leucine forming the Δ helicate. The helicate cages are also shown to be self-selecting, as the reaction of a mixture of L-leucine and D-leucine substituted ligands forms the Δ and Λ cages with no product containing both ligands. The chirality of the helicates can be disrupted by two different methods, to form a mesocate which lacks helical chirality. When the achiral glycine-derived ligand is used a quadruple stranded mesocate is formed (analogous to the chiral Cu4L4 cages) in which the ligands run straight 'up-and-down' the complex rather than in a helical manner. When a racemic DL-leucine-substituted ligand is used a similar mesocate is formed.

Poster Session 2 - Board: BT-10 / **101**

The AXXS Upgrade Proposal

Author(s): Dr. BOLAND, Mark[1]
Co-author(s): Dr. DOWD, Rohan [1] ; TAN, Eugene [1] ; CHARLES, Tessa [1] ; Dr. ZHU, David [1] ; Mr. LEBLANC, Greg [1]

[1] *Australian Synchrotron*

Corresponding Author(s): mark.boland@synchrotron.org.au

The Australian Synchrotron has been in operation for users since 2007 while the first electron beam was achieved ten years ago. This proposal is for an upgrade to the accelerator systems and improve the source for the next set of beamlines proposed in Science Case Two to keep the facility state-of-the-art for the decades to come. The concept is to replace the existing storage ring with a Diffraction Limited Storage Ring, upgrade the injection system to a full energy x-band linac which can be used for an X-Ray Free Electron Laser. The project to develop these plans is entitled Australian X-Band X-Ray Source (AXXS).

Poster Session 1 - Board: BT-07 / **68**

FDMX: Full-Potential Calculations of EXAFS for Extraction of Structural, Thermal, and Electronic Properties from Absolute Accuracy Measurements

Author(s): Dr. BOURKE, Jay D[1]
Co-author(s): Prof. CHANTLER, Christopher Thomas [2]

[1] *U Melbourne*

[2] *University of Melbourne*

Corresponding Author(s): jayb@unimelb.edu.au, chantler@unimelb.edu.au

We present the new computational package FDMX; a full-potential code for accurate robust calculations of x-ray absorption fine structure across all energies from below the edge to the smooth atom-like absorption region. Full-potential modeling of condensed matter systems is a critical tool for analysis of x-ray absorption near-edge structure (XANES) spectra [1,2]. Despite demonstrated advantages in the low-energy regime [3], these tools are still not generally applied to EXAFS analysis. We present here the new package FDMX, a development of the Finite Difference Method for Near-Edge Structure (FDMNES) package [2], for use in the calculation of extended XAFS spectra. FDMX features new implementations of thermal and electron scattering parameters [4], core-hole and outer-shell absorption effects. FDMX calculates high-accuracy XAFS spectra for large energy ranges in both elemental and complex molecular systems. Material parameters such as bond lengths, electron inelastic mean free paths [5], and Debye-Waller factors [6] may be extracted using full-potential modeling. 1 P Blaha etal., Comput. Phys. Commun. 59 339 (1990) [2] Y Joly, Phys. Rev. B 63 125120 (2001) [3] JL Glover, CT Chantler, AV Soldatov, G Smolentsez and MC Feiters, AIP Conf. Proc. 882(2007)625 [4] JD Bourke, CT Chantler, J. Phys. Chem. Lett. 6(2015)314 [5] JD Bourke, CT Chantler, Phys. Rev. Lett. 104(2010)206601 [6] LJ Tantau, CT Chantler, JD Bourke, MT Islam, AT Payne, NA Rae, CQ Tran, J. Phys.Condens.Mat.27(2015)266301

Poster Session 1 - Board: EE-09 / **116**

THERMAL EXPANSION OF MONOCLINIC NATROJAROSITE: A COMBINED TIME-OF-FLIGHT NEUTRON AND SYNCHROTRON POWDER DIFFRACTION STUDY.

Author(s): Dr. BRAND, Helen[1]
Co-author(s): Ms. SCARLETT, Nicola [2] ; Dr. GREY, Ian E. [2] ; Dr. KNIGHT, Kevin S. [3]

[1] *Australian Synchrotron.*

[2] *CSIRO*

[3] *ISIS neutron and Muon source*

Corresponding Author(s): helen.brand@synchrotron.org.au

Jarosites and related minerals are of great interest to a range of mineral processing and research applications. In some industrial settings jarosite formation is encouraged; for example to aid the removal of iron species from solutions in hydrometallurgical processes. There has been a recent resurgence in interest in jarosite minerals since their detection on Mars by the MER rover Opportunity. In this context, the presence of jarosite has been recognised as a likely indicator of the presence of water on Mars in the past. It is hoped that study of their formation mechanisms, stability and thermoelastic properties will provide insight into the environmental history of Mars as well as informing terrestrial industrial concerns. To this end we are engaged in a program to study jarosites, their formation and stability behaviour, over a range of conditions. This contribution describes in situ powder diffraction experiments to determine the thermal expansion of a deuterated natrojarosite. Data were collected on the HRPD beamline at the ISIS spallation source where the natrojarosite sample was heated from 10–700K, and at the powder diffraction beamline at the Australian synchrotron where the sample was heated from 80-700K. Equations of state have been fitted to the data and the thermal expansion tenor determined. Full structural refinements show that anisotropic expansion of the structure is driven by the hydrogen bonding network. Details of the combined neutron-synchrotron analysis approach will be discussed.

Poster Session 1 - Board: SB-09 / **149**

Structural Insights into Bak Activation and Oligomerisation

Author(s): Mr. BROUWER, Jason[1]
Co-author(s): Dr. CZABOTAR, Peter [2] ; Dr. ROBIN, Adeline [3] ; Prof. COLMAN, Peter [1]

[1] *Walter and Eliza Hall Institute of Medical Research*

[2] *Walter and Eliza Hall Institute*

[3] *WEHI*

Corresponding Author(s): brouwer@wehi.edu.au

Apoptotic stimuli activate and oligomerise the pro-apoptotic proteins Bak and Bax resulting in mitochondrial outer membrane permeabilisation and subsequent cell death. Crystal structures by Czabotar et al. (2013) provided novel insights into BH3-only induced Bax activation and oligomerisation, namely the separation of the core and latch domains, followed by core domain dimerisation. Here we provide complementary studies on the related protein Bak. We present the crystal structures of Bak core-latch domain swapped dimers and demonstrate their dissociation upon Bak activation. A second crystal structure of the Bak core domain provides the first high-resolution details for this key dimerisation unit upon which the larger Bak oligomer builds. Cellular assays, guided by the presented crystal structures, confirm the physiological relevance of these key events in the intrinsic apoptotic pathway (Brouwer et al. 2014). These studies confirmed an analogous mechanism for activation and dimerisation of Bak and Bax in response to BH3-only peptides. More recently we have performed structural studies on the direct interaction of BH3 only peptides with Bak. We have gained insight into the differences between interactions of BH3 only proteins with Bak compared to the pro-survival proteins; these findings may inform the design of novel therapeutics to manipulate cell death.

Poster Session 2 - Board: RR-02 / **71**

Characterization of a novel 3D silicon strip detector for Microbeam Radiation Therapy (MRT) quality assurance

Author(s): Mr. CAMERON, Matthew[1]
Co-author(s): Dr. CORNELIUS, Iwan [2] ; Dr. GUATELLI, Susanna [1] ; Prof. LERCH, Michael [1] ; Dr. PETASECCA, Marco [1] ; Prof. ROSENFELD, Anatoly [1]

[1] *University of Wollongong*

[2] *Imaging and Medical Beamline, Australian Synchrotron*

Corresponding Author(s): mc815@uowmail.edu.au

Microbeam Radiation Therapy (MRT) is a promising radiotherapy modality that uses arrays of spatially fractionated micrometre sized beams of synchrotron radiation to irradiate tumours. A typical MRT radiation field consists of an array of microbeams, each with a FWHM of 50 μm and a pitch of 200 μm. The small field size and the steep dose gradient at the peaks poses a challenge for dosimetry due to the required spatial resolution of 1 micrometer. Use of silicon detectors in an edge-on configuration has been investigated as a way to increase spatial resolution 1 but this introduces a non-water equivalent response due to interactions in the silicon surrounding the sensitive volume. The Centre for Medical Radiation Physics (CMRP), University of Wollongong (UOW), and collaborators have produced two configurations of novel silicon single strip detector (SSD) aiming to improve tissue equivalency of the detector. It has been achieved by fabrication the 3D MESA sensitive volume of SSD erected on top of SiO2 by etching away silicon surrounding the sensitive volume. Detector Topology was examined using a scanning electron microscope at the Australian Institute of Innovative Materials (AIIM). Electrical characterization of the detector was accomplished using I-V and C-V measurements. Preirradiation to stabilize radiation response of the 3D SSD followed by acquisition of microbeam dose profiles were performed at the Autralian Synchrotron's Imaging and Medical Beamline (IMBL) using CMRP's X-Tream dosimetry system [2]. Electrical characteristics, topology, and microbeam dose profiles will be presented in this poster.

Poster Session 2 - Board: AM-02 / **6**

Incorporation of N-heterocyclic carbene moieties into MOFs

Author(s): Mr. CAPON, Patrick[1]
Co-author(s): Prof. SUMBY, Chris [2] ; Dr. BURGUN, Alexandre [2]

[1] *The University of Adelaide*

[2] *University of Adelaide*

Corresponding Author(s): patrick.capon@adelaide.edu.au

Metal-organic frameworks (MOFs) are a class of porous materials that can be synthesised through judicious combination of metal salts and organic linkers. MOFs are constructed from a bottom up approach, where variation of the starting materials can yield a vast array of structures with varying pore sizes, shapes, and chemistry. The high versatility of MOFs makes them a highly desirable target in the fields of gas storage and separation, as well as catalysis. Recently, there has been significant interest in incorporating N-heterocyclic carbene (NHC) precursors into MOFs for use in catalysis. NHCs can be readily synthetically modified, making them an interesting functional group to incorporate into MOFs in order to develop new catalysts, or fine tune existing molecular catalysts.
In this contribution, a series of MOFs incorporating a substituted NHC precursor as the organic linker will be reported. By choice of the starting metal salt different MOFs may be accessed, in which NHC precursor azolium linkers are retained or substituted NHC complexes are generated. For example, reactions with Zn(II) (and an added Cu(I) source) and Cu(II) give MOF materials with concomitant Cu(I) metalation of the NHC moiety. The degree of metalation is currently being studied by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) and Single Crystal X-Ray Diffraction (SCXRD). The chemistry of these and several other related NHC MOFs will be presented in this contribution.

Structural Biology / 170

Is diffraction limited by the crystal or beam? A comparison of FEL vrs Synchrotron protein diffraction data.

Author(s): CARADOC-DAVIES, Tom[1]
Co-author(s): Dr. LAW, Ruby [2] ; Dr. PANG, Siew Siew [2]

[1] *Australian Synchrotron.*

[2] *Monash University*

Corresponding Author(s): tom.caradoc-davies@synchrotron.org.au

The development of X-ray Free-Electron Lasers (XFELs) has created a range of novel crystallography experiments such as the use of liquid-jet injectors. The use of goniometer-based FEL experiments(1) allows the direct comparison of diffraction from the same or similar crystals at both sources. The diffraction of a set of crystals tested on the MX2 beamline at the Australian Synchrotron and the XPP beamline at the Linear Coherent Light Source (LCLS) will be presented. The diffraction for most crystals was found to be similar with a small increase in observed resolution limit for some samples. The cases where a significant increase in diffraction is expected to be seen when using an XFEL will be discussed along with other experiments that can only be done on an XFEL. Data collection at an XFEL poses a series of significant challenges. The samples are vaporised by the beam and the resulting diffraction image covers an extremely small rocking curve. These data suggest that for most "standard" MX crystals the increase in resolution expected at an XFEL over a microfocus MX beamline is marginal. For the collection of samples presented, the intrinsic diffraction limit of the crystals and not the intensity of the source was the limiting factor. These data suggest the use of XFELs will be most effective for well-ordered micro crystals or systems where the radiation damage "free" nature of XFEL data is required for characterisation of states such as oxidised and reduced forms of metallo-enzymes.

Structural Biology / 52

The BHP2 protein - an evolutionary perspective on the intrinsic apoptotic pathway

Author(s): Dr. CARIA, Sofia[1]
Co-author(s): Dr. KVANSAKUL, Marc [1]

[1] *La Trobe University*

Corresponding Author(s): s.caria@latrobe.edu.au

Apoptosis or programmed cell death is a crucial response to perturbations in physiological conditions, allowing an organism to determine if a given cell can be eliminated when unneeded, damaged or dangerous for the organism. In this mechanism the B-cell lymphoma 2 (Bcl-2) protein family plays an important role in regulating the homeostasis 1.
Sponges are the phylogenetically oldest existent members of the Metazoa phylum. It has been demonstrated that *Geodia cydonium* (*G. cydonium*) and *Suberites domuncula* possesses polypeptide sequences with high sequence similarity to Bcl-2 protein members [2]. The study of these proteins is highly relevant for the understanding of the evolution of apoptosis across species. BHP2, a *G. cydonium* pro-survival Bcl-2 protein, has been shown to be involved in apoptotic pathway [3].
In this study the BHP2 protein biochemical characterisation using ITC as well as its structure determination in complex with a BH3-only peptide has enable us to shine light on the sponges apoptosis mechanism and compare it to others previously characterized such as the mammalian and viral. A better understanding of how apoptosis evolved across species might yield value information for rational drug design.
References: 1- Kvansakul M et al. (2014) *Method Enzymol.* 544, 44-79. [2]- Wiens M et al. (2000) *J. Mol. Evol.* 50, 520-531. [3]- Wiens M et al. (2001) *Cell Death Differ.* 8, 887-98.

Structural Biology / 141

The solution structure of Sr33

Author(s): Mr. CASEY, Lachlan[1]
Co-author(s): Prof. KOBE, Bostjan [2] ; Dr. WILLIAMS, Simon [2] ; BENTHAM, Adam [3] ; Mr. LAVRENCIC, Peter [2]

[1] *University of Queensland*

[2] *The University of Queensland*

[3] *Flinders University*

Corresponding Author(s): lachlan.casey@uqconnect.edu.au

The recognition of fungal effectors by plant NOD-like receptors (NLRs) is an important step in defense. The coiled-coil (CC) domains of these proteins are known to be necessary and sufficient for response. Two structures have previously been solved, which show highly divergent conformations. The CC domain of the potato NLR, Rx, adopts a compact, monomeric four-helix bundle, while that of a barley protein, Mla10, was observed as an extended homodimer which was thought to be constitutively present, posing problems for mechanisms of self-association induced signaling.

We have solved the solution structure of the CC domain from the related wheat resistance protein Sr33 by NMR spectroscopy. This protein has high sequence similarity to Mla10, but our structure reveals a compact, Rx-like four-helical bundle. We subsequently analysed all three proteins by synchrotron SAXS, supported by MALS and analytical ultracentrifugation. We found that the CC-domains of Sr33, Mla10 and Rx are in fact monomeric in solution, with some evidence of weak self-association. Furthermore, the NMR structure of Sr33 is consistent with the dilute scattering from all three proteins.

Our work thus reconciles the Mla10 structure with existing models of signalling by demonstrating that a stable monomeric fold exists. We suggest that the conformation in the Mla10 crystal is a rare state that may be involved in signaling, and that the combination of this with the NMR structure of Sr335-120 provides a more complete model of the system.

Poster Session 1 - Board: BT-05 / **63**

Quality Improvements for Fluorescence Detected XAFS Spectra of Ferrocene

Author(s): Prof. CHANTLER, Christopher Thomas[1]
Co-author(s): Prof. WANG, Feng [2] ; Mr. ISLAM, M Tauhidul [3] ; Dr. BEST, Stephen P [3] ; Dr. TRAN, Chanh Q [4]

[1] *University of Melbourne*

[2] *Swinburne University of Technology*

[3] *U Melbourne*

[4] *La Trobe*

Corresponding Author(s): chantler@unimelb.edu.au, fwang@swin.edu.au, m.islam3@student.unimelb.edu.au, spb@unimelb.edu.au, cq.tran@latrobe.edu.au

Methods for the quantification of statistically valid measures of the uncertainties associated with X-ray absorption fine structure (XAFS) data obtained from dilute solutions using fluorescence measurements are developed. Several systematics (e.g. self-absorption) associated in fluorescence detection cannot yet be corrected automatically. Multielement fluorescence detectors provide a set of absolute spectra depending on the geometry of the detector channels with different apparent sensitivities. Error analysis performing the characterization and correction of systematics (self-absorption, energy calibration, photoreduction, air path attenuation etc.) can measure statistical accuracy. Experimental data obtained from 10 mM solutions of the organometallic compound ferrocene, Fe(C5H5)2, are analysed within this framework and give robust estimates of the standard errors of the individual measurements. Incorporation of experimental uncertainties into an IFEFFIT-like analysis yield refinement statistics for the staggered and eclipsed forms of ferrocene which show a far more realistic preference for the eclipsed form which accurately reflects the reliability of the analysis. Moreover, the more strongly founded estimates of the refined parameter uncertainties allow more direct comparison with those obtained by other techniques. These XAFS-based estimates of the bond distances have accuracies comparable with those obtained using single-crystal diffraction techniques and are superior in terms of their use in comparisons of experimental and computed structures [CT Chantler, NA Rae, MT Islam, SP Best, J Yeo, LF Smale, J Hester, N Mohammadi, F Wang, Stereochemical analysis of Ferrocene and the uncertainty of fluorescence XAFS data, J Synch. Rad. 19 (2012) 145-158].

Advanced Materials I / 65

The Hybrid technique for accurate transmission XAS on 1-10mM Ni solutions

Author(s): Prof. CHANTLER, Christopher Thomas[1]
Co-author(s): Mr. ISLAM, M Tauhidul [2] ; Dr. STEPHEN P, Best [2] ; Dr. TRAN, Chanh Q [3]

[1] *University of Melbourne*

[2] *U Melbourne*

[3] *La Trobe*

Corresponding Author(s): chantler@unimelb.edu.au, m.islam3@student.unimelb.edu.au, spb@unimelb.edu.au, cq.tran@latrobe.edu.au

XAFS can now be used to investigate electron inelastic mean free paths, dynamical and thermal bonding, to measure nanoroughness and most importantly to assess the significance of alternate hypotheses with derived experimental uncertainty. These key developments will be discussed. A new approach is introduced for determining XAS spectra on absolute and relative scales using multiple solutions with different concentrations by the characterisation and correction for experimental systematics. This hybrid-technique (HBT) is a development of standard XAFS along the lines of high-accuracy XERT but with applicability to solutions, dilute systems and cold cell environments. We have applied this methodology to determining absolute XAS of [bis(N-n-propyl-salicylaldiminato)] nickel(II) and [bis(N-i-propyl-salicylaldiminato)] nickel(II) complexes with square planar and tetrahedral structures in 15 mM and 1.5 mM dilute solutions. Dilute systems provide excellent XANES and XAFS spectra by transmission, and we confirm that transmission measurements can be superior to conventional fluorescence measurements even for dilute systems. For the first time, we have determined XAS of the isomers from low concentration solutions on an absolute scale with a 1%-5% accuracy, and with relative precision to 0.1% to 0.2% in the active XANES and XAFS regions after inclusion of systematic corrections [CT Chantler, MT Islam, SP Best, LJ Tantau, CQ Tran, MH Cheah, AT Payne, High accuracy X-ray Absorption Spectra of mM solutions of nickel(II) complexes with multiple solutions using transmission XAS. Journal of Synchrotron Radiation 22 (2015) 1008-1021].

Poster Session 2 - Board: BT-06 / **67**

X-ray Spectroscopic Advances in Condensed Matter Interactions with X-rays

Prof. CHANTLER, Christopher Thomas[1]

[1] *University of Melbourne*

Corresponding Author(s): chantler@unimelb.edu.au

Exciting fundamental problems and advanced applications have emerged in X-ray Spectroscopy. Accuracy of absorption coefficients to 0.02% have led to insights into atomic form factors1, XAFS dynamical bonding[2], electron inelastic mean free paths[3] and nanoroughness[4], with technological offshoots into detector and synchrotron diagnostics. As a consequence, the accurate characterization of fluorescence spectroscopy is developing, together with the accurate investigation of organometallic complexes. Burgeoning applications in RIXS and ultrafast techniques have led to insight into chemical intermediates. Advances are beginning to be able to investigate polarization, alignment, nanostructures, and dynamic and static disorder. 1 MD de Jonge, CQ Tran, CT Chantler, Z Barnea et al, Measurement of the x-ray mass attenuation coefficient and determination of the imaginary component of the atomic form-factor of tin over the energy range of 29 keV – 60 keV, Phys. Rev. A75 (2007) 032702 [2] JL Glover, CT Chantler, Z Barnea, NA Rae, CQ Tran, Measurement of the X-ray mass-attenuation coefficients of gold, derived quantities between 14 keV and 21 keV and determination of the bond lengths of gold, J. Phys. B 43 (2010) 085001 [3] CT Chantler, JD Bourke, X-ray Spectroscopic Measurement of the Photoelectron Inelastic Mean Free Paths in Molybdenum, Journal of Physical Chemistry Letters 1 (2010) 2422; JD Bourke and CT Chantler, Phys. Rev. Lett. 104, 206601 (2010) [4] JL Glover, CT Chantler, MD de Jonge, Nano-roughness in gold revealed from X-ray signature, Phys. Lett. A373 (2009) 1177

Poster Session 2 - Board: SB-02 / **72**

Why only pyrimidine serves in DNA amongst its diazine isomers?

Author(s): Mr. CHATTERJEE, Subhojyoti[1]
Co-author(s): Mr. WINNETT, Alex [1] ; Prof. WANG, Feng [1]

[1] *Faculty of Science, Engineering and Technology and Molecular Model Discovery Laboratory, Swinburne University of Technology, Victoria, Australia.*

Corresponding Author(s): subhojyotichatterjee@swin.edu.au

X-ray photoemission spectra (XPS), their nuclear magnetic resonance (NMR) spectra and solvent effects of pyrimidine (1,3-diazine) and its other diazine structural isomers (1,2-diazine and 1,4-diazine) are studied using density function theory (DFT) based B3LYP/aug-ccVTZ quantum mechanical calculations, in order to reveal the structure and property information why only pyrimidine serves in DNA, i.e., cytosine (C), thymine (T) and uracil (U) are pyrimidine derivatives, amongst its diazine isomers (Pyridazine (1,2-), Pyrazine (1,4-)). To further elucidate the effects of the structural and the properties differences when interaction with environment, the present work also studies the effect of the solvents (i.e. carbon tetrachloride (CCl4) and water (H2O)) on the structure and vibrational spectra of the diazine isomers along. The preliminary results indicate that the C1s and N1s spectra of the diazine isomers indeed show apparent differences reflecting their nitrogen positions in the ring, which agrees with the calculated molecular electrostatic potentials (MEPs) and NMR chemical shift. Significant blue shifts of the vibrational spectra of the tautomers were observed in the vibrations of C-H bonds due to structures of the N-positions. Finally, the chemical graph LU decomposition matrix from graph theory also indicates that the connection of pyrimidine is quite different from its diazine isomers.

Poster Session 2 - Board: BT-14 / **124**

The Quick-scanning EXAFS Beamline at Taiwan Photon Source

Author(s): Dr. CHEN, Jeng-Lung[1]
Co-author(s): Dr. LEE, Jyh-Fu [1] ; Dr. HUANG, Yu-Shan [1] ; Dr. PAO, Chih-Wen [1] ; Ms. CHUANG, Hui-Fang [1] ; Dr. HUANG, Chi-Yi [1]

[1] *National Synchrotron Radiation Research Center*

Corresponding Author(s): chen.jl@nsrrc.org.tw

The quick-scanning EXAFS beamline using bending magnet at Taiwan Photon Source (TPS) features a quick-scanning monochromator (Q-Mono) for time-resolved studies in series with a conventional double crystal monochromator (DCM). This beamline covers a wide energy range from 4.5 up to 34 keV. The quick-scanning capability allows the collection of a full spectrum in millisecond range. All installed optical components can be used for both quick-scanning and conventional step-by-step modes. There will be different coatings (Si, Rh, Pt) on both collimating mirror (CM) and toroidal focusing mirror (TFM) for high-order harmonic rejection. Additionally, a micro beam will be achieved by Kirkpatrick-Baez (K-B) mirrors for the microprobe analysis. The expected peak photon flux is 5 × 10ˆ{11} photons/s at 10 keV from SHADOW and XOP simulation with the beam size of 66 (h) × 195 (v) μmˆ{2} in FWHM. It can be further reduced down to 20 × 20 μmˆ{2} (FWHM) after K-B mirrors.

Poster Session 2 - Board: BT-04 / **59**

High Resolution Powder X-ray Diffraction beamline at Taiwan Photon Source: Structural Characterization and Dynamics

Author(s): Dr. CHUANG, Yu-Chun[1]
Co-author(s): Mr. CHANG, Chung-Kai Chang [1] ; Dr. YU, Kuan-Li [1] ; Mr. LEE, Longlife [1] ; Dr. SHEU, Hwo-Shuenn [1]

[1] *National Synchrotron Radiation Research Center*

Corresponding Author(s): chuang.yc@nsrrc.org.tw

The low emittance (1.6 nm·rad) synchrotron radiation ring, Taiwan Photon Source (TPS), has reached the design value of 3 GeV and delivered its first synchrotron light on the last day of 2014. In phase I, TPS comprises seven frontier beamlines, which will be constructed and completed commission before the end of 2015. At the excited moments, a dedicated high resolution powder X-ray diffraction beamline is pro-posed to satisfy extensive PXRD user demand. Structure and kinetics of materials are always the attrac-tive and fundamental issues for scientists. To satisfy versatile researches in chemistry, physics and mate-rials, a highly collimated and intense X-ray source will be produced by an in-vacuum undulator (IU22) to obtain the highest possible brilliance in the range of 5-30 keV. A large concentric 3-circle diffractometer equipped with a multi-crystal analyzer system and a fast position sensitive detector (MYTHEN 24K) were designed for high angular resolution and time-resolved studies respectively. The polycrystalline materials under different non-ambient conditions, such as high/low temperature, high pressure and gas de/adsorption, will be provided to investigate structural transformation. In addition, to enhance the beam-line efficiency, a high throughput robot will be installed to allow automated sample mounting. The in situ and time-resolved experiments as well as structure determination from powder diffraction data will be emphasized in this beamline.

Poster Session 1 - Board: EE-07 / **69**

Characterisation of the localisation and speciation of radionuclides at the former nuclear weapons testing site of Maralinga, South Australia.

Author(s): Dr. COLLINS, Richard[1]
Co-author(s): Dr. JOHANSEN, mathew [2]

[1] *The University of New South Wales*

[2] *ANSTO*

Corresponding Author(s): richard.collins@unsw.edu.au

In the 1950s-60s the Maralinga Lands were used by the British/Australian governments for the testing and development of nuclear weapons. Four clean-up programs have been undertaken at Maralinga with the last, concluding in 2000, having the objective to release the former nuclear test sites for use by the traditional owners. As part of a wider scientific program examining soil-to-animal radionuclide transfer, the localisation and speciation of radionuclides in the soils were investigated by XFM and XAS. In samples from atomic bomb detonation sites, Sr-90 was mostly localised in 'fused' sand formed during the explosions. Its distribution within the silicate melt particles was extremely heterogeneous, however, XANES imaging demonstrated that its speciation was homogeneous and EXAFS analyses confirmed it to be similar to Sr incorporated into hydrous silicate glasses. At a site where about 8 tonnes of natural/depleted uranium were exploded, uranium was found to be heterogeneously distributed as discrete micron-sized particles. XFM revealed that no other heavy elements were associated with these particles and XANES imaging demonstrated that uranium was solely present in the particles as U(VI) in uranyl geometry. EXAFS analyses confirmed the XANES imaging results, but due to significant scattering from the 2nd coordination shell, the chemical speciation of uranium was not unequivocally identified. Whilst identification of these particles's mineralogy is on-going, these results have demonstrated that the soil-to-animal transfer of these radionuclides through inhalation, the dominant uptake process in mammals, will be minimal.

Energy Materials II / 233

Radionuclide speciation at former nuclear weapons testing sites and in situ technologies to immobilise aqueous uranium

Corresponding Author(s): richard.collins@unsw.edu.au

Poster Session 1 - Board: RR-09 / **213**

Patient Safety System for Micro Radiation Therapy at the Australian Synchrotron

Author(s): Mr. KARNAGHAN, Bryce[1]
Co-author(s): Mr. CONESA-ZAMORA, Gonzalo [1] ; Dr. LIVINGSTONE, Jayde [1] ; Dr. CLIFT, Mark [1] ; Mr. MCKINLAY, Jonathan [1] ; Mr. ARIAS, Jaime [2] ; Mr. LE GUEN, Rick [1] ; Dr. NEMOZ, Christian [3] ; Dr. CORNELIUS, Iwan [4] ; Dr. BERKVENS, Paul [3]

[1] *Australian Synchrotron*

[2] *Australian Sychrotron*

[3] *ESRF*

[4] *Imaging and Medical Beamline, Australian Synchrotron*

Corresponding Author(s): gonzalo.c-z@synchrotron.org.au

The Imaging and Medical Therapy Beamline at the Australian Synchrotron is progressing with Micro Radiation Therapy studies, to enable the Beamline to be used to treat human patients in the future. These studies provide a number of technical challenges for the Engineering Teams due to the high dose rates accompanying this technique. Trial systems are under development using small rodents as a step along the path to human treatment. This paper provides an overview of the Patient Safety System (PaSS) being developed to support the MRT application on the Medical Therapy Beamline. The system is based on the Beckhoff TwinCAT distributed hardware platform utilising safety I/O in conjunction with a Multipurpose Unit for Synchronisation Sequencing and Triggering (MUSST) developed by the ESRF. In this paper, the key challenge of meeting the timing requirements of 2 ms and maintaining a system that can provide a known Probability of Failure to Dangerous, will be examined

Poster Session 2 - Board: IM-12 / **165**

Radiation damage in a micron-sized protein crystal studied via reciprocal space mapping and Bragg coherent diffractive imaging

Author(s): Ms. COUGHLAN, Hannah[1]
Co-author(s): Dr. DARMANIN, Connie [2] ; Mr. PHILLIPS, Nicholas [3] ; Dr. VAN RIESSEN, Grant [1] ; Prof. ABBEY, Brian [4] ; Dr. HARDER, Ross [5]

[1] *La Trobe University*

[2] *La Trobe*

[3] *LTU/CXS*

[4] *LTU/ImagingCOE*

[5] *Argonne National Laboratory*

Corresponding Author(s): hdcoughlan@students.latrobe.edu.au

For laboratory and synchrotron based X-ray sources, radiation damage has posed a significant barrier to obtaining high-resolution structural data from biological macromolecules. The problem is particularly acute for micron-sized crystals where the weaker signal often necessitates the use of higher intensity beams to obtain the relevant data. Here, we employ a combination of techniques, including Bragg coherent diffractive imaging to characterise the radiation induced damage in a micron-sized protein crystal over time using beam line 34-ID-C at the Advanced Photon Source. The approach we adopt here could help screen for potential protein crystal candidates for measurement at X-ray free election laser sources.

Poster Session 2 - Board: SB-08 / **143**

Structural Investigation of Bax Oligomerisation

Author(s): Mr. COWAN, Angus[1]
Co-author(s): Dr. CZABOTAR, Peter [2] ; Prof. COLMAN, Peter [2]

[1] *The Walter and Eliza Hall Institute*

[2] *Walter and Eliza Hall Institute*

Corresponding Author(s): cowan.a@wehi.edu.au

The Bcl-2 protein family regulates the intrinsic apoptotic pathway and the critical step of mitochondrial outer membrane permeabilisation (MOMP). MOMP results in the release of Cytochrome *c* and other molecules from the intermembrane space, leading to the formation of the apoptosome and caspase activation. Bax and Bak are structurally and functionally homologous pro-apoptotic Bcl-2 proteins that facilitate MOMP. BH3-only proteins such as Bim transiently bind to and activate Bax and/or Bak resulting in their homodimerisation and oligomerisation. The large Bax/Bak oligomers disrupt the mitochondrial outer membrane causing MOMP. BH3-only protein binding causes the dissociation of Bax/Bak into two distinct domains known as the "core" and "latch" domains. The structures of both homodimerised Bax and homodimerised Bak core domains, with a GFP fusion tag to aid crystallisation, have been solved. The core domains dimerise through a symmetrical interface involving the reciprocal insertion of the BH3 domain alpha helix of one Bax/Bak molecule into the hydrophobic groove of the partner Bax/Bak molecule. To further investigate the Bax core domain, we have expressed it as a GST fusion protein and removed the GST tag. The cleaved core domain remains soluble and runs as a multimer (likely a hexamer or an octamer) on a size exclusion column. The structure of this multimer could provide insight into the nature of the large Bax oligomers that have remained structurally enigmatic despite decades of investigation.

Collaborating with Industry - the perils and the pleasure / 133

Using the Australian Synchrotron – A clinical perspective

Dr. KANNAR, David[1]

[1] *Monash University*

Corresponding Author(s): john.cullen@au.aspenpharma.com

While synchrotron science is well beyond most clinicians, our research suggests it will become an important tool in future clinical research. Although there is a lot of science behind the clinical and pharmacological understanding of drug products formulation, what actually happens inside the tablet before and during the administration process is mostly empirical and sometimes "mystical". The Australian Synchrotron has progressed understanding of the science of tablet formulation with benefits in formulation development, enabling us to understand the three dimensional structure of various tablet matrices – something that has never been a factor for consideration – allowing better control of drug release as a function of excipients and delivery route. While drug release from tablet matrices, for example, is relatively simple and studied in a standard dissolution apparatus, release rate is traditionally varied by combination of binders, fillers, compression and interaction with specific membranes.

This knowledge of how the tablet works and the effects various components have on each other and on biological transport has also provided significant protection of our intellectual property. As a result, the science of future tablet formulation will more likely involve the synchrotron.

A brief review will be shared on how our multi-disciplinary team collaborated to solve a clinical problem and, importantly, attracted support from state and federal government grants.

Poster Session 1 - Board: EM-17 / **212**

Uranium speciation and mineralogy within an organic-rich ore deposit (Mulga Rock, WA); implications for U mobility and extraction

Author(s): CUMBERLAND, Susan[1]
Co-author(s): Dr. FISHER, Louise [2] ; Dr. DE JONGE, Martin [1] ; HOWARD, Daryl [1] ; Dr. MOREAU, John [3] ; Dr. KAPPEN, Peter [1] ; Dr. DOUGLAS, Grant [4] ; Dr. EVANS, Katy [5]

[1] *Australian Synchrotron*

[2] *CSIRO, Mineral Resources, CSIRO, Bentley 6102, Perth, Western Australia*

[3] *School of Earth Sciences, University of Melbourne, Parkville 3010, Victoria*

[4] *CSIRO, Land and Water, Wembley 6913, Perth, Western Australia*

[5] *School of Applied Geology, Curtin University, Bentley 6845, Perth, Western Australia*

Corresponding Author(s): susan.cumberland@synchrotron.org.au

Uranium (U) is internationally important as a low carbon energy source, however, its extraction and radioactive waste legacies require continuing research into the factors controlling U mobility. Uranium mobility is strongly influenced by its oxidation state: U(VI) (e.g., U(VI)-carbonate) is more soluble than U(IV), which mineralises as coffinite [USiO4] or uraninite [UO2]. By identifying the U-species present in natural systems, insights can be gained into ore formation, U extractability (e.g. in-situ leaching) and contaminated site management. The influence of U by organic matter (OM) on both uranium mobility and fixation is interesting, as within deposits higher U concentrations often coincide with OM-rich zones. Alternatively, OM may also inhibit sorption of U via formation of soluble complexes. Analytical challenges include identifying U-species within OM-rich samples. Synchrotron radiation, in particular X-ray Absorption Spectroscopy (XAS) and X-ray fluorescence microscopy (XFM), have proven advantageous in studying oxidation state and coordination. Here, we present the results of XAS analyses of Mulga Rock cores, an OM-hosted U-deposit in WA. We show that within OM, uranium is finely dispersed displaying simple monomeric structures analogous to uranyl silicate, suggesting potential for U extractability. However, where uranium is locally concentrated, coffinite predominates. Results of XFM-XANES and XRD transects also document a redox gradient of U(IV) to U(VI) across a U-pyrite boundary.

Poster Session 2 - Board: BS-04 / **88**

Development of a synchrotron FTIR microspectroscopy approach to evaluate the efficacy of candidate multiple sclerosis therapeutics

Author(s): Mr. DANG, Phuc[1]
Co-author(s): Dr. BAMBERY, Keith [2] ; Mr. JIMENEZ, Antonio [1] ; Dr. PUSKAR, Ljiljana [3] ; Dr. ORIAN, Jacqueline [1]

[1] *La Trobe University*

[2] *Australian Synchrotron*

[3] *Helmholtz-Zentrum Berlin*

Corresponding Author(s): timithydvl@gmail.com

The sphingosine-1-phosphate receptor 1 (S1PR1) is a target for the multiple sclerosis drug FTY720, a functional antagonist causing sequestration of autoreactive immune cells. Conventional approaches with the experimental autoimmune encephalomyelitis (EAE) model do not provide an overall index of drug efficacy, hence the use of FTIR microspectroscopy. Experimental groups included vehicle-only, EAE+placebo (EAE+P) and EAE+FTY720 (EAE+FTY). Spinal cord grey (gm) and white matter (wm) changes were evaluated and compared with data from conventional techniques. Different profiles of tissue destruction and FTY720-mediated damage prevention were documented. In gm, spectra showed significantly increased protein and lipid content in the EAE+P group relative to controls, in agreement with cellular infiltration. However the EAE+FTY group showed significantly higher protein but lower lipid content relative to the EAE+P group, suggesting reduced infiltration, but combined with upregulation of repair pathways. In wm, spectra showed significantly lower protein, but higher lipid content, suggesting that protein and lipid increases associated with cellular infiltration are exceeded by tissue destruction. The EAE+FTY group showed significantly higher lipid content, but no significant protein difference with controls, in agreement with both reduced infiltration and tissue destruction. The complexity and size of the acquired spectral data set warrants a multivariate approach to the analysis. We are currently applying principal component analysis (PCA) with the aim of building a model capable of further discriminating biochemical differences between the experimental groups for application to second-generation S1PR1-targeted drugs.

Poster Session 1 - Board: BT-11 / **104**

Scanning the night away – stage upgrade at the XFM beamline

Author(s): Dr. DE JONGE, Martin[1]
Co-author(s): HOWARD, Daryl [1] ; WALSH, Adam [1] ; Ms. SHEPHERD, Emma [1] ; FAULKS, Andrew [2] ; PATERSON, David [1] ; Mr. AFSHAR, Nader [3] ; Dr. RYAN, Chris [2] ; STARRITT, Andrew [1] ; Mr. KIRKHAM, Robin [2] ; Mr. STEPHENSON, Macleay [1] ; Mr. MICHALCZYK, Adam [1] ; Mr. BASTEN, Noel [1]

[1] *Australian Synchrotron*

[2] *CSIRO*

[3] *Controls Engineer*

Corresponding Author(s): martin.dejonge@synchrotron.org.au

X-ray Fluorescence Microscopy uses a focussed beam and an energy resolving detector to map trace metals at exquisite sensitivity and resolution for a broad diversity of research programmes. Our possession of the Maia detector enables us to acquire high-sensitivity data at incredible pixel rates, and this in turn has enabled higher-dimensional techniques, such as fluorescence tomography, XANES imaging, and XANES-tomography. The beamline has solid impact, punching well above its weight.
From the beamline's inception (late 2008) up to May 2015, beamline data acquisition was limited by a range of mechanical and controls parameters, including stage resolution, speed, and acceleration. We have recently completed phase 1 of a project to bring fast scanning to the XFM beamline. The new build substantially improves data acquisition rates and accuracy, and frees limitations on the measurement parameter-space, enabling a range of entirely new investigations. Here we report on the design, build, and testing of the updated stages, and discuss a range of further improvements that will make this an optimised workhorse of the XFM beamline. We welcome feedback about the future capabilities of the equipment from the user community.

Poster Session 2 - Board: BT-12 / **105**

Lost in transmission? Recent outcomes with fast-framing cameras at the XFM beamline.

Author(s): Dr. DE JONGE, Martin[1]
Co-author(s): Dr. JONES, Michael [1] ; Dr. LYNCH, Peter [2] ; Dr. ABBEY, Brian [3] ; Dr. MUDIE, Stephen [1] ; Mr. PHILLIPS, Nicholas [4] ; Dr. RYAN, Chris [5] ; KIRKHAM, Robin [5] ; HOWARD, Daryl [1] ; PATERSON, David [1]

[1] *Australian Synchrotron*

[2] *Deakin University*

[3] *LaTrobe University*

[4] *LTU/CXS*

[5] *CSIRO*

Corresponding Author(s): martin.dejonge@synchrotron.org.au

X-ray Fluorescence Microscopy uses a focussed beam and an energy resolving detector to map trace metals at exquisite sensitivity and resolution for a broad diversity of research programmes. For the majority of investigations in the biological and environmental sciences, over 90% of the beam intensity goes straight through the specimen. At a minimum, this beam is detected and used to determine an absorption map of the specimen.
We have recently had an opportunity to use two different x-ray cameras: a PixiRad-1 and and Eiger 1M. Over around 4 weeks of merit beamtime these were used for a wide variety of experiments, including: micro-SAXS, micro diffraction, scanning x-ray diffraction microscopy, differential phase contrast, and to observe Kossel lines. Here we present some results from each of these, along with some cost-benefit analysis of the various camera options for the beamline. Please come and tell us if you have another use for a transmission camera in the microprobe geometry!

Soft Matter / **62**

Influence of different side-chains on the morphology and device physics of all-polymer solar cells.

Author(s): Mr. DESHMUKH, Kedar[1]
Co-author(s): Dr. GAAN, Eliot [2] ; Dr. PRASAD, Shyamal [3] ; Dr. LIU, Amelia [1] ; Prof. HODGKISS, Justin [3] ; Prof. MCNEILL, Chris [1]

[1] *Monash University*

[2] *Australian Synchrotron*

[3] *Victoria University Wellington*

Corresponding Author(s): kedar.deshmukh@monash.edu

Semiconducting polymers are interesting materials that can be used as the active layer in light-emitting diodes, transistors and solar cells. In a polymer solar cell, the blending of donor and acceptor materials is required to achieve effective charge generation. Historically, fullerene derivatives have been used as the acceptor material due their high electron affinity, but fullerenes only weakly absorb light and are more expensive than semiconducting polymers. Recently significant progress has been made with so-called all-polymer solar cells that use semiconducting polymers as both donor and acceptor, with power conversion efficiencies of 7.7% recently reported. Key to this recent increase in cell efficiency has been the tailoring of the chemical structure of the polymeric materials, in particular the structure of the side-chains used to solubilise these materials.
In this study, we study seek to understand the increase in cell efficiency that accompanies the replacement of oxygen atoms with thiophene moieties in the side chains of the donor polymer PTB7. Devices fabricated with PTB7 as the donor show an efficiency of 2.2%, while devices fabricated with the thiophene-substituted PBDTTT-EFT have an efficiency of 5%. A combination of lab-based (AFM, TEM) and synchrotron-based (NEXAFS spectroscopy, GIWAXS, R-SoXS) are used to characterise thin film microstructure, which is related to device physics and photophysics to paint a clear picture of the factors aiding in improvement of the performance.

Poster Session 1 - Board: RR-03 / **95**

MRT Dosimetry at the Australian Synchrotron using the X-Tream System

Author(s): Mr. DIPUGLIA, Andrew[1]
Co-author(s): Dr. CORNELIUS, Iwan [2] ; Ms. FOURNIER, Pauline [3] ; Dr. STEVENSON, Andrew [4] ; Dr. HALL, Chris [5] ; HAUSERMANN, Daniel ; Dr. ROSENFELD, Anatoly [3] ; Dr. LERCH, Michael [3] ; Dr. PETASECCA, Marco [3]

[1] *University of Wollongong*

[2] *Imaging and Medical Beamline, Australian Synchrotron*

[3] *Centre for Medical Radiation Physics*

[4] *Australian Synchrotron/ CSIRO*

[5] *Australian Synchrotron*

Corresponding Author(s): ad150@uowmail.edu.au

Microbeam Radiation Therapy (MRT) uses synchrotron-generated X-rays to deliver a treatment dose at a very high dose rate via collimated planar, parallel array of microbeams. The synchrotron X-ray beam on the Imaging and Medical Beamline (IMBL) at the Australian Synchrotron (AS) is spatially fractionated by a tungsten carbide/kapton multislit collimator (MSC) giving beam dimensions of either 25 or 50μm FWHM microbeams with center-to-center spacing of 200μm. Using these beam dimensions the dose volume effect is evident and results in a tissue sparing effect. One consequence of this effect, is healthy tissue sparing whilst maintaining tumor control. Due to the high dose rate and complex structure of the radiation field, current traditional dosimeters are not optimal for dosimetry as they lack the required high spatial resolution, and/or real-time readout. The X-Tream dosimetry system, is a system based on a Silicon Strip Detector (SSD) with real-time readout and high spatial resolution, and has been developed at the Centre of

Medical and Radiation Physics (CMRP). Preliminary dosimetric measurements at the AS, for both broad beam and microbeams, were investigated using the X-Tream system and Pinpoint ionization chamber for dose calibration. The Peak-to-Valley-Dose-Ratios (PVDRs), which are vital dosimetry parameters in the Quality Assurance (QA) in MRT, were acquired and evaluated at a variety of depths for both water and solid-water phantoms using a variety of field sizes using both microbeam dimensions.

Poster Session 1 - Board: SB-11 / **222**

Deuterated recombinant protein production: A high yield, robust and reliable method using Escherichia coli

Author(s): Dr. DUFF, Anthony[1]
Co-author(s): Ms. WILDE, Karyn [1] ; Dr. REKAS, Agata [1] ; Dr. DAVYDOVA, Natalia [1] ; Dr. HOLDEN, Peter [1]

[1] *ANSTO*

Corresponding Author(s): anthony.duff@ansto.gov.au

In support of neutron scattering studies of proteins, we use a highly reliable method for the deuteration of a broad range of proteins by recombinant expression in Escherichia coli BL21. Typical biomass yields are 40-80 g/L wet weight, yielding 50-500 mg/L purified protein. This method uses a simple, relatively inexpensive defined medium, and routinely results in a high yield expression without need for optimisation. The key elements are: very tight control of expression, careful starter culture adaption steps, media composition and strict maintenance of aerobic conditions ensuring exponential growth. Culture temperature is reduced as required to prevent biological oxygen demand exceeding maximum aeration capacity. The defined medium has glycerol as the sole carbon source and we have not encountered an upper limit for the size of proteins that can be expressed, achieving excellent expression for proteins from 11-154 kDa. The quantity produced at 1L scale ensures that no small angle neutron scattering (SANS), nuclear magnetic resonance (NMR) or neutron crystallography experiment is limited by the amount of deuterated material available. Where difficulties remain, these tend to be cases of altered protein solubility due to high protein concentration and a D2O-based environment. This method is also applied to the recombinant multiple labelling (13C, 15N, 2H) of proteins for NMR investigations.

Poster Session 2 - Board: EM-18 / **226**

In-Situ Investigation of Electrodeposited Manganese Dioxide Thin Film Electrodes using Powder Diffraction

Author(s): Ms. DUPONT, Madeleine[1]
Co-author(s): Mr. GIBSON, Andrew [1] ; Mr. DOSE, Wesley [1] ; Prof. DONNE, Scott [1]

[1] *University of Newcastle*

Corresponding Author(s): madeleine.dupont@uon.edu.au

Manganese dioxide has proven to be an excellent electrode material for electrochemical capacitors due to its high capacitance, low cost and low toxicity. In particular, thin film electrodes have been shown to exhibit extremely high capacitance values, which may be attributed to their low resistance and good electrolyte accessibility.
Anodic electrodeposition of manganese dioxide from an acidic solution of Mn2+ ions has produced electrodes with specific capacitance in excess of 2000 F/g. However, it has often been observed that the capacitive performance of thin film electrodes decreases significantly as film thickness increases. This effect has been partially attributed to the decrease in specific surface area that occurs with longer deposition times, but is also expected to be affected by other material properties such as crystal structure. In this work, the crystal structure of manganese dioxide films was examined in-situ using powder diffraction. Manganese dioxide films were deposited anodically from a solution of MnSO4 in H2SO4 (of varying concentrations) for up to 3 hours. The effect of deposition conditions on the crystal structure was determined and the films were performance tested to identify any relationship between the material structure and the capacitive performance.

These results will lead to a better understanding of how the deposition conditions can be tailored to optimise the performance of electrodeposited thin films.
Consequently, an understanding of the deposition mechanism and its effects on the crystal structure are vital for improving the performance of electrodeposited manganese dioxide electrodes.

Energy Materials I / 79

Analysis of Manganese Dioxide Electrochemical Capacitors using Synchrotron Methods: Determining the Effects of Material Properties on Electrochemical Performance

Author(s): Ms. DUPONT, Madeleine[1]
Co-author(s): Mr. GIBSON, Andrew [1] ; Dr. DOSE, Wesley [1] ; Prof. DONNE, Scott [1]

[1] *University of Newcastle*

Corresponding Author(s): madeleine.dupont@uon.edu.au

Energy storage devices are an increasingly important technology due to the growing demand for energy. This demand, combined with the depletion of non-renewable resources, has increased the need for renewable energy and energy-saving technologies. These systems rely heavily on energy storage. Renewable energy sources, including wind and solar power, require storage to mitigate the effects of a fluctuating energy supply and energy storage devices can increase energy efficiency in many applications.
Electrochemical capacitors (ECs) are a promising energy storage device due to their good performance, safety and reliability. ECs store charge in the electrical double layer formed at the interface between an electrolyte and a polarized electrode. In manganese dioxide electrodes, fast, reversible redox reactions also take place which contribute to its high capacitance.
The charge storage capabilities of manganese dioxide are influenced by material properties including crystal structure, pore size distribution, surface area and morphology [1, 2]. Improving electrode performance relies on understanding the effects of material properties on performance. In this work, we focus on characterising manganese dioxide in both the material synthesis stage and during electrode cycling using SAXS and powder diffraction. By determining the effects of the synthesis conditions on material properties, and furthermore, the effects of material properties on performance, we aim to optimise the performance of these devices.

1. M. Dupont, A. F. Hollenkamp and S. W. Donne, Electrochimica Acta, 104 (2013) 140-147
2. M. F. Dupont and S. W. Donne, Journal of The Electrochemical Society, 162 (2015) A5096-A5105

Poster Session 1 - Board: AM-17 / **137**

Coordination Polymers from Amine-Based Ligands

Author(s): Mr. EMERSON, Adrian[1]
Co-author(s): Dr. TURNER, David [1] ; Prof. BATTEN, Stuart [1]

[1] *Monash University*

Corresponding Author(s): adrian.emerson@monash.edu

This research has developed amine-based porous coordination polymers (PCPs) as materials for CO2 capture from coal-fired power plants. PCPs are a class of framework materials built from a combination of organic linkers and metal ions which display a wide range of desirable properties for gas adsorption, including high thermal stability and adjustable chemical functionality. One of the key aims is to improve the adsorption selectivity of PCPs towards CO2 over other common flue-gas components such as N2, O2 and H2O by incorporating polar amine functionality into the polymer framework.
The use of diethylenetriamine derived ligands has led to the synthesis of a series of three-dimensional coordination polymers. The solid-state structure of each coordination polymer

was characterised using single crystal X-ray diffraction at the Australian Synchrotron using the Macromolecular beamlines. These framework materials can be classified as microporous, with the largest pore size observed measuring 9 Å in diameter. Each framework has been tested for thermal stability, with decomposition of the frameworks observed above 300 °C. Adsorption experiments using N2 at 77 K and CO2 at 273 K have been performed, with a promising uptake of CO2 observed.

Poster Session 2 - Board: BT-22 / **179**

A study of beam stability improvements delivered by a monochromator upgrade to the Australian Synchrotron MX2 beamline

Author(s): ERIKSSON, Daniel[1] ; Dr. ARAGAO, David[1]
Co-author(s): CHERUKUVADA, Hima [1] ; Dr. HARROP, Stephen [1] ; CLARKEN, Robbie ; EASDON, Alan [1] ; Dr. PANJIKAR, Santosh [1] ; WILLIAMSON, Rachel [1] ; Dr. PRICE, Jason [1] ; MACEDO, Sofia [1] ; CARADOC-DAVIES, Tom [2]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron.*

Corresponding Author(s): daniel.eriksson@synchrotron.org.au, david.aragao@synchrotron.org.au, tom.caradoc-davies@synchrotron.org.au

MX2 is an in-vacuum undulator based crystallography beamline at the 3 GeV Australian Synchrotron. The beamline delivers hard x-rays in the energy range from 5.5 - 21 KeV to a focal spot at the sample position of ˜15 microns FWHM. At 13 KeV the flux at the sample is typically 2.0 x 10ˆ12 ph/sec. This beamline is ideal for weakly-diffracting, hard-to-crystallise proteins, viruses, protein assemblies and nucleic acids as well as smaller molecules such as inorganic catalysts and organic drug molecules. However, as a decrease in beam size generally has positive effect on smaller crystals or disordered larger crystals the beam vibration can have an effect in beam position with consequent decrease in data quality. These considerations are particularly true for small crystals such as from GPCRs or grown by the lipidic cubic phase methodologies where wedges of data from multiple crystals is required to build a complete set of data. A description of the latest upgrade on the monochromator including a pre- and post upgrade beam vibration analysis is presented. The results show a more robust beamline to both external vibrations as well as reduce intrinsic vibration.

Instrumentation / **185**

24h with a pixel detector - assessment of a Dectris 1M EIGER unit on loan to MX2

Author(s): Dr. ERIKSSON, Daniel[1]
Co-author(s): Dr. ARAGAO, David [1] ; Dr. CARADOC-DAVIES, Tom [2] ; Dr. HARROP, Stephen [1] ; Dr. PANJIKAR, Santosh [1] ; Dr. PRICE, Jason [1] ; MUDIE, Stephen [1] ; Dr. WILLIAMSON, Rachel [1] ; Dr. MACEDO, Sofia [1]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron.*

Corresponding Author(s): daniel.eriksson@synchrotron.org.au, david.aragao@synchrotron.org.au, tom.caradoc-davies@synchrotron.org.au

The EIGER series of hybrid photon detectors constitute an interesting alternative to the more established Pilatus technology. As a means to assess their potential, Dectris kindly lent the Australian Synchrotron their smallest unit for a short period, to be tested at a range of beamlines. The EIGER has a range of properties suitable for deployment at an MX beamline such as kilohertz frame rate; no read-out noise; very low point-spread function; and continuous readout with 3 μs dead-time. Here we present the findings of working with this detector during a 24 hour window on MX2. Preliminary data suggest that the unit is suitable for high frame-rate, fine-sliced, shutterless data collection for PX and CX with a merging R-factor on par with our current setup. With a temporary and unoptimized installation, our insulin test crystals could be

solved by trivial molecular replacement from data collected at 13 keV at 10 Hz to 200 Hz using 200 degrees oscillation keeping the dose constant. At 8 keV, 200 degrees of data was enough for S-SAD phasing. Overall impressions are positive, and any concerns that a pixel detector can be installed and commissioned on MX2 in a timely manner have been allayed.

Poster Session 1 - Board: AM-15 / **108**

EXAFS study on the structural properties of In and In + C implanted Ge

Author(s): Mr. FENG, Ruixing[1]
Co-author(s): Dr. KREMER, Felipe [1] ; Dr. SPROUSTER, David [1] ; Ms. MIRZAEI, sahar [2] ; Dr. MEDLING, Scott [1] ; Prof. RIDGWAY, Mark [1]

[1] *Australian National University*

[2] *PhD student*

Corresponding Author(s): ruixing.feng@anu.edu.au

Ge has been increasingly important in semiconductor application in the recent years, since it has the potential to be an alternative material replacing Si in fabricating metal-oxide semiconductor field-effect-transistor for future metal oxide semiconductor devices. Here we study the effect of Indium concentration on the structural and electrical properties of Ge with or without C co-doping. By using extended x-ray absorption fine structure and x-ray absorption near-edge spectroscopy, we found that in the case of In implanted Ge, In atoms occupy a substitutional site in the Ge lattice with In concentration ≤ 0.3 at. %, yet when In concentration is ≥ 1 at. %, In precipitates to from metallic particles as confirmed by transmission electron microscopy, evidence of an In – Vacancy complex is also apparent with EXAFS. With C co-implantation, x-ray absorption spectra show that In precipitation was suppressed when the In and C concentration are ≥ 1 at. % (also supported by transmission electron microscopy), and evidence of In – C pairing formation was found in EXAFS. Hall Effect measurement also showed that the carrier density significantly increased and In atom activation ratio was improved with C co-implantation. Density Functional Theory was applied to calculate the binding energies of In – In, In – Vacancy and In – C clusters, and it was found that In atoms have a preference to pair with vacancies and C in Ge. The lattice structure of the samples were simulated using Density Functional Theory and compared with the reulsts of XAS.

Radiotherapy and Radiobiology / **85**

The innate immune system is associated with gene expression modulation in skin distant from irradiated sites.

Author(s): Dr. FORRESTER, Helen[1]
Co-author(s): Dr. STEVENSON, Andrew [2] ; Dr. HALL, Chris [3] ; Dr. LOBACHEVSKY, Pavel [4] ; Prof. HAMILTON, John [5] ; MARTIN, Olga [4] ; Dr. SPRUNG, Carl [1]

[1] *Hudson Institute of Medical Research*

[2] *Australian Synchrotron/ CSIRO*

[3] *Australian Synchrotron*

[4] *Peter MacCallum Cancer Centre*

[5] *The University of Melbourne/Royal Melbourne Hospital*

Corresponding Author(s): helen.forrester@hudson.org.au

Microbeam radiotherapy (MRT) utilizes high intensity synchrotron generated X-rays collimated planar microbeams (˜25 μm). MRT showns promise for cancer treatment, effectively ablating tumours while causing less normal tissue damage compared to conventional broadbeam (BB) radiotherapy. Synchrotron radiation also has low scattering making it ideal to investigate non-targeted, systemic radiation effects (i.e., abscopal effects). Although abscopal effects such as non-targeted tumour shrinkage and DNA damage are observed in distant tissue, the molecular mechanism is unknown. To investigate the molecular radiation response in distant non-target tissue, hind flanks of C57BL/6J mice were irradiated with synchrotron MRT and BB and gene

expression levels were measured in distant skin. DNA damage response genes, Trp53 and Mdm2, are decreased in distant skin after both BB and MRT. To determine if these effects are due to the innate immune system, immunodeficient mice were irradiated with MRT. These mice showed no decrease in the Trp53 and Mdm2 genes in distant skin. Furthermore, Trp53 increases in distant skin from macrophage depleted mice. Also, in distant skin from Ccl2 deficient mice, the levels of Mdm2 and the inflammatory genes, Tgfb1, Tnfa, and Ccl22 increases. In conclusion, the innate immune system is associated with suppression of genes in distant tissue which otherwise may induce inflammation in response to radiation-induced cytokines.

Poster Session 2 - Board: EM-16 / **211**

Comparing and Contrasting the Anomalous Structural Phase Transformations Between the Isostructural Orthorhombic and Rhombohedral Forms of CdUO4 and SrUO¬4

Author(s): Mr. GABRIEL, Murphy[1]
Co-author(s): Prof. KENNEDY, Brendan [2]

[1] *University of Sydney*

[2] *The University of Sydney*

Corresponding Author(s): gmur5714@uni.sydney.edu.au

The resurgence of interest that is currently enveloping the nuclear power industry has reinvigorated research attempts into optimising current UO2 based fuel. However, little progress has been made regarding the understanding of the solid state chemistry of UO2 fuels matrices, the interaction they have with fission daughters such as Sr-90/Cs-137 and the solid-phases that form during fission. This has resulted in significant challenges for nuclear waste treatment methods, with no viable long term solutions for nuclear waste. We have investigated the ternary uranium oxide systems of CdUO4 and SrUO4 using in situ synchrotron X-ray powder diffraction and absorption spectroscopy (XAS). We have found that both oxides can form isomorphous rhombohedral and orthorhombic structures. Despite these structural similarities, we found that the structural phase transformation that occurs between the rhombohedral and orthorhombic forms is anomalous and considerably contrasting. In SrUO4, we found the rhombohedral form is a metastable structure that seeks to transform to the orthorhombic form, but is impeded by a large thermodynamic barrier. This barrier can be reduced by formation of vacancies in the oxygen sub-lattice allowing the rhombohedral structure to transform to the stable orthorhombic form with subsequent oxygen reabsorption. In CdUO4, we see opposite, the orthorhombic form is metastable and the rhombohedral is the preferred low energy configuration. However in both instances the transformation does proceed with the generation of vacancies in the oxygen sub-lattice with in situ XAS measurements revealing the reduction of U(VI) to U(V).

Radiotherapy and Radiobiology / 146

Nanoparticle Dose Enhancement of Synchrotron Beams on the IMBL

Author(s): Mr. GAGLIARDI, Frank[1]
Co-author(s): Dr. STEVENSON, Andrew [2] ; Prof. FRANICH, Rick [3] ; Prof. GESO, Moshi [3]

[1] *William Buckland Radiotherapy Centre*

[2] *Australian Synchrotron/ CSIRO*

[3] *RMIT University*

Corresponding Author(s): frank.gagliardi@wbrc.org.au

Nanoparticles with high atomic number (Z) have a larger x-ray cross section than biological tissues. Synchrotron beams interact with the nanoparticles to produce Auger electrons which deposit their energy over a short range, typically less than a micron. This characteristic offers the ability to enhance the dose delivered to tumors by synchrotron broad beam (BB) or microbeam radiation therapy (MRT). High Z nanoparticles can also be used as a contrast agent for in-vivo x-ray imaging during the treatment setup. Here we present our initial findings on the dose enhancement effect

for synchrotron beams on the IMBL using UV/Vis spectroscopy with radiosensitive dosimeters irradiated with and without nanoparticles.

Poster Session 2 - Board: RR-04 / **144**

Dose Distributions and Treatment Planning System Verification of Synchrotron Beams on the IMBL

Author(s): Mr. GAGLIARDI, Frank[1]
Co-author(s): Dr. POOLE, Christopher [2] ; Dr. CROSBIE, Jeff [3] ; Prof. FRANICH, Rick [3] ; Prof. GESO, Moshi [3]

[1] *William Buckland Radiotherapy Centre*

[2] *RMIT*

[3] *RMIT University*

Corresponding Author(s): frank.gagliardi@wbrc.org.au

Radiation therapy requires vigorous validation of the treatment planning system (TPS) before patient treatments can be accurately performed. Typically this is done by comparing dose calculations of the TPS with ionisation chamber or film measurements in various phantoms. Researchers from RMIT University and the Australian Synchrotron's IMBL have developed a TPS based on the Eclipse TPS (Varian Medical Systems of Palo Alto, California, USA). The Eclipse algorithms which calculate the dose distributions for megavoltage (MV) radiation therapy have been substituted for Monte Carlo algorithms that model the dose distribution generated by the kilovoltage (kV) synchrotron beams on the IMBL. The major difficulty in validating the dose distributions calculated with the new TPS is the dynamical nature of the IMBL treatments. Only a single ionisation chamber measurement or a 2D representation with film may be performed at a time. Dosimetric properties of synchrotron beams on the IMBL have been measured in 3D with water equivalent radiosensitive dosimeters and optical CT scanning. The results have been compared with ion chamber measurements performed on the IMBL and calculations with the new TPS.

Advanced Materials II / 145

Observation of crystalline orthogonal self-stratification in spin-coated conjugated polymer thin films with depth-sensitive X-ray scattering

Author(s): Dr. GANN, Eliot[1]
Co-author(s): Prof. MCNEILL, Chris [2]

[1] *Australian Synchrotron*

[2] *Monash University*

Corresponding Author(s): eliot.gann@synchrotron.org.au

We report the observation of an orthogonally realigned crystalline surface layer in a spin-coated conjugated polymer film as used in organic field-effect transistors. The ability of Grazing Incidence Wide Angle X-ray Scattering to provide some surface sensitivity of scattering features within thin films is known, but until now an unambiguous orthogonal stratified crystalline microstructure in high performance polymeric materials has not been demonstrated. By comparing angle-resolved scattering intensity collected at the SAXS/WAXS beamline of the Australian Synchrotron to simulated X-ray electric field intensity within a 72 nm thin polymer film, we find the data is consistent with 9 nm of edge-on aligned crystallites on top of 63 nm of highly crystalline face-on crystallites. We propose that a balance of air-polymer, polymer-polymer, and substrate-polymer interactions encourage edge-on surface realignment and stratification. This type of surface reorganization and alignment will be increasingly important to measure and predict as further organic electronic devices are developed.

Advanced Materials III / 161

Biomimetic antibacterial surfaces - fatty acid molecular packing and surface topology on HOPG by grazing incidence diffraction

Author(s): Dr. GARVEY, Chris[1]
Co-author(s): Ms. NGUYEN, Song Ha [2] ; Dr. WEBB, Hayden [2] ; Prof. MAINWARING, David [2] ; Prof. CRAWFORD, Russell [2] ; Prof. IVANOVA, Elena [3]

[1] *ANSTO*

[2] *Swinburne University of Technology*

[3] *Swinburne Univeristy of Technology*

Corresponding Author(s): cjg@ansto.gov.au

The distinctive topology on the wings of some insects may provide a physical anti-bacterial action based on the penetration of the cell wall/membrane and the disruption of the integrity of the intra-cellular solution. Surfaces which mimic the topology of the insect anti-bacterial surface may be produced by the crystallization of fatty acid molecules on a highly ordered pyrolytic graphite (HOPG) substrate. Based on the nature of the chains which pack on the surface, different topologies may be produced. In this study we use synchrotron grazing incidence x-ray diffraction (GID) to understand the packing of molecules on the surface and their preferred orientation. The work indicates the potential of GID investigations to provide an understanding on the relationship between crystal growth on the surface and the topology of the resultant surface.

Poster Session 2 / 163

Structural Changes Induced by Uniaxial Deformation and Photodegradation in Low Density Polyethylene

Author(s): Dr. GARVEY, Chris[1]
Co-author(s): Dr. HSU, Yu-Chieh [2] ; Dr. WEIR, Michael [3] ; Dr. TRUSS, Rowan [4] ; Dr. NICHOLSON, Timothy [4] ; Prof. HALLEY, Peter [4]

[1] *ANSTO*

[2] *3M Australia Pty Ltd*

[3] *Department of Physics and Astronomy, The University of Sheffield*

[4] *School of Chemical Engineering, The University of Queensland*

Corresponding Author(s): cjg@ansto.gov.au

In previous work we have used synchrotron based small angle x-ray scattering (SAXS) and a transform of the radially averaged SAXS data, the linear correlation function (LCF)1, to study the structural changes in the semi-crystalline lamellae of low density polyethylene (PE) during photo-oxidative degradation2. Typical SAXS patterns consisted of decay with a superposed broad diffraction feature indicative of the semi-crystalline lamellae. Key parameters extracted from the transformation of data into the LCF were the lamellar spacing, relative volumes of crystalline and amorphous regions in the lamellar region. In this work we use the LCF of data sector averaged in a direction parallel and normal to the direction of tensile deformation to characterise the structural changes in low-density PE during uniaxial tensile deformation from in-situ synchrotron SAXS measurements from both as provided and samples subject to controlled degradation. As provided samples show a region of the tensile curve where the lamellar structure is deformed elastically and a region of plastic deformation where there is considerable deformation of the semi-crystalline lamellar structure. The photo-degraded material shows an elastic deformation of the lamellae before failure.

1. Goderis, B.; Reynaers, H.; Koch, M. H. J.; Mathot, V. B. F., Journal of Polymer Science Part B-Polymer Physics 1999, 37 (14), 1715-1738.

2. Hsu, Y. C.; Weir, M. P.; Truss, R. W.; Garvey, C. J.; Nicholson, T. M.; Halley, P. J., Polymer 2012, 53 (12), 2385-2393.

Poster Session 2 - Board: EM-02 / **78**

Analysis of manganese dioxide electrochemical capacitors using synchrotron methods: in-situ analysis of electrodeposition.

Author(s): Mr. GIBSON, Andrew[1]
Co-author(s): Ms. DUPONT, Madeleine [1] ; Prof. DONNE, Scott [1] ; Mr. DOSE, Wesley [1]

[1] *University of Newcastle*

Corresponding Author(s): andrew.gibson@uon.edu.au

Manganese oxides (MnO2, MnOOH) are promising materials for electrochemical capacitors due to their low cost and toxicity, coupled with their attractive energy storage properties, and are hence well represented in the literature 1. Thin films of MnO2 prepared by electrodeposition are capable of achieving high values for gravimetric specific capacitance (>2000 F/g) [2]. Material activity, as well as material morphology play an important role in determining the capacitive behaviour of a material [3]. Thus, it is important to understand the role the electrodeposition solution has on the resultant structure and morphology of the deposited manganese oxides.
In this poster, the in-situ application of three different synchrotron techniques to the electrodeposition of manganese oxides will be discussed. The beamlines utilised for the experiments described in this poster are powder diffraction, small angle x-ray scattering and x-ray absorption spectroscopy. In all cases, the electrodeposited manganese oxides have been prepared from a solution containing between 0.001 - 0.1 M MnSO4 and 0.01 – 1 M H2SO4.

1. Wei, W., et al., Manganese oxide-based materials as electrochemical supercapacitor electrodes. Chemical Society Reviews, 2011(40): p. 1697 - 1721.

2. Andrew Cross, A.M., Ariana Cormie, Tony Hollenkamp, Scott Donne, Enhanced Manganese Dioxide Supercapacitor Electrodes Produced by Electrodeposition. Journal of Power Sources, 2011. 196: p. 7847 - 7853.

3. Conway, B.E., Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications. 1999, New York: Springer.

Poster Session 2 - Board: BT-32 / **210**

Optimisation of a Ge pixel detector – how low can we go?

Author(s): Dr. GLOVER, Chris[1]
Co-author(s): JOHANNESSEN, Bernt [1] ; Dr. KAPPEN, Peter [1]

[1] *Australian Synchrotron*

Corresponding Author(s): chris.glover@synchrotron.org.au

The Australian Synchrotron has one hard X-ray XAS beamline. This was constructed to service the majority of the local scientific community needs, which notably consists of a significant component of Bio-XAS and materials studies where the elements of interest are often very dilute (< 0.5 ppm). This is balanced with users with more typical experimental needs (eg several 0.1%'s concentration fluorescence or transmission measurements). As such, a high flux (up to 10^13 photons/sec) beamline, matched to a 100 element Germanium pixel array detector (PAD) was seen as the best experimental match for the community for routine operation. On occasion, the sensitivity limit for XANES is around 100-200 ppb. At such low concentrations, many aspects of the PAD are critical. Areas we are constantly exploring include: using Z-1 filters and soller slits / collimators, masking adjoining pixel interstitial region, optimized electronic filter parameters, per element deadtime corrections, maximum countrate and linearity tradeoffs, peaking time vs resolution tradeoff and fitting the full fluorescence signal/background to provide better normalization. Results from selected investigations will be presented focusing on the resulting quality and reliability of the normalized XAS signals, influenced bythe question –"How low in concentration can we reliably go?"

Advanced Materials II / 148

Synchrotron XPS, EXAFS and IR studies of atomically precise chemically made clusters

Author(s): Dr. GOLOVKO, Vladimir[1]
Co-author(s): Prof. METHA, Greg [2] ; Prof. ANDERSSON, Gunther [3] ; Dr. ANDERSON, David [1] ; Dr. ADNAN, Rohul [1] ; Mr. BENNETT, Trystan [2] ; Dr. DONOEVA, Baira [1]

[1] *University of Canterbury*

[2] *University of Adelaide*

[3] *Flinders University*

Corresponding Author(s): vladimir.golovko@canterbury.ac.nz

We are exploring the use of atomically-precise, chemically-synthesised metal clusters deposited on various forms of oxides with a view to understanding how and why they perform as catalysts and sensors.1, 2 Although measurement of their catalytic activity is important, it is vital to identify and understand the geometric and electronic structure of the active sites to make further gains in photocatalytic efficiency and efficacy. Consequently, theoretical modelling on atomically precise co-catalysts can provide understanding to interpret and explain experimental analysis and observation.
Results of recent synchrotron XPS/EXAFS studies of pure and supported clusters and colloids reveal their unique electronic properties and highlight the importance of support chemistry in controlling aggregation of clusters.3, 4 We applied density functional theory to model a wide range of clusters in order to assign core and core-ligand vibrations in experimentally obtained spectra for the first time.5,6

1. R. H. Adnan et al., Catalysis Science & Technology, 2015, 5, 1323-1333.
2. M. Z. Ahmad et al., International Journal of Hydrogen Energy, 2013, 38, 12865-12877.
3. D. P. Anderson et al., Physical Chemistry Chemical Physics, 2013, 15, 14806-14813.
4. D. P. Anderson et al., Physical Chemistry Chemical Physics, 2013, 15, 3917-3929.
5. J. F. Alvino et al., RSC Advances, 2013, 3, 22140-22149.
6. T. Bennett et al., Inorganic Chemistry, 2014, 53, 4340-4349.

Poster Session 2 - Board: IM-04 / **53**

Improved Absorption and Phase Contrast PIV Via Multi-Source Imaging Techniques

Author(s): Mr. GOONAN, George[1]
Co-author(s): Dr. DUBSKY, Stephen [1] ; Prof. FOURAS, Andreas [1] ; Mr. CARNIBELLA, Richard [1]

[1] *Monash University*

Corresponding Author(s): george.goonan@monash.edu

Previous research in the field of Particle Image Velocimetry (PIV) has highlighted the need for high spatio-temporal resolution [[1]] as well as a distinction between static and dynamic imaging optimization [2]. Traditional single-source imaging systems optimized for small spot sizes are constrained by physical limitations, such as maximum anode power density. By utilising multiple sources with small spot sizes, anode power density is maintained while increasing overall brightness. The resultant image (see Figure 1), while not necessarily suitable for static imaging, provides increased information density for more accurate PIV analysis.
Presented here is the preliminary investigation into multi-source PIV imaging regimes. Two forms of this technology are displayed; Aperture-type applications (see Figure 1), and the characteristically equivalent flat-panel array source applications. Through computational simulations experimentally validated using a liquid metal jet source, we demonstrate this novel technology's

capability for significantly increased PIV accuracy with reduced source luminosity. We further demonstrate that these properties can be greatly enhanced by judicious selection of source location and system geometry.

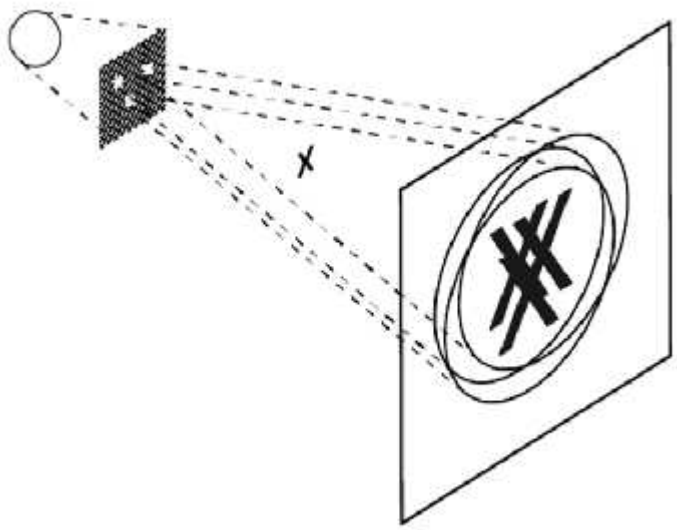

Figure 1: Aperture-type Multi-Source Imaging. The overlapping images, whilst creating blur for static imaging, increases information density for dynamic imaging. Source credit: Rajeev Samarage

[[1]] S. Dubsky, S. B. Hooper, K. K. W. Siu, and A. Fouras: J. R. Soc. Interface 9 (2012) 2213.
[2] I. Ng, D. M. Paganin and A. Fouras, J. Appl. Phys., vol. 112, no. 074701, pp. 1-11, 2012.

Poster Session 1 - Board: SM-17 / **130**

High throughput synthesis and Characterisation of Protic Ionic Liquids

Author(s): Dr. GREAVES, Tamar[1]
Co-author(s): Ms. HA, Krystal [1] ; Dr. MUIR, Benjamin [2] ; Dr. HOWARD, Shaun [2] ; Mr. WEERAWARDENA, Asoka [1] ; Dr. KIRBY, Nigel [3] ; Prof. DRUMMOND, Calum [1]

[1] *RMIT University*

[2] *CSIRO*

[3] *Australian Synchrotron*

Corresponding Author(s): tamar.greaves@rmit.edu.au

Ionic liquids (ILs) are tailorable solvents with a vast number of potential cation and anion combinations. ILs have many potential applications in fuel cells, organic and inorganic synthesis and as biological solvents. Currently the tailorability of ILs is underutilised with most studies optimising the choice of IL for a specific application using < 20 candidates. Protic ILs (PILs) are a subset of ILs which are simple to synthesise, through proton transfer from a Bronsted acid to a Bronsted base. Here we developed a high throughput (HT) automated method to synthesis and dry a library of 48 PILs, comprising alkyl carboxylic acids paired with alkylamines.1 Desirable properties were identified using visual screens for surface tension, viscosity and melting points. HT analysis of their liquid nanostructure was obtained using small and wide angle X-ray scattering (SAXS/WAXS) at the Australian Synchrotron. The nanostructure consisted of polar and non-polar domains, with intercalation of the alkyl chains on the cation and anion and charge alternation of the polar groups. The nanostructure depended on the relative length of the alkyl chain on the cation and anion, and to our knowledge has not previously been reported. The HT methodology and screens are widely applicable to the synthesis and drying of PILs, are at least

20 times faster, and significantly less labour intensive than conventional techniques. Our method can be scaled up and combined with design of experiment methodologies to develop vast libraries of PILs . Greaves et al. Phys. Chem. Chem. Phys. 2015, 17, 2357.

Poster Session 2 - Board: EM-10 / **136**

In-situ hydrogen absorption/desorption behaviour of Mg based alloys

Author(s): Mr. TRAN, Xuan Quy[1]
Co-author(s): Dr. MCDONALD, Stuart [1] ; Dr. GU, Qinfen [2] ; Prof. MATSUMURA, Syo [3] ; Dr. NOGITA, Kazuhiro [1]

[1] *Nihon Superior Centre for the Manufacture of Electronic Materials (NS CMEM), School of Mechanical and Mining Engineering, The University of Queensland, Australia*

[2] *Australian Synchrotron*

[3] *Department of Applied Quantum Physics and Nuclear Engineering and the Ultramicroscopy Research Center, Kyushu University, Fukuoka, 819-0395, Japan*

Corresponding Author(s): qinfen.gu@synchrotron.org.au

Hydrogen has the potential to power much of the modern world with only water as a by-product, but storing hydrogen safely and efficiently in solid form such as magnesium hydride remains a major obstacle. Here we use in-situ synchrotron powder X-ray diffraction to investigate the mechanisms of the hydrogen absorption and desorption in bulk Mg-Ni alloys. Our study shows that the hydrogenation of Na-doped hypoeutectic Mg-Ni alloys can be identified at a temperature as low as 260oC via an interface-controlled nucleation and growth mechanism without any prior activation while dehydrogenation occurrs at about 370oC. The sequence of phase transformations associated with these reactions as well as the expansion properties of individual phases during hydrogen sorption reactions as provided by high resolution X-ray diffraction data are also discussed. Furthermore, as evidenced by an in-situ ultra-high voltage transmission electron microscopy study, we find that the hydrogen release mechanism from bulk (2 m) MgH2 particles is based on the growth of multiple pre-existing Mg crystallites within the MgH2 matrix, present due to the difficulty of one hundred percent hydrogenation. In contrast, in thin samples analogous to nano-powders, dehydriding occurs by a ‘shrinking core’ mechanism.

Poster Session 2 - Board: EM-08 / **117**

The influence of Ni and Zn additions on microstructure and phase transformations in SnCu solder joints

Author(s): Dr. GU, Qinfen[1]
Co-author(s): Dr. ZENG, guang [2] ; Prof. NOGITA, kazuhiro [3] ; Dr. MCDONALD, Stuart [3]

[1] *Australian Synchrotron*

[2] *Univeristy of queensland*

[3] *University of Queensland*

Corresponding Author(s): qinfen.gu@synchrotron.org.au

Microalloying, in which the solidification structure is preferably and significantly modified by trace elements, is a key method for improving Pb-free interconnections in electronic devices. Microalloying Ni or Zn is expected to modify the Sn–0.7Cu alloy in different ways. This research examines the influences of minor/trace additions of Ni and Zn concurrently on the development of the microstructure, the interfacial reactions and the stability of the intermetallics in Sn–0.7Cu solder alloys and associated joints, using X-ray radiography, X-ray florescence analysis, X-ray diffraction and electron microscopy. It shows that minor Zn additions (∼0.15 wt.%) result in the formation of a CuZn intermetallic in the interdendritic region during solidification, whereas a small amount of Ni completely changes the solidification mode and a eutectic microstructure is obtained. When Ni is added, small particles of primary (Cu,Ni)6Sn5 intermetallic forms in advance of the solidification front. Microalloying Ni and Zn concurrently refines the microstructure and leads to a more continuous, finer-grained and stable interfacial Cu6Sn5 intermetallic and suppresses

the growth of Cu3Sn. The Ni and Zn are homogeneously distributed in interfacial Cu6Sn5 and inhibit the polymorphic phase transformation of Cu6Sn5. This stabilizing effect minimizes the thermal expansion mismatch between interfacial Cu6Sn5 and the Cu substrate. The findings have important implications for the manufacture of high-reliability lead-free microjoints.

Poster Session 2 - Board: EM-12 / **166**

Phase evolution and structural transformation of electrodes for Li- and Na-ion batteries upon cycling

Author(s): Dr. PANG, Wei Kong[1]
Co-author(s): PETERSON, Vanessa [2] ; Prof. GUO, Zaiping [1] ; Mr. KALLURI, Sujith [1] ; SHARMA, Neeraj [3] ; JOHANNESSEN, Bernt [4] ; Dr. KIMPTON, Justin [4]

[1] *University of Wollongong*

[2] *ANSTO*

[3] *UNSW*

[4] *Australian Synchrotron*

Corresponding Author(s): zguo@uow.edu.au

Li-ion batteries (LIBs) are the primary choice of power source for portable electronic devices, including mobile phones, laptops, as well as electric vehicles. The working principle of a LIB is to store electric energy in chemical form by using charge-balancing Li ions that reversibly insert into the electrodes. On the other hand, Na-ion batteries (NIBs) are also considered one of the best alternatives to LIB technology, due to their similar electrochemistry, potentially non-toxicity, and the greater elemental abundance of sodium leading to low-cost. In both LIB and NIB, the structure and chemistry of the electrodes are closely related and determine its functional mechanism. A mechanistic understanding of the charge-carrier insertion/extraction process in electrode materials is necessary to understand the electrochemical properties that underpin battery function. In this presentation, we showcase examples of operando studies of both LIB and SIB using synchrotron X-ray powder diffraction (PD) and X-ray absorption (XAS) data, collected on PD and XAS beamlines, with sufficient information to extract detail of the insertion/extraction mechanism and to give rational improvements for the developments .

Advanced Materials III / **10**

SAXS Investigation of SiO2 Nano-Pore Membranes

Author(s): Ms. HADLEY, Andrea[1]
Co-author(s): Mr. PROFT, Max [2] ; Dr. MEDLING, Scott [2] ; Dr. HAWLEY, Adrian [3] ; Dr. KLUTH, Patrick [2] ; SCHAURIES, Daniel [1] ; Mrs. NADZRI, Allina [4] ; Mr. MOTA SANTIAGO, Pablo [2]

[1] *ANU*

[2] *Australian National University*

[3] *Australian Synchrotron*

[4] *Australian National University (ANU)*

Corresponding Author(s): andrea.hadley@anu.edu.au

Membranes with nano-sized pores are ideal for many advanced applications including bio-sensing, filtration processes, nano-fluidics, nano-electronic and nano-optic devices. To effectively realise these applications, pores with controlled shapes and narrow size distributions are needed. Irradiation with high energy heavy ions and subsequent chemical etching can be used to form highly uniform nano-porous membranes in a variety of materials, including polymers like polycarbonate, PET and polyimide, and in solid state materials such as silicon dioxide (SiO2). SiO2 membranes can be integrated with routine semiconductor fabrication processes, and they exhibit superior thermal stability compared to polymer membranes. We are currently developing a technology for controlled fabrication of nano-pore membranes using 0.5-2 μm thin SiO2 layers. Freestanding membranes were irradiated with 185 MeV Au ions and etched in dilute HF solution, preferentially etching the radiation damage to form the pores. SAXS, in combination with advanced Monte-Carlo (MC) simulation techniques, provides an ideal method for characterisation of the

complex pore structures formed in SiO2 . These structures can exhibit conical or double conical shapes, depending on the etching conditions. Compared to cross-sectional transmission and scanning electron microscopy, SAXS in combination with MC simulations enables a more accurate reconstruction of the size and shape of the pores, taking advantage of superior statistics since a large number of pores may be measured simultaneously. This information is essential for development of the membrane technology.

Imaging I / 33

Combining SR Computed Tomography and Fluoresence X-Ray Computed Tomography

Author(s): Dr. HALL, Chris[1]
Co-author(s): ACRES, Robert [1] ; Mr. WINNETT, Alex [2] ; Prof. WANG, Feng [2]

[1] *Australian Synchrotron*

[2] *Swinburne University of Technology*

Corresponding Author(s): chris.hall@synchrotron.org.au

An x-ray image highlighting technique which might prove more sensitive than simple attenuation alteration, is imaging the x-ray fluorescence from specific markers. This technique is exploited to great effect on x-ray fluorescence microscopy beam lines like our XFM facility. On IMBL we would like to develop a lower resolution, but wider field of view method of reconstructing 3-D fluorescence imaging compatible with SRCT.
A beam modulation technique has been proposed previously to allow fluorescence CT (FXCT) and SRCT data to be collected simultaneously 1. This work resulted in some proof of concept modelling and a simple experiment test system.
Since seminal papers on the subject were published in 2008, there has been significant activity around Compressive Sensing (CS). Ideas in CS have been proven for imaging at optical and infra-red wavelengths. CS has also caused a lot of excitement in the medical imaging community. However, to date not much has been published on using CS techniques in SR x-ray imaging. We believe CS imaging techniques suit IMBL and may overcome the issues in combining SRCT and FXCT.
We present some recent data, and model outputs which demonstrate the reconstruction of low resolution iodine fluorescence maps of realistic phantoms from data collected with a single point detector during a CT scan on IMBL.
1 - C. Hall, 'Combined x-ray fluorescence and absorption computed tomography using a synchrotron beam', 2013, Journal of Instrumentation. doi:10.1088/1748-0221/8/06/C06007

Cheiron School Student Presentations / 220

Mg-carbonate minerals trap potentially toxic trace metals and CO2 at Woodsreef Mine, New South Wales

Author(s): HAMILTON, Jessica[1]
Co-author(s): WILSON, Sasha [1] ; Dr. MORGAN, Bree [2] ; Mr. TURVEY, Connor [1] ; MCCUTCHEON, Jenine [3] ; PATERSON, David [4] ; SOUTHAM, Gordon [3]

[1] *Monash University*

[2] *CSIRO*

[3] *University of Queensland*

[4] *Australian Synchrotron*

Corresponding Author(s): jessica.hamilton@monash.edu

Carbon mineralisation has been recognised as a safe and long-term means of trapping and storing CO2 within mineral structures. The stockpiles of reactive, finely pulverised mine tailings produced by ultramafic-hosted mines are ideal settings in which to observe and promote carbonation. This can be achieved by reaction of Mg-rich waste minerals with atmospheric or industrial CO2.

Consequently, there has been much interest in enhancing the rate of natural weathering processes at mine sites.
We have recently (October 2015) deployed the first ever field-scale experiments to accelerate CO2 sequestration by enhanced weathering at the Woodsreef Chrysotile Mine in NSW, Australia. Mine tailings commonly contain significant concentrations of potentially toxic metals (e.g., Cr, Co, Cu, Ni), found within the crystal structures of Mg-silicates, sulfides, oxides and metal alloys. Because our field trial involves leaching tailings with acidic solutions, which may enhance metal mobility, it was crucial that we first understand the ultimate fate of trace metals during enhanced weathering.
Synchrotron X-ray fluorescence mapping indicated that recently precipitated (since 1983) carbonate minerals are sequestering first-row transition metals (i.e., Cr, Ni, Mn, Co, Cu) trace metals, likely via substitution for Mg, within their crystal structures. This demonstrates that accelerated carbonation of metal-rich industrial wastes or mine tailings, such as those at Woodsreef Mine, is unlikely to generate metalliferous drainage and will not pose an environmental risk.

Poster Session 1 - Board: EE-05 / **56**

Using the Synchrotron IR beam to develop optical markers for the characterisation of coal and other components in urban dust samples

Author(s): Mr. GREGOIRE, Krahenbuhl[1]
Co-author(s): Mr. BAMBERY, Keith [2] ; Mr. O'BRIEN, Graham [1] ; Mrs. KARRYN, Warren [1] ; Mrs. HAPUGODA, Priyanthi [1] ; Mr. HAPUGODA, Sarath [1]

[1] *CSIRO*

[2] *Australian Synchrotron*

Corresponding Author(s): priyanthi.hapugoda@csiro.au

Establishing health impacts of urban dust require quantitative particle size and composition information. For the coal industry, dust is a significant responsibility. Coal dust originates from mining, transportation and coal usage. Public concern is greatest where mines are in proximity to towns, rail corridors and ports. Although coal may only be one of the dust constituents, there is an (often incorrect) perception that all black dust is coal; it is therefore important to to present dust analysis information in a way which can obtain acceptance.
We used the Australian Synchrotron Infrared Microscopy beamline to obtain chemical information for particulates including coal, diesel soot, rubber, organic matter, plastic, paint, rust, dirt and determined their proportions in urban dust samples collected in the coal transport corridor and coal ports.
The high spatial resolution of the Synchrotron IRM is ideally suited for the particles of interest which are in the 1-10 micron range. The Synchrotron is particularly useful to identify matter (e.g. organic) that is otherwise difficult to characterise. Sample spectra were recorded at the beamline microscope in Attenuated Total Reflection mode which allows enhanced spatial resolution due to the high refractive index of the ATR crystal element.
Once the particles are identified we use them used as a ground-truth to train a supervised learning algorithm that will allow identification of dust components based on optical microscopy. The optical images also provide the size information of individual particles and a method for presenting quantitative information on the makeup of dust.

Instrumentation / **35**

X-ray Imaging Detector for X-ray Free-Electron Lasers (XFELs) and Diffraction Limited Storage Rings (DLSRs)

Dr. HATSUI, Takaki[1]

[1] *RIKEN*

Corresponding Author(s): hatsui@spring8.or.jp

X-ray Free-Electron Lasers (XFELs) are now bringing new opportunities in coherent X-ray Science (CXS). Future X-ray sources such as high-repetition XFELs and Diffraction Limited Storage Rings (DLSRs) are anticipated to advance CXS further by delivering higher repetition rate and higher brilliance of coherent X-ray beam. In this talk, we first review the detector development for XFELs 1 with an emphasis of physical and technology limitation. Then we try to outlook the future opportunities from the viewpoint of X-ray imaging detectors. As a concrete example, we will describe the target performance of the detector for upgraded SPring-8 facility with a continuous frame rate of 20 kHz, and a few 10 ns time resolution in burst mode [2].
References 1 T. Hatsui and H. Graafsma, "X-ray imaging detectors for synchrotron and XFEL sources", IUCrJ, Vol. 2, p371. [2] SPring-8-II Conceptual Design Report, http://rsc.riken.jp/pdf/SPring-8-II.pdf

Beamline update and discussion / 29

Beamline update and discussion: IMBL

Author(s): HAUSERMANN, Daniel[None]
Co-author(s): Dr. HALL, Chris [1]

[1] *Australian Synchrotron*

Corresponding Author(s): daniel.hausermann@synchrotron.org.au

This session will provide an update on activities and capabilities at IMBL. The session aims to provide users with the opportunity to discuss current and future needs with the beamline team.

Imaging II: Sponsored by MASSIVE / 191

Overview of the 'New' Imaging and Medical Beamline

Author(s): HAUSERMANN, Daniel[1]
Co-author(s): Dr. HALL, Chris [1] ; Dr. MAKSIMENKO, Anton [1] ; Dr. LIVINGSTONE, Jayde [1] ; Dr. STEVENSON, Andrew [2] ; Dr. PEARSON, James [3] ; ACRES, Robert [1] ; Dr. PELLICCIA, Daniele [4]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron/ CSIRO*

[3] *IMBL / Monash University*

[4] *RMIT University*

Corresponding Author(s): daniel.hausermann@synchrotron.org.au

The Imaging and Medical Beamline (IMBL) opened for users in October 2012. In 2013 June 2015 was set as milestone for completing the Phase II research infrastructure funded by NHMRC. To achieve this we embarked on an ambitious design and implementation programme requiring 50% of the beamtime for development and commissioning, a considerable loss for our users. We however reached our objectives by June 2015 so that new and/or higher performance research techniques and facilities are now commissioned. Consequently 75% of the beamtime is now available to users, 90% in 2016. We therefore encourage new and established users from material science to clinical research to apply enthusiastically for beamtime. With this in mind we will describe the new facilities in detail and illustrate their performance with results from recent experiments. Meanwhile a recap of the main IMBL characteristics and facilities is given below.

- Source to sample distance up to 135m, beam size up to 4cm x 50cm (white and monochromatic).
- 7 detectors with a wide range of field of view, resolution, efficiency and speed.
- Extensive research infrastructure for *in vivo* studies with animals ranging from rodents to sheep.

- 3 main modes of operation: High dose step-and-shoot microbeam radiation therapy at 20m; High speed computed tomography (CT) and dynamic MRT at 35m; High resolution imaging and CT at 135m.

Poster Session 2 - Board: SM-04 / **231**

Small angle scattering examination of structures self-assembled during milk digestion

Author(s): Dr. HAWLEY, Adrian[1] ; Prof. BOYD, Ben[2]
Co-author(s): Dr. SALENTINIG, Stefan [2] ; Ms. PHAN, Stephanie [2]

[1] *Australian Synchrotron*

[2] *Monash Institute of Pharmaceutical Sciences*

Corresponding Author(s): adrian.hawley@synchrotron.org.au

Milk is a critical source of nutrition in the diet of many people, especially for infants for whom milk is the complete diet the first months of life. Milk contains both water soluble and water insoluble components all of which are made bioavailable during digestion to provide everything needed for growth and development. Recent work at the Australian Synchrotron SAXS beamline reported the discovery of self-assembled structures during the in-situ digestion of bovine and human milks. The progression through a range of different highly organized self-assembled structures has been studied using small angle scattering to follow the formation and progression of the structures in real time during digestion. Cryo-TEM was also used to study the phases formed. The lipophilic environment inside milk fat globules was found to gradually transition to more hydrophilic surfaces in highly ordered structure with high internal surface area. Digestion conditions were found to change the rate of transition. These transitions in self-assembled structures are likely to be key to making water insoluble species bioavailable in the gastrointestinal tract. Further small angle scattering studies will allow a greater understanding of how individual components in milks impact the digestion and whether additional species, e.g. adding sparingly soluble vitamins, changes the digestion stages. Understanding the different stages and structures of digestion offers scope to develop improved nutritional supplements or controlled release drug delivery systems.

Poster Session 1 - Board: AM-27 / **227**

Rational Design of Porous Coordination Polymers for Catalysis

Mr. HICKS, Jamie[1] ; Prof. BATTEN, Stuart[1] ; Dr. TURNER, David[1]

[1] *Monash University*

Corresponding Author(s): jamie.hicks@monash.edu

Over the past couple of decades, Porous Coordination Polymers (PCPs) have been extensively studied due to their variety of applications including gas storage, small molecule separations and sensors. Furthermore, heterogeneous catalysis using PCP's has recently become an area of considerable interest, as tuning the pore size can lead to selective catalysis in mixtures of reagents. However, these catalytically active PCP's often require post synthetic modification of an existing framework with a catalytically active metal.

A number of novel dicarboxylate ligands have been synthesised, which include an additional metal coordination site within the main body of the ligand itself, such as a diazabutadiene moiety. Having this additional coordination site allows for coordination of a catalytically active metal centre to the ligand, hence forming a metalloligand, before the synthesis of the coordination polymer.

With the intention of using this relatively unexplored route to rationally design PCP's, a range of metalloligands containing second row transition metal species have been developed. One such ligand, containing a Mo(CO)4 fragment, has successful been utilised in the formation of a heterometallic molybdenum/cadmium PCP, with approximately 43% void volume. The Mo(CO)4

fragments line the edges of 1D solvent channels within the structure and therefore should be accessible to substrates.

Energy Materials II / 44

What Geochemistry teaches us about Catalyst Design

Author(s): HOCKING, Rosalie[1]
Co-author(s): Ms. SCHALGENHAUFF, Sara [1] ; Ms. KING, Hannah [1]

[1] *James Cook University*

Corresponding Author(s): rosalie.hocking@jcu.edu.au

One of the greatest challenges of the 21st century will be securing cheap and renewable sources of energy. One of the most promising approaches to this challenge is to design catalysts from earth abundant materials capable of implementing key chemical reactions including splitting water into hydrogen and oxygen (H2O → 2H+ + O2); and both the oxidation (H2→ 2H+) and reduction (2H+→ H2) of hydrogen the reduction of CO2 hydrocarbons.
Some of the most promising catalyst materials for these reactions are metal oxides and sulfides which commonly exist in nature. Despite the fact that these materials are common, their structures, stability are often poorly understood. This is in part because of the reliance on traditional analytical techniques (particularly X-ray diffraction) for materials characterisation. The molecular structure of functional metal oxide and metal sulfide based catalysts can be probed in situ by combining X-ray Absorption Spectroscopy (XAS) and Transmission Electron Microscopy (TEM) to provide new insights into catalyst structure and function. We find some interesting correlations between these materials in their functional state and the geochemical cycles which form these materials in nature, implicating "kinetic destabilised forms" of these common materials. Our work provides important clues to a possible role these materials may have played in the evolution of metallo-protein type catalysis.

Poster Session 1 - Board: BT-29 / **203**

Development of cell for in situ electric-field-dependent structural and macroscopic strain measurements

Author(s): Mr. HOSSAIN, Mohammad Jahangir[1]
Co-author(s): Ms. WANG, Lijun [2] ; Dr. WANG, Zhiyang [3] ; Mr. KHANSUR, Neamul [4] ; Dr. HINTERSTEIN, Manuel [2] ; Dr. KIMPTON, Justin [5] ; DANIELS, John [4]

[1] *The School of Materials Science and Engineering, UNSW Australia*

[2] *School of Materials Science and Engineering, UNSW Australia, Sydney, NSW 2052, Australia*

[3] *School of Materials Science and Engineering, UNSW Australia & The Powder Diffraction Beamline, Australian Synchrotron*

[4] *UNSW*

[5] *Australian Synchrotron*

Corresponding Author(s): hossainjahangir1988@gmail.com, zhiyang.wang@synchrotron.org.au

Piezoelectric ceramics are playing an important role as sensor and actuator materials in many modern smart devices. When studying these functional materials, understanding the structural changes during the actuation process is necessary for gaining a complete picture of the structure-property relationship. Structures of such materials may be meta-stable during actuation, thus must be observed using in situ characterisation methods. In situ diffraction methods offer a powerful and direct means of quantifying the structural contributions to the strain generation mechanisms of these materials. Here, we demonstrate a sample cell equipped with a linear displacement sensor (LDS) capable of measuring the structural variations of electro-ceramic materials under high electric field, while simultaneously collecting macroscopic strain data. The results show that the macroscopic strain measured using the cells LDS can be directly correlated with the microscopic response of the material as observed by powder diffraction methods. The cell has been successfully demonstrated at the powder diffraction beamline of the Australian Synchrotron.

Poster Session 2 - Board: IM-08 / **132**

High Definition X-ray Fluorescence Elemental Mapping of Historic Photographs

Author(s): HOWARD, Daryl[1]
Co-author(s): PATERSON, David [1] ; Dr. DE JONGE, Martin [1] ; Mr. THURROWGOOD, David [2]

[1] *Australian Synchrotron*

[2] *Queen Victoria Museum and Art Gallery*

Corresponding Author(s): daryl.howard@synchrotron.org.au

In the 19th century, photography rapidly advanced with the continuous development of light-sensitive chemical-based processes. As such, some photographic processes were in use for less than a decade before being rendered obsolete. Some of these historic processes are sensitive to image degradation, and many photographic images are considered lost due to severe fading.
We have non-destructively analysed several historic photograph types at the X-ray fluorescence microscopy beamline of the Australian Synchrotron to investigate the spatially resolved elemental distributions and their relationship to image permanence and the photographic processes used. The analysis also tested the hypothesis that besides providing chemical information about the photographs, image retrieval is also possible. We propose that scanning X-ray fluorescence methods may prove practical in recovering images that are faded beyond recognition.

Poster Session 2 - Board: BT-20 / **164**

Successful outreach at the AS and work-integrated learning

Author(s): Dr. HOXLEY, David[1]
Co-author(s): Dr. KAPPEN, Peter [2] ; Mr. GRAEME, Oliver [1]

[1] *La Trobe University*

[2] *Australian Synchrotron*

Corresponding Author(s): d.hoxley@latrobe.edu.au

The Chief Scientist of Australia, amongst others, has observed that student engagement (and hence learning) in Science, Technology, Engineering and Maths (STEM) wanes despite the growing importance of a technologically literate population. It is widely held that disengagement flows from disconnection between students' experience in the classroom and science as professionally practised.
A connection to science as a human endeavour can be repaired by involving students in research at large facilities such as the AS, where elite groups of scientists are brought together in well-supported, cross-disciplinary teams to conduct well-planned, intensive experiments using very modern equipment. It is thus natural to invite novice scientists to the facility for pedagogical purposes (i.e. 'outreach').Care must be taken that students do not become mere bystanders in science. While hands-on involvement is engaging, it is difficult to imagine in such a delicate scientific environment. Other barriers are transport, teacher relief, and facility time.
We summarises the state of the art in synchrotron outreach, at the AS and elsewhere, and suggest solutions to the problem of scaling and engagement beyond one-off excursions. These include remote access, targeted leadership programs, and wider community engagement. We consider the evidence for and against the effectiveness of various forms of outreach to engage student learning, and argue that effective outreach can be considered as a form of Workplace Integrated Learning (WIL).

Poster Session 2 - Board: BT-24 / **188**

TPS-05A1 Protein Microcrystallography Beamline at the National Synchrotron Radiation Research Center

Author(s): Dr. HUANG, Chun-Hsiang[1]
Co-author(s): Dr. JEAN, Yuch-Cheng [1]

[1] *National Synchrotron Radiation Research Center*

Corresponding Author(s): huang.conann@nsrrc.org.tw

The routine use of synchrotron radiation for single crystal diffraction study in the past decades has revolutionized macromolecular structural biology. However, crystals of important macromolecules, such as membrane proteins and viruses, are usually small in sizes and have poor diffraction quality. Advances in synchrotron radiation sources, detectors, and software are necessary to tackle these challenging problems. This beamline aims to provide such a tool for difficult structures as well as routine data collection. The X-ray source of TPS-05A1 is a three meters long in-vacuum undulator (IU22), producing a high-brilliant X-ray beam. The X-rays are monochromated by a liquid-nitrogen-cooling Si double-crystal monochromator, and focused by a pair of Kirkpatrick–Baez mirrors. The focused beam size at the sample is 50 μm (H) x 20 μm (V) with a photon flux of 6 x 10^12 photons/s. Apertures are used to collimate the beam in the range of 50–5 μm. The beam divergence at the sample is less than 500 μrad (H) and 100 μrad (V), and the energy range is from 5.7 to 20 keV (wavelength 2.175-0.62 Å). TPS-05A1 will be equipped with a high speed CCD area detector and a robotic sample changer for automatically sample mounting and centering, making the data acquisition more efficient. The optional mini-κ goniometer of the high precision micro-diffractometer enables crystal reorientation for challenging experiments. The design and constructing status of this beamline is given in this article.

Poster Session 1 - Board: EM-07 / **112**

Probing molecular and crystalline orientation in solution-processed perovskite solar cells

Author(s): Mr. HUANG, Wenchao[1]
Co-author(s): GANN, Eliot [2] ; MCNEILL, Chris [1]

[1] *Monash University*

[2] *Australian Synchrotron*

Corresponding Author(s): wenchao.huang@monash.edu

We investigate the microstructure of solution-processed organometallic lead halide perovskite thin films using a combination of synchrotron based techniques. Using a combination of GIWAXS and NEXAFS spectroscopy we separately probe the orientational alignment of CH3NH3PbI3 crystallites and CH3NH3+ cations. The GIWAXS results reveal that the orientation of CH3NH3PbI3 crystallites is sensitive to film thickness, solvent evaporation rate, and the underlying TiO2 morphology. In perovskite films prepared by a gas-assisted method, oriented perovskite crystallites are detected in thin films (˜60nm) deposited on a dense TiO2 blocking layer. As the thickness of the perovskite layer is increased to ˜250 nm, however, this preferential orientation of perovskite crystals disappears. In contrast, for both thin and thick perovskite films deposited on an underlying mesoporous TiO2 layer randomly orientated crystallites are observed. NEXAFS measurements on all samples prepared by the gas-assisted method found that CH3NH3+ cations exhibit a random molecular orientation with respect to the substrate, independent of the TiO2 architecture and the perovskite film thickness. The lack of any NEXAFS dichroism for the thin CH3NH3PbI3 layer deposited on planar TiO2 in particular indicates the absence of any preferential orientation of CH3NH3+ cations within the CH3NH3PbI3 unit cell for as-prepared layers (that is, without any poling). Solar cells based on the thicker (˜ 250 nm) perovskite films were also prepared to enable correlation with microstructural results, with solar cells based on planar TiO2 achieving an efficiency of 14.3% compared to 12% for cells fabricated with mesoporous TiO2 layers.

Poster Session 1 - Board: BT-15 / **128**

Beamline Plan at Taiwan Photon Source

Dr. HUANG, Yu-Shan[1]

[1] *National Synchrotron Radiation Research Center*

Corresponding Author(s): jade@nsrrc.org.tw

Taiwan Photon Source is designed to emphasize electron beams of small emittance and great brilliance for generating ex-tremely bright photon beams. The superior characteristics of TPS have opened avenues for novel scien-tific opportunities and experimental techniques. The advanced techniques of seven phase-I beamlines include temporally coherent X-ray diffraction, protein microcrystollography, submicron soft X-ray spec-troscopy, coherent X-ray scattering, submicron X-ray diffraction, X-ray nanoprobe, and resonant soft X-ray scattering. Taking full advantage of the highly brilliant photon source, the phase-I beamlines will aim for the forefront of science. These beamlines cover diverse researches in physics, chemistry, biology, and material science, in the energy range from soft to hard X-rays for advanced research in spectroscopy, scattering and imaging. Scientific opportunities provided by the beamlines will no doubt boost Taiwan frontier researches. Moreover, phase-II beamline plan at TPS is under discussion. The eighteen phase-II beamlines will address complementary advanced techniques to phase-I beamlines and relocate the fruitful scientific activities at Taiwan Light Source to the TPS.

Structural Biology / 1

Structural basis for hijacking CBFβ and CUL5 E3 ligase complex by HIV-1 Vif

Author(s): Mrs. GUO, Yingying[1] ; Mr. DONG, Liyong[1] ; Ms. QIU, Xiaolin[1]
Co-author(s): Ms. LIU, Hongnan [1] ; Ms. ZANG, Yi [1] ; Mr. YU, You [2] ; Prof. YANG, Maojun [2] ; Prof. HUANG, Zhiwei [1] ; Ms. WANG, Yishu [1] ; Ms. ZHANG, Bailing [1]

[1] *Harbin Institute of Technology*

[2] *Tsinghua University*

Corresponding Author(s): huangzhiwei@hit.edu.cn

The HIV-1 Vif protein is a key regulator of viral infection and absolutely required for HIV-1 replication, rendering the viral protein an important target for anti-viral drug development. HIV-1 Vif was recently shown to dually hijack core-binding factor subunit beta (CBFβ) and CUL5 E3 ligase complex simultaneously to form an HIV-1 Vif-CBFβ-CUL5-ELOB-ELOC complex for degradation of viral restriction factors, including APOBEC3G (A3G) and all other Vif-sensitive human A3 proteins, thus preserving HIV-1's infectivity. Despite the important roles of Vif in viral infection and more than 30 years of intensive studies, the structural information of HIV-1 Vif alone or in the context of a functional complex is still elusive. We recently determined the crystal structure of the Vif-CBFβ-CUL5-ELOB-ELOC complex. The structure reveals the nearly full-length structure of Vif for the first time and provides significant insights into the mechanisms employed by HIV-1 Vif to dually hijack CBFβ and E3 ligase complex CUL5-ELOB-ELOC simultaneously. Clearly, our structure paves the way for designing and developing novel antiviral drugs that can target Vif and the pentameric complex as well. We believe that our structure represents a breakthrough in the field of HIV and will interest scientists from both academia and industry.

Advanced Materials I / 26

Fluorine-Substituted Metal Hydrides for Thermal Energy Applications

Author(s): Dr. HUMPHRIES, Terry[1]
Co-author(s): Dr. SHEPPARD, Drew A. [1] ; Dr. ROWLES, Matthew R. [1] ; Prof. BUCKLEY, Craig E. [1]

[1] *Curtin University*

Corresponding Author(s): terry.humphries@curtin.edu.au

Metal hydrides have long been explored for their potential application in a variety of technological applications including hydrogen storage materials for energy applications, fast-ion conductors and sensors. For thermal energy storage, such as concentrating solar thermal energy storage, metal hydrides are required to operate at temperatures in excess of 500 °C 1. This temperature is too high for even the more stable, reversible hydrogen storage materials, and as such, work has been undertaken to synthesise metal hydrides that are stable and reversible at these high temperatures.

One proven strategic method to stabilise these materials is to substitute fluorine atoms for hydrogen [2]. Fluorides are more stable than their hydride equivalents and this can be exploited to increase the stability of metal hydrides by partially substituting hydrogen for fluorine. For example, for the NaMgH3-xFx system, pure NaMgH3 releases H2 at ˜400 °C, whereas NaMgH2F decomposes at ˜478 °C [2]. This effect has been employed for a number of potential thermal energy storage metal hydrides, such as NaH, Mg2FeH6 and Na2Mg2FeH8, allowing for greater tuning of their thermal properties by hydrogen/fluorine substitution.
References

1. D. N. Harries et al., Proceedings of the IEEE, 2012, 100, 539.

2. D. A. Sheppard et al., RSC Adv., 2014, 4, 26552.

Surface Science / 20

Functionalization of graphene via foreign atoms intercalation

Dr. HWANG, Chan-Cuk[1]

[1] *Pohang Accelerator Laboratory*

Corresponding Author(s): cchwang@postech.ac.kr

Graphene has many intriguing characteristics in its electronic structure. Its conduction and valence bands meet at a Dirac point and the energy depends linearly on the wave vector near the K-points, similar to a relativistic particle. The massless Dirac fermions have also chirality, suppressing electron backscattering. However, real graphenes often show different electronic structures depending on what they are facing. We provide angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) results of graphenes grown on different substrates, such as Ni, Cu, SiC, etc. The electronic structures can be modified by adsorbing or intercalating foreign atoms. Since the intercalation could be useful to give a special function to graphene such as superconductivity, we show some experimental data for the intercalation of several atoms between graphene and substrate together with the role of steps, defects, domain boundaries in real graphenes.

Advanced Materials III / 34

GISAXS of pre-crystallisation events in the formation of CO2 corrosion products on steel

Author(s): Dr. INGHAM, Bridget[1]
Co-author(s): Dr. KO, Monika [2] ; Dr. LAYCOCK, Nick [3] ; Prof. WILLIAMS, David [4]

[1] *Callaghan Innovation*

[2] *Quest Integrity Group*

[3] *Qatar Shell Research & Technology Centre*

[4] *University of Auckland*

Corresponding Author(s): bridget.ingham@callaghaninnovation.govt.nz

The corrosion of steel in aqueous saturated CO2 environments is a major industrial problem. Under certain conditions a highly protective scale of siderite (FeCO3) is formed; however, there is little information available regarding the initial nucleation processes. In recent years we have performed a number of in situ synchrotron X-ray diffraction studies using electrochemistry to accelerate the corrosion rate, exploring the effect of temperature 1, corrosion inhibitor species and concentrations [2-3], addition of Mg2+ [4] and Cr3+ [5], and steel microstructure [6] on the growth rates of crystalline FeCO3 films. These experiments all showed a significant induction period before a signal was observed. Recently we used grazing incidence small-angle X-ray scattering (GISAXS) and obtained evidence for an amorphous gel film that forms at much shorter times [7]. Our current hypothesis is that this amorphous gel then crystallises into either chukanovite (Fe2(OH)2CO3) or siderite, possibly via amorphous chukanovite as an intermediate phase. 1

Ingham, Ko, Kear et al., Corr. Sci. 52 (2010) 3052. [2] Ko, Laycock, Ingham & Williams, Corrosion 68 (2012) 1085. [3] Ko, Laycock, Ingham & Williams, NACE Int. Corrosion Conf. Ser. 5 (2012) 3662. [4] Ingham, Ko, Laycock et al., Corr. Sci. 56 (2012) 96. [5] Ko, Ingham, Laycock & Williams, Corr. Sci. 80 (2014) 237. [6] Ko, Ingham, Laycock & Williams, Corr. Sci. 90 (2015) 192. [7] Ingham, Ko, Kirby, Laycock & Williams, Faraday Discuss. In press (2015). DOI: 10.1039/C4FD00218K.

Poster Session 2 - Board: SS-04 / **89**

Dynamic Self-organisation of Gluconobacter oxydans in Three-Dimensional Electron-transferring Network

Prof. IVANOVA, Elena[1] ; Dr. TRUONG, Vi Khanh[2] ; Dr. GARVEY, Chris[3] ; Ms. BHADRA, chris[4] ; Dr. AL KOBAISI, Mohammad[5] ; Mr. NGUYEN, Khuong Duy[6] ; Ms. PERERA, Palalle[5] ; Prof. MAINWARING, David[5] ; Prof. JUODKAZIS, Saulius[5] ; Prof. CRAWFORD, Russell J.[5]

[1] *Swinburne Univeristy of Technology*

[2] *School of Science, Faculty of Science, Engineering and Technology, Swinburne University of Technology*

[3] *ANSTO*

[4] *swinburne university of technology*

[5] *School of Science, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Hawthorn, Victoria, 3122 Australia*

[6] *School of Science, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Hawthorn, Victoria, 3122 Australi*

Corresponding Author(s): eivanova@swin.edu.au, vtruong@swin.edu.au, cbhadra@swin.edu.au

Electro-catalytic microorganisms are an essential component in bioelectro-catalytic systems such as microbial fuel cells. *Gluconobacter oxydans* has been widely used in such applications. In this study, we employed scanning electron microscopy, confocal laser scanning microscopy and ultra-small angle neutron scattering to investigate the dynamic self-organisation of *G. oxydans* cells into a three dimensional network within a hydrogel that had been constricted using linear poly(vinyl alcohol) and the crosslinker N-vinyl pyrroliodne (VP) (PVA-VP). It was found that the *G. oxydans* utilised the polymeric chains of the PVA-VP to form micro-wires that were capable of transferring electrons. The *G. oxydans* cells formed short chains on the micro-wires over a period of one hour, followed by these short chains undergoing self-assembly to form a three-dimensional network of electron-transferring micro-wires. The formation of this micro-wire network resulted in a twofold increase power generation bring obtained. This discovery has the potential to lead to the development of new, more efficient bioelectrocatalytic systems.

Poster Session 1 - Board: SS-05 / **111**

Silica nanoparticles acting as light nanocondensers

Prof. CRAWFORD, Russell J.[1] ; Prof. IVANOVA, Elena P.[1] ; Mr. STEFANOVIC, Miljan[1] ; Dr. TRUONG, Vi Khanh[2] ; Dr. MACLAUGHLIN, Shane[3] ; Dr. TOBIN, Mark[4]

[1] *School of Science, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Hawthorn, Vic, Australia, 3122*

[2] *School of Science, Faculty of Science, Engineering and Technology, Swinburne University of Technology*

[3] *BlueScope Steel Research, Port Kembla, NSW, Australia*

[4] *Australian Synchrotron*

Corresponding Author(s): eivanova@swin.edu.au, 5373271@student.swin.edu.au, vtruong@swin.edu.au

The development of functional nanocoating is crucial in the manufacturing process, possessing the potential to increase both surface corrosion and deterioration resistance properties. In particular, silica nanoparticle (SiO2 NP) coatings have been widely used to increase corrosion-, wear- and tear-resistance. For instance, in industrial applications, steel surfaces are initially coated with polyester polymers and then further coated with SiO2 NPs. However, the effect of environmental factors upon these dual protection layers pertaining to steel substrata still remains unknown.

In this study, we employed various surface characterization techniques to ascertain both the physical and chemical properties of SiO2 NP-coatings on a polyester-coated steel substratum. The modified substrata were exposed to hot and humid environments with high levels of UV-light irradiation over a period of five years. It is found that surfaces coated with SiO2 NPs, lead to an increased surface roughness on the nano-scale, as inferred from atomic force microscopy and optical profilometry. The rate at which surface roughness increased was found to be five times greater than that of substrata without SiO2 NP coatings. Furthermore, chemical characterization of SiO2 NPs-coated steel substrata was performed using X-ray photoelectron spectroscopy and synchrotron IR micro-spectroscopy. Despite coating degradation, SiO2 NPs were found to be present on the surfaces. One innovative mechanism proposed in this study, is that SiO2 NPs act as light nanocondensers, enhancing the UV-light effect upon the degradation of polymer-coating between SiO2 NPs.

Poster Session 2 - Board: EE-06 / **57**

XANES Iron K-Edge Speciation of Corroded Tube upon Victorian Brown Coal Oxy-Fuel Combustion

Author(s): Mrs. JABAZ, Iman[1]
Co-author(s): Dr. CHEN, Juan [2] ; Dr. BARBARA, Etschmann [3] ; Prof. NINOMIYA, Yoshihiko [2] ; Dr. ZHANG, Lian [4]

[1] *Department of Chemical Engineering, Monash University*

[2] *Department of Applied Chemistry, Chubu University, Japan*

[3] *Department of Geosciences, Monash University*

[4] *Deaprtment of Chemical Engineering, Monash University*

Corresponding Author(s): iman.jabaz@monash.edu, lian.zhang@monash.edu

Oxy-fuel combustion is the burning of coal in the mixture of recirculated flue gas and high-purity oxygen, so as to reduce the carbon emission from coal-fired power plant. The fly ash - related fouling and corrosion are some of the most crucial issues encountered in this process. Understanding tube corrosion in this new combustion process is pivotal for a successful adoption of this technology by the existing power plants. In this work, we have employed a horizontal furnace to study the fly ash-related tube corrosion at 650 oC for the duration of 50 hr in air versus oxy-fuel combustion mode. Six tubes and five different ashes have been tested. The cross-section of the tube after exposure test was studied by using optical microscopy (OM), scanning electron microscopy (SEM) coupled with energy dispersive spectroscopy (EDS), and synchrotron X-ray absorption near edge spectroscopy (XANES). As have been confirmed, the corrosion of tube surfaces was substantially accelerated under the oxy-fuel combustion condition, as compared to air. The ash composition also affected the extent of the tube corrosion. With regard to different tube materials, it was found that, SUS347 and T23 steel were corroded most intensively, whereas SS400 was affected slightly by flue-gas composition.

Soft Matter / 158

Investigations of Self-Assembling Block Copolymer/Ionic Liquid Blends

Author(s): Dr. JACK, Kevin[1]
Co-author(s): Mr. BENNETT, Thomas [2] ; Dr. THURECHT, Kristofer [2] ; Dr. BLAKEY, Idriss [2]

[1] *University of Queensland*

[2] *The University of Queensland*

Corresponding Author(s): k.jack@uq.edu.au

Block copolymers are ubiquitous materials with a vast range of applications, e.g. in drug delivery, photolithography, chemical sensors, surfactants, and as templates for the production of hard materials. The properties of these materials and hence the range of potential applications arise from the ability to combine an array of chemical functionalities and architectures that can be synthesised using contemporary polymerisation techniques. More recently, the addition of low

molecular weight diluents has been shown to modify as well as allow for the control of the microstructures adopted by these systems.
Recent advancements in characterisation methods have opened up the possibility to interrogate these materials at the molecular- and nano-scale and to, therefore, better understand structure-property-performance relationships within them. This work will focus on recent studies by us carried out in part at the Australian Synchrotron (e.g. using high-throughput and grazing-incidence SAXS) on a range of block copolymers/ionic liquid blends in which it is possible to manipulate both the accessible block copolymer phases and the resulting properties of the materials. These studies have provided both insights into physical properties, e.g. scaling properties of the polymers, and practical methods for fabricating microphases such as co-continuous phases.

Energy Materials I / **84**

Synchrotron imaging of metallurgical coke for analysis of coke quality

Author(s): Dr. JENKINS, David[1]
Co-author(s): Dr. MAHONEY, Merrick [2] ; Dr. STEEL, Karen [3] ; Mrs. WARREN, Karryn [4] ; Dr. LOMAS, Hannah [2] ; Dr. ROEST, Richard [2] ; Mr. PEARCE, Robin [4] ; Dr. MAYO, Sherry [4]

[1] *CSIRO Digital Productivity Flagship*

[2] *University of Newcastle*

[3] *University of Queensland*

[4] *CSIRO*

Corresponding Author(s): david.jenkins@csiro.au

Metallurgical coal is a major Australian commodity export, worth more than A$20b *per annum*. It is used to make coke, a vital component in steelmaking. High quality coke is important for successful operation of modern ironmaking blast furnaces. Crucial to coke quality is the strength and reactivity of this porous composite material. There is a close relationship between coke quality and its microstructure, which varies at micron scale. As part of a comprehensive study of the factors that affect coke quality, from the properties of the original coal, through the processing into coke and then its utility in the blast furnace, we have used the Imaging and Medical Beam Line at the Australian Synchrotron to study the relationship between coke quality and its microstructure. In three separate projects, we have (a) imaged coke to determine its cold strength (b) imaged laboratory prepared samples to examine the transformation into coke and (c) imaged progressively reacted coke at high temperatures to examine its behaviour in the blast furnace. In this presentation we will present brief results from each of these studies, to illustrate the benefit of synchrotron science to the coking coal industry in Australia.

Poster Session 1 - Board: EM-15 / **205**

Growth of catalytic Au nanoparticles upon electrochemical ageing

Author(s): Mr. STEVEN, Jared[1]
Co-author(s): Dr. GOLOVKO, Vladimir [1] ; JOHANNESSEN, Bernt [2] ; Dr. MARSHALL, Aaron [1]

[1] *University of Canterbury*

[2] *Australian Synchrotron*

Corresponding Author(s): bernt.j@synchrotron.org.au

Au nanoparticles, potential catalysts in fuel cells, were produced following a published chemical method. As-made nanoparticles were then adsorbed to carbon black supports and an electrochemical ageing sequence was applied. Of interest to this study was to observe and quantify the long term stability of Au nanoparticles upon ageing and as a function of nanoparticle size. To this end X-ray absorption spectroscopy and complementary methods were applied. Interestingly, it was found that small (2.4 and 3.1 nm diameter) nanoparticles grew in size as a result of the ageing process, whilst larger (4.6 nm) nanoparticles did not grow appreciably. Our results have implication on the suitability of Au nanoparticles as commercially viable catalytic material.

Techniques I / 60

New developments at the XFM beamline: Get more from your research, for free

Author(s): Dr. JONES, Michael[1]
Co-author(s): Dr. DE JONGE, Martin [1] ; Dr. VAN RIESSEN, Grant [2] ; Mr. PHILLIPS, Nicholas [3] ; Dr. BALAUR, Eugeniu [2] ; PATERSON, David [1] ; HOWARD, Daryl [1] ; Dr. VINE, David [4] ; Dr. NASHED, Youssef [5] ; Dr. MCCOLL, Gawain [6] ; Dr. MUDIE, Stephen [1]

[1] *Australian Synchrotron*

[2] *La Trobe University*

[3] *LTU/CXS*

[4] *Advanced Photon Source, Argonne National Laboratory*

[5] *Argonne National Laboratory*

[6] *The Florey Institute*

Corresponding Author(s): michael.jones@synchrotron.org.au

The XFM beamline at the Australian Synchrotron typically operates in the backscatter geometry using the Maia detector and fast scanning stages, allowing rapid and efficient collection of fluorescent X-ray photons. In most cases, the transmitted beam is collected by a photodiode to give at best a poor measure of the thickness of the specimen. However, the transmitted beam carries much more information than is currently being used. In this presentation, I will show you simultaneously collected fluorescence and ptychography data which not only gives you a sub 100 nm resolution phase contrast image of your sample but allows you to increase your fluorescence resolution as well. Further developments in this area will allow simultaneous ptychography data to be collected across a wide range of samples at no additional time cost to standard fluorescence data collection.

Advanced Materials I / 142

EXAFS insights into the crystal-chemistry of nickel in tropical ultramafic areas: A survey at the molecular environmental level in New Caledonia.

Author(s): Dr. JUILLOT, Farid[1]
Co-author(s): Dr. MORIN, Guillaume [1] ; Dr. PROUX, Olivier [2] ; Dr. HAZEMANN, Jean-Louis [2] ; Dr. OLIVI, Luca [3] ; Mr. MARAKOVIC, Gregory [4] ; Dr. BROWN JR., Gordon [5] ; Dr. FRITSCH, Emmanuel [1] ; Dr. DUBLET, Gabrielle [1] ; Dr. NOEL, Vincent [1] ; Dr. ONA-NGUEMA, Georges [1] ; Dr. MARCHAND, Cyril [1] ; Ms. BREST, Jessica [1] ; Ms. IKOGOU, Maya [1] ; Dr. BELIN, Stephanie [6]

[1] *Institut de Mineralogie, de Physique des Materiaux et de Cosmochimie IMPMC, UMR CNRS 7590, UR IRD 206, Universite Pierre et Marie Curie UPMC, 75005 Paris, France*

[2] *European Synchrotron Radiation Facility (ESRF), FAME Beamline, F-38043 Grenoble Cedex, France*

[3] *Sincrotrone Trieste (ELETTRA), Area Science Park, Strada Statale, 34012 Basovizza, Trieste, Italy*

[4] *Koniambo Nickel SAS (KNS), 98860 Kone, New Caledonia*

[5] *Department of Geological & Environmental Sciences, Stanford University, Stanford CA 94305-2115, USA*

[6] *Synchrotron SOLEIL, SAMBA Beamline, L'Orme des Merisiers Saint-Aubin - 91192 Gif-sur-Yvette Cedex, France*

Corresponding Author(s): farid.juillot@ird.fr

In this presentation, we will show how Ni K-edge EXAFS data from the Australian Synchrotron (Melbourne) and several facilities worldwide (ESRF-France, ELETTRA-Italy, SOLEIL-France, SSRL-USA) helped us to depict the crystal-chemistry of nickel in New Caledonia, the third nickel producer in the world thanks to its geological setting (one-third of the surface covered with lateritic regoliths resulting from the long-term weathering of peridotites under tropical conditions). This survey at the molecular environmental level will start in the peridotites (the source of nickel) with data that help to better understand the formation of the hydrous Mg/Ni silicate deposits (i.e. known as garnierite) of New Caledonia. It will follow in the lateritic regoliths with data

that emphasize the vertical change of nickel speciation from Ni-bearing phyllosilicates in the bottom ultramafic bedrock towards Ni-bearing goethite in the upper lateritic horizons (Dublet et al., 2012; 2014; 2015). Finally, it will end in the mangrove ecosystem with data that show the vertical change of nickel speciation from Ni-bearing goethite towards Ni-bearing pyrite when going from the oxic surface horizons towards the anoxic deep horizons of mangrove sediments located downstream lateritic regoliths (Noel et al., 2014; 2015). Beyond the single case of New Caledonia, all these informations on the crystal-chemistry of nickel in ultramafic environments shall help building a sustainable exploitation of nickel laterites (60 to 70% of the world's Ni resources ; Butt and Cluzel, 2013).

Poster Session 2 - Board: AM-22 / **174**

Investigation of the Phase Transition of CuSb2O6 at High Temperatures by Synchrotron Powder Measurements

Author(s): KANG, Hyung-Been[1]
Co-author(s): Dr. SOEHNEL, Tilo [1] ; Dr. FINLAYSON, Trevor [2] ; Prof. LING, Chris [3] ; Dr. AVDEEV, Maxim [4] ; Dr. PILTZ, Ross [4] ; Dr. GU, Qinfen [5]

[1] *The University of Auckland*

[2] *University of Melbourne*

[3] *University of Sydney*

[4] *ANSTO*

[5] *Australian Synchrotron*

Corresponding Author(s): hkan026@aucklanduni.ac.nz

The phase transition of CuSb2O6 has been described previously as a transition from tetragonal trirutile to distorted monoclinic trirutile structure. Cu2+ as a d9 system forms the square lattice oxide layer, which leads to a second order phase transition (Jahn-Teller distortion) 1. The systematic reduction in symmetry would require the existence of an orthorhombic modification between the two modifications, surpressed in many structures. From synchrotron high temperature measurements, the phase transition in CuSb2O6 can be clearly observed and a possible two modification model (orthorhombic modification (Pnnm) and tetragonal modification (P42/mnm)) can be refined from 200 °C to 900°C data. The direct phase transition from the monoclinic to the tetragonal modification is clearly surpressed over a large temperature range. The measurements show an unusual thermal behaviour. Some groups of diffraction peaks show an increase of the intensity as the temperature increases and others show a relative decrease of the intensity, but the thermal broadening decreases as the temperature increases. This is related to the ratio of the two high temperature modifications present at all temperature. The refined ratio of orthorhombic modification to tetragonal modification decreases from 200°C to 900°C but the phase transition is still not completed at 900°C. The refined lattice parameters indicate a normal thermal expansion of the unit cell, whereas the thermal broadening of the diffraction shows the opposite trend.
1 A.V. Prokofiev, F. Ritter, W. Assmus, B.J. Gibson and R.K. Kremer, J. Cryst. Growth. 247, 457 (2003).

Beamline update and discussion / 31

Beamline update and discussion: XAS

Dr. KAPPEN, Peter[1]

[1] *Australian Synchrotron*

Corresponding Author(s): peter.kappen@synchrotron.org.au

This session will provide an update on activities and capabilities at the XAS beamline. The session aims to provide users with the opportunity to discuss current and future needs with the beamline team.

Poster Session 1 - Board: AM-01 / **2**

Towards Iron-Carbon Multi-Functional Nanomaterials

Author(s): Dr. KAPPEN, Peter[1]
Co-author(s): Dr. RIDER, Andrew [2] ; Dr. BRACK, Narelle [3]

[1] *Australian Synchrotron*

[2] *Defence Science and Technology Organisation, DSTO*

[3] *La Trobe University*

Corresponding Author(s): peter.kappen@synchrotron.org.au

Carbon nanotubes (CNTs) have attracted significant attention and in many cases they have been used as a single-function additive to modify a specific property of a material, such as the mechanical strength of a composite. It is interesting to extend those properties by coupling them with properties of other materials, thus generating systems that can serve more complex functions (e.g., magnetic or metallic functions coupled with strength).
We report here on progress in a research activity directed at generating multi-functional materials based on CNTs and iron. The activity is focussed on controlling the production of the iron-carbon nanomaterials and is influenced by practical aspects of the production processes.
Towards multi-functional materials, we explore the synthesis of iron-containing multi-walled CNTs using chemical vapour deposition, where XAS data show the presence of metallic Fe phases under certain deposition conditions. Long-term storage and implications for the shelf-life of metallic iron inside CNTs will be discussed. Taking into account practical considerations, such as process scalability and energy efficiency, the deposition of magnetic Fe nanoparticles on oxygen functionalised multi-walled CNTs will be explored. Results from XAS, XPS and SEM show that short deposition times lead to thin, discontinuous iron films with a high proportion of Fe(II/III). As the deposition time increases, so do film thickness and Fe(0) content. Furthermore, magnetic measurements show a reduction in coercivity with increased deposition time, however, not to the extent expected for bulk metallic Fe.

Plenary / **8**

Radioactive? Tick; Toxic? Tick; Explosive? Tick. What could possibly go wrong?

Prof. KENNEDY, Brendan[1]

[1] *The University of Sydney*

Corresponding Author(s): brendan.kennedy@sydney.edu.au

Innovation drives science, and synchrotrons are often a critical tool in this. Consequently many experiments done at synchrotrons are pioneering and/or unique. Despite the impression we may form when completing a Risk Assessment prior to an experiment, Synchrotrons are the antipathy of the nanny state. The Australian Synchrotron frequently allows experiments under extreme conditions with extremely reactive or toxic materials. As the title says what could possibly go wrong when heating a radioactive material under a hydrogen atmosphere? In this presentation I will describe our journey to the riskier side of chemistry, looking at structural transformations in uranium, technetium and osmium oxides. Each of these elements present unique handling challenges that are further compounded since we are interested in the response of the materials to changes in temperature and environment. Whilst my tool of choice is generally high resolution powder diffraction there is often the need to supplement this with spectroscopic information; moving hazards from one beamline to the next, always with the hope of being allowed back.

Poster Session 2 - Board: AM-16 / **110**

A structural study and magnetic properties of electrospun carbon/manganese ferrite (C/MnFe2O4) composite nanofibers

Dr. KIDKHUNTHOD, Pinit[1]

[1] *Synchrotron Light Research Institute (Public Organiztion)*

Corresponding Author(s): p.kidkhunthod@gmail.com

Carbon/manganese ferrite (C/MnFe2O4) composite nanofibers were fabricated using electrospinning technique followed by carbonization process under mixed of air and argon atmosphere at 400, 600 and 800 ˚C, respectively. The prepared composite nanofibers were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), vibrating sample magnetometry (VSM) and X-ray absorption spectroscopy (XAS) including X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS). After calcination at 800 ˚C, the composite nanofibers of C/MnFe2O4 were obtained with a mean diameter of nanofibers of approximately 700 - 800 nm. The structure of MnFe2O4 was successfully studied using XAS technique and was found to be cubic spinel with a coupling of Mn2/Mn3+ and Fe3+ oxidation states . All composite nanofibers exhibited ferromagnetic behavior especially after being calcined at 800 ˚C. This ferromagnetic properties were related to the distribution of cations over tetrahedral and octahedral sites as revealed by EXAFS results.

Poster Session 1 - Board: BT-19 / **162**

Mechanical design of a various included angle Hetterick style monochromator covering tender X-rays

Author(s): Dr. KIM, Jae-Young[1]
Co-author(s): Mr. KIM, Hyo-Yoon [1] ; Mr. YANG, Seongseon [2]

[1] *Pohang Accelerator Laboratory*

[2] *Vactron, Daegu, Korea*

Corresponding Author(s): hykim@postech.ac.kr

A soft X-ray monochromator covering, so called, tender X-rays is realized with grating optics. The monochromator is composed of two reflection optics of a deflection mirror and a grating and they are configured to work at highly grazing incidence angles to guarantee moderate reflectivity even in the tender X-ray energy range. By the limitation of grazing incidence angles, the energy scan should be also completed within the highly limited rotation range of grating angle, which gives us very tight mechanical tolerances for the angles of the deflection mirror and the grating. The problem is solved by combining nano-motors and a special pivot. The various included angles on the grating is made by an off-axis rotation of the deflection mirror. In order to minimize the size of the entire chamber, the distance of the rotation axes is designed as small as a few millimeters. In this presentation, we would like to show the design details and test results.

Poster Session 1 - Board: BT-17 / **157**

Middle energy beamline for Max-Planck Korean initiative at Pohang Light Source

Author(s): Dr. KIM, Jae-Young[1]
Co-author(s): Mr. KIM, Hyo-Yoon [1] ; Mr. HO-YOUNG, Kim [2] ; Prof. JAE-HOON, Park [2]

[1] *Pohang Accelerator Laboratory*

[2] *MPPC_CPM, POSTECH*

Corresponding Author(s): masson@postech.ac.kr

The construction of a beamline covering a wide energy range of 250 eV ~ 3000 eV is going on at Pohang Light Source (PLS). In order to provide sufficient photon flux up to 3000 eV with grating optics, the beamline is designed to use just four reflection optics with highly grazing angles. A Hetterick style monochromator with various incident angles is adopted under entrance slitless configuration. The first and the last mirrors are toroidal and they are configured to compensate the line curvature errors of them to each other. The beamline is dedicated for X-ray Magnetic Circular Dichroism (XMCD) and soft X-ray scattering (SXS). All the optical parameters are optimized by an analytical code based on the optical path function theory. The grating efficiency is also calculated rigorously by differential methods. The calculation is verified by ray-tracing too. The construction is going on under the program of Max-Planck Korean Initiative and will be

done by June, 2016. In this talk, the design details and the current construction status will be presented.

Poster Session 2 - Board: BT-18 / **160**

Construction status of PAL-XFEL

Mr. KIM, Seungnam[1]

[1] *Pohang Accelerator Laboratory*

Corresponding Author(s): ksn@postech.ac.kr

The PAL-XFEL project was launched construction at the Pohang Accelerator Laboratory, Korea in April 2011, with the planned user service of 2017. PAL-XFEL will provides FEL beams over the energy range of 250 eV to 20.4 keV using the fundamental, with the pulse energies of at ˜1 mJ depending on the pulse duration and photon energy. We will present the current construction status of PAL-XFEL including accelerator and beamlines (HX1, SX1) and the focused scientific programs.

Poster Session 2 - Board: AM-20 / **159**

Anion ordering in complex perovskite oxynitrides AM0.2Ta0.8O2.8N0. (A = Sr, Ba; M = Li, Na)

Author(s): Prof. KIM, Young-Il[1]
Co-author(s): Dr. AVDEEV, Maxim [2] ; Dr. YOUNKEE, Paik [3]

[1] *Yeungnam University*

[2] *Bragg Institute, ANSTO*

[3] *Korea Basic Science Institute*

Corresponding Author(s): yikim@ynu.ac.kr

Oxynitride-type complex perovskites, AM0.2Ta0.8O2.8N0.2 (A = Sr, Ba; M = Li, Na), were synthesized by the ammonolytic heating of a layered perovskite, A5Ta4O15, with 0.5M2CO3. A Rietveld refinement of the synchrotron X-ray and neutron powder diffraction patterns confirmed the complete structural transformation from a hexagonal layered-perovskite to a three-dimensional perovskite type, as well as the stabilization of alkali cations on the octahedral sites rather than on the dodecahedral sites in the latter. In all four compounds, M+ and Ta5+ were disordered completely despite a charge difference as much as 4. The crystal symmetry of the average structure depended on the size of the dodecahedral cation; simple cubic for BaM0.2Ta0.8O2.8N0.2, and body-centered tetragonal for SrM0.2Ta0.8O2.8N0.2. This trend coincides with the symmetry transition from BaTaO2N (Pm3 [U+0305]m) to SrTaO2N (I4/mcm). In both SrM0.2Ta0.8O2.8N0.2, nitrogen atom preferentially occupied the c-axial 4a site of the tetragonal cell. Solid state magic angle spinning nuclear magnetic resonance spectroscopy showed that SrNa0.2Ta0.8O2.8N0.2 and BaNa0.2Ta0.8O2.8N0.2 exhibited marked downfield shifts of 23Na, manifesting an octahedral coordination. On the other hand, the 7Li NMR of SrLi0.2Ta0.8O2.8N0.2 and BaLi0.2Ta0.8O2.8N0.2 indicated a highly symmetrical coordination environment of Li.

Beamline updates / 113

Developments on the Powder Diffraction Beamline at the Australian Synchrotron

Author(s): Dr. KIMPTON, Justin[1]
Co-author(s): Dr. GU, Qinfen [1] ; Dr. BRAND, Helen [2] ; Dr. WANG, Zhiyang [3]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron.*

[3] *School of Materials Science and Engineering, UNSW Australia & The Powder Diffraction Beamline, Australian Synchrotron*

Corresponding Author(s): justin.kimpton@synchrotron.org.au

The Powder Diffraction (PD) beamline at the Australian Synchrotron has successfully operated its User Programme since 2007 enabling many research teams to produce world-class outcomes. The rapid data collection capabilities coupled with the wide array of sample stages and environments permit an expansive range of *in situ* powder diffraction experiments. This presentation describes recent upgrades, new developments and future plans for the PD beamline that will enhance experiment capability. The hardware and software upgrades to the MYTHEN detector are discussed as well as the integration and performance of the new Mar345 image plate detector with a bespoke adjustable stand. The image plate area detector will be used for experiments where two-dimensional data collection is required (e.g. high pressure diamond anvil cell, texture... etc.) and offers compatibility with existing sample stages and environments, and improved configuration flexibility. The presentation will also cover upgrades to existing equipment that will benefit most ambient and high-temperature capillary experiments. A new multi-position coin cell battery sample stage and several planned future beamline upgrades designed to increase sample throughput will also be presented.

Beamline update and discussion / 30

Beamline update and discussion: SAXS/WAXS

Author(s): Dr. KIRBY, Nigel[1]
Co-author(s): MUDIE, Stephen [1] ; Dr. HAWLEY, Adrian [1]

[1] *Australian Synchrotron*

Corresponding Author(s): nigel.kirby@synchrotron.org.au

This session will provide an update on activities and capabilities at the SAXS/WAXS beamline. The session aims to provide users with the opportunity to discuss current and future needs with the beamline team.

Instrumentation / 171

Orientation and strain determination using the Maia detector

Author(s): Mr. KIRKWOOD, Henry[1]
Co-author(s): Dr. VAN RIESSEN, Grant [1] ; Dr. DE JONGE, Martin [2] ; HOWARD, Daryl [2] ; Dr. RYAN, Chris [3] ; Dr. ROWLES, Matthew [4] ; Dr. HOFMANN, Felix [5] ; Dr. BRIAN, Abbey [1]

[1] *La Trobe University*

[2] *Australian Synchrotron*

[3] *CSIRO*

[4] *Curtin University*

[5] *University of Oxford*

Corresponding Author(s): h.kirkwood@latrobe.edu.au

X-ray micro-beam Laue diffraction is a powerful tool for mapping the orientation and elastic strain within polycrystalline materials. Microscale interactions between neighbouring grains influence the macroscale behaviour of a material, particularly its deformation behaviour and damage mechanisms such as cracking which is often initiated in the intercrystalline regions. Widely used deformation models are often inconsistent with experimental observations of fatigue behaviour in polycrystalline and multiphase materials and raise intriguing questions about deformation behaviour at the microscale. Here we report on recent experiments using energy scanning diffraction of a polycrystalline nickel foil at the XFM microprobe. We find that the elastic back scatter measured in the pixelated Maia detector permits determination of the local crystallographic orientation within the polycrystalline foil. The shape and location of the Bragg peaks measured in the energy scan is shown to reveal information about the strain state of the sample. The results highlight how the combination of spatial and energy resolution offered by the Maia detector enables new types of experiments to be performed not possible with either conventional 1D energy-resolving, or 2D monochromatic detectors.

Advanced Materials III / 5

Characterisation of Ion Tracks using Small Angle Scattering

Author(s): Dr. KLUTH, Patrick[1]
Co-author(s): SCHAURIES, Daniel [2] ; Mr. MOTA SANTIAGO, Pablo [1] ; Mrs. NADZRI, Allina [3] ; Mr. PROFT, Max [1] ; Dr. MEDLING, Scott [1] ; Mrs. HADLEY, Andrea [1] ; Dr. KIRBY, Nigel [4] ; Dr. HAWLEY, Adrian [4] ; Dr. MUDIE, Stephen [4]

[1] *Australian National University*

[2] *ANU*

[3] *Australian National University (ANU)*

[4] *Australian Synchrotron*

Corresponding Author(s): patrick.kluth@anu.edu.au

Ion tracks are narrow trails of permanent damage generated along the paths of highly energetic heavy ions. These tracks are generally between 5-10 nm in diameter and can be tens of micrometers long. They have applications in many disciplines including materials science and engineering, nuclear physics, geochronology, archaeology, and interplanetary science.
If generated in an accelerator, an ensemble of ion tracks comprises parallel, (almost) identical nano-sized objects with negligible overlap. Due to their high monodispersity, small angle scattering, albeit measuring typically ~10^7 ion tracks, can yield information about the individual track structure averaging out fluctuations on an atomic level. Parallel alignment and stochastic distribution of the tracks reduces the analysis to simple form-factor scattering, yet due to their high aspect the 'small angle approximation' is no longer valid.
Over the last years we have demonstrated that SAS can resolve details of ion tracks in many materials inaccessible to other techniques [e.g. see 1-3]. This includes implementation of innovative capabilities at the Australian Synchrotron SAXS/WAXS beamline, including the use of diamond anvil cells in combination with in situ annealing to study ion track recovery of minerals under high pressure. More recently we developed a Monte-Carlo code to calculate scattering from complex track morphologies.
This presentation will give an overview of our work on ion tracks highlighting the new capabilities we have developed.

1. Phys. Rev B **90** (2014) 224108
2. Phys. Rev. Lett. **101** (2008) 175503
3. Phys. Rev. Lett. **110** (2013) 245502

Plenary / 194

Status of PAL-XFEL Project

Prof. KO, In Soo[1]

[1] *PAL*

Corresponding Author(s): isko@postech.ac.kr

PAL-XFEL project is aiming to produce 0.1 nm coherent X-ray laser to photon beam users. In order to produce such photons, there are 10-GeV electron linac based on S-band normal conducting accelerating structures and a 150-m long out-vacuum undulator system. The project was already started in April 2011, and the 1.11 km-long building is completed, and many parts of the linac and undulator systems are being installed. The beam commissioning is expected to be started in January 2017. In this talk, I will briefly introduce the project in general.

Techniques II / 14

100 nm 3D Laue Diffraction Technique for Ultra-High Spatial and Strain Resolution Combined with Versatile Analytical Probes

Dr. KU, Ching-Shun[1]

[1] *National Synchrotron Radiation Research Center*

Corresponding Author(s): csku@nsrrc.org.tw

This beamline is one of the phase-I projects for Taiwan Photon Source (TPS). Construction of the beamline will complete before July 2015 and commissioning for optics and end-station will follow. The beamline is dedicated to white/mono-beam Laue diffraction for structural analysis. For instance, users could obtain the 2D and 3D distribution of phases, orientation, residual strain, stress, and dislocations for materials in a complex form without destructing the samples during measurement. The estimated spatial resolution could be better than 100x100x50 nm.Furthermore, this end-station provided many complementary tools. Quadro-probe stages collect optical, electrical, surface properties of specimens; the fluorescence detector provides elemental information and the cryo-stage integrated with heater for temperature dependence experiments. Particularly, it is also the first time in synchrotron history to integrate an online real-time scanning electron microscopy (SEM) as a navigator. With spatial resolution down to 4 nm, it is able to find out the interest region with tiny structure on samples and arrange the position for different probes.This end-station can function either in vacuum or ambient environments depending on the user's demands. The station mounts an adjustment structure and settles on an active vibration cancellation optical table which minimizes the vibration level. In summary, this beamline and end-station will provide not only 2D/3D-XRD but also XRF, XAS, XEOL/CL, SPM and SEM information for diverse research programs. The end-station is scheduled to open to user in early 2016.

Techniques I / **114**

Three dimensional visualization of nanoscale structure: High contrast X-ray nanotomographic imaging at Pohang Light Source II

Author(s): Dr. LEE, Sangsul[1]
Co-author(s): Dr. LIM, Jun [2]

[1] *Pohang Accelerator Laboratory, POSTECH*

[2] *Pohang Accelerator Laboratory*

Corresponding Author(s): sangsul@postech.ac.kr

The synchrotron-based hard X-ray nanotomography beamline, named X-ray Nano Imaging (XNI), has been established since 2011 at sector 7C of Pohang Light Source-II (PLS-II). The XNI beamline was constructed primarily as a full-field X-ray microscopy for the inner structures study of biology and material science. Normal operation mode provides 46 nm resolution for still images and 100 nm resolution for tomographic images, with a 40 μm field of view using objective zone plate which has 50nm outer most zone width. Additionally, for large-scale application, it is capable of a 110 μm field of view with an intermediate resolution. Currently 7C XNI upgrade is scheduled to deliver high flux X-rays to transmission X-ray microscopy (TXM) system for cutting edge science and industrial application with three dimensional visualization. In this talk, we present current application and upgrade status including optics design, key instruments and extended applications.

Poster Session 1 - Board: BS-05 / **109**

MECHANISMS OF L-SULFORAPHANE-INDUCED ANTI-INFLAMMATORY EFFECTS DURING PNEUMOCOCCAL ADHERENCE.

Author(s): LIANG, Julia[1]
Co-author(s): Ms. VERVERIS, Katherine [2] ; Dr. VONGSVIVUT, Jitraporn (Pimm) [3] ; Dr. BAMBERY, Keith [3] ; Dr. LICCIARDI, Paul V [4] ; Dr. KARAGIANNIS, Tom C [5]

[1] *Baker IDI*

[2] *Baker IDI Heart and Diabetes Institute*

[3] *Australian Synchrotron*

[4] *Allergy and Immune Disorders, Murdoch Childrens Research Institute, Royal Children's Hospital, Flemington Road, Parkville, Victoria, Australia*

[5] *Epigenomic Medicine, Baker IDI Heart and Diabetes Institute, Melbourne, VIC, Australia*

Corresponding Author(s): julia.liang@bakeridi.edu.au

Pneumococcal disease caused by Streptococcus pneumoniae, a bacterium found in the upper respiratory tract, remains a leading cause of childhood mortality worldwide. Colonisation of the nasopharynx is essential in pathogenesis, facilitated by interactions between specific bacterial and host factors. During this process, receptors and intracellular proteins stimulate a local inflammatory response. While vaccines are effective, efficacy is limited where colonisation is established. Similarly, widespread antibiotic use has led to increased rates of multi-drug resistant pneumococci. Hence, alternative strategies are urgently required. L-sulforaphane (LSF), a compound derived from broccoli, possesses anti-cancer, anti-oxidant, and anti-inflammatory properties. Our previous findings demonstrate LSF can inhibit pneumococcal adherence to respiratory epithelial cells, however mechanisms are still unclear. We hypothesise that LSF inhibits pneumococcal adherence to human respiratory epithelial cells via modulation of host cell surface receptors, and/or inflammatory pathways. Using computational modelling in silico we developed molecular models of LSF and analogues to determine binding affinities to potential receptor targets of pneumococcal virulence factors. To investigate cell surface receptor expression on epithelial cells, we used immunofluorescence detection and western blotting to measure polymeric immunoglobulin receptor (PIGR), platelet-activating factor receptor (PAFR) and toll-like receptor 4 (TLR4). Finally, we used Fourier transform infrared microspectroscopy (FTIR) at the Australian Synchrotron to gain molecular and chemical spectra of human lung epithelial adenocarcinoma A549 cells to gain mechanistic insights of LSF prevention of pneumococcal inflammation. Understanding mechanisms of LSF in a model of will potentially have a major impact on child health.

Poster Session 1 - Board: BT-23 / **187**

Photon beam stabilization at the beamline 6C Bio Medical Imaging of PLS-II

Author(s): Dr. LIM, Jae-Hong[1]
Co-author(s): Mr. KIM, Hyo-Yun [1] ; Dr. LEE, Sangsul [2] ; Mr. SEO, In Deuk [1] ; Mr. LEE, Chae-soon [1] ; Dr. PARK, Youngjun [1] ; Mr. RYU, Chun Kil [1]

[1] *Pohang Accelerator Laboratory*

[2] *Pohang Accelerator Laboratory, POSTECH*

Corresponding Author(s): limjh@postech.ac.kr

Photon beam stabilization is a basic issue for reliable data acquisition. The beamline 6C Bio Medical Imaging of Pohang Light Source-II (PLS-II) is a dedicated station for full-field X-ray projection imaging at micron spatial resolutions. It uses Bragg-crystal monochromators which have a beam expanding capability. Although the beam size is relatively large, about one centimeter vertically, we still experience severe photon beam instability which is manifested as beam position drifting in the vertical direction. The instability appears thermal in origin because it initiates with changes of the heat load on crystals and gets stabilized over time. In order to study the instability in detail, we recently installed an ion chamber just downstream of the beam exit for real time monitoring of the beam intensity. Surprisingly, we found that the beam position drifting can be corrected by adjusting the pitch of the second crystal of the monochromator in a direction that keeps the ion current constant. By repeatedly applying this simple measure, the photon beam position is kept stable and the time-consuming CT data acquisition can now be performed quite reliably. This presentation describes the feedback control system along with the brief introduction of the beamline and its activity.

Poster Session 2 - Board: AM-10 / **66**

Determination of sulfur in natural rubber for reversion process

Author(s): Dr. LIMPHIRAT, Wanwisa[1]
Co-author(s): Dr. BOONKERD, Kanoktip [2]

[1] *SLRI*

[2] *Chulalongkorn University*

Corresponding Author(s): wanwisa@slri.or.th

The correlation amongst the sulfur to reversion resistances of natural rubber (NR) compound was investigated using X-ray absorption near edge spectroscopy. The NR samples were prepared which is varied accelerator DCBS and CBS ratio. It was found that the reversion of the NR compounds was not simply proportional to the increase of the sulfur to accelerator ratios no matter which accelerator was used. The increase of reversion indicating by the shorter plateau region and higher reversion rate was observed only when the sulfur to accelerator ratios were initially increased. At certain point, further increasing the sulfur to accelerator ratios in turn gave the NR compounds with higher reversion resistance. The important thing revealed here by XANES was the amount of polysulfidic linkage in the NR compounds passed through the maximum with the increasing of the sulfur to accelerator ratios. Therefore that the rubber compounds with higher polysulfidic linkages show the higher reversion are still valid. But the relation between the sulfur to accelerator ratio and the distribution of polysulfidic crosslinks was proved here that it was not simply proportional, thus causing the relation between the sulfur to accelerator ratio and reversion behavior not simply proportional too.

Poster Session 2 - Board: AM-24 / **184**

Determination of kinetics of pores formation during temperature controlled chemical de-alloying of Au-Ag50 alloys by in-situ SAXS/WAXS

Author(s): Mr. LIN, Bao[1]
Co-author(s): Dr. DUMÉE, Ludovic [1] ; Prof. KONG, Lingxue [1] ; Prof. HODGSON, Peter [1]

[1] *Deakin University*

Corresponding Author(s): baol@deakin.edu.au

The formation of nano-porous Au structures has potential for the design of advanced sensors, catalysts and bio-compatible separation media. Here, chemical de-alloying of Au-Ag50 alloy thin films were performed at different temperatures to alter the pore formation kinetics as well as the final morphology of the materials. Fractal dimensions at low q were significantly reduced with increasing temperatures affecting the fractal geometry of the pore propagation from surface fractal to volume fractal. The SAXS/WAXS in situ tests performed at the Australian Synchrotron were completed with scanning electron micrographs, x-ray diffraction, Kelvin probe and atomic force microscopy roughness determinations to produce a highly versatile nano-porous formation route. Following the Porod scattering model, the de-alloyed structures were found to be mathematically self-similar rather than amorphous and the pure Au ligaments dimension and the through pores size were found to increase by up to 50 % with increasing solutions temperature while the overall porosity was found to remain constant.

Instrumentation / **16**

Recent Developments in MRT at IMBL

Author(s): Dr. LIVINGSTONE, Jayde[1]
Co-author(s): Dr. STEVENSON, Andrew [2] ; Dr. HALL, Chris [1] ; Dr. PELLICCIA, Daniele [3] ; Dr. HAUSERMANN, Daniel [1]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron/ CSIRO*

[3] *Australian Synchrotron/RMIT*

Corresponding Author(s): jayde.livingstone@synchrotron.org.au

Microbeam radiation therapy (MRT) is a preclinical treatment modality utilising medium energy x-rays from a third generation synchrotron source. The x-rays are collimated into parallel beams which are typically 25-100 μm wide with a pitch of 10-400 μm. Spatial fractionation of the beam allows the delivery of high doses with preferential damage to cancerous tissue and sparing of surrounding radiosensitive normal tissues.
A dedicated MRT system designed for preclinical small animal trials was installed and commissioned in Hutch 2B of the Imaging and Medical Beamline in April 2015. The system consists of a vertical multislit collimator made from tungsten with 50 μm slits and pitch of 400 μm, two thin silicon beam monitors for monitoring dose rate upstream and downstream of the collimator and stage with integrated conformal mask array and visual positioning system.
During commissioning, dosimetry studies were conducted with the aim of developing dosimetry and treatment protocols. Broadbeam dosimetry has been performed on the new system using gafchromic film, various ionisation chambers and diamond detector to compare detector responses in various size and shaped fields. Good agreement was found between detectors for a reference field, and between solid and liquid water phantoms. Microbeam dosimetry has also been performed to characterise the vertical multislit collimator. The thin silicon beam monitors have been characterised and have also been tested with the Patient Safety System which is under development. In this presentation, the updates to MRT on IMBL will be discussed and dosimetry results presented.

Earth and Environment / 195

Transformation of silver nanoparticles in the environment

Author(s): Dr. LOMBI, Enzo[1]
Co-author(s): Ms. KHAKSAR, Maryam [1] ; Dr. SEKINE, Ryo [1] ; Dr. DONNER, Erica [1] ; Dr. BRUNETTI, Gianluca [1] ; Dr. SCHECKEL, Kirk [2] ; Dr. VASILEV, Krasimir [1] ; Dr. KAPPEN, Peter [3] ; Dr. GLOVER, Chris [3] ; JOHANNESSEN, Bernt [3]

[1] *University of South Australia*

[2] *US EPA*

[3] *Australian Synchrotron*

Corresponding Author(s): enzo.lombi@unisa.edu.au

The transformation of manufactured nanoparticles under natural conditions is a challenging area of research due to the environmental low concentrations that can be expected at present time. We have investigated the transformation of nanoparticles from consumer products and along the wastewater, biosolid soil pathway using a range of approaches. For instance, we developed and tested a nano in situ deployment device (nIDD) in which plasma polymerization is used to immobilize Ag-NPs on a substrate which allows us to analyse, through XANES, nanoparticles upon exposure and retrieval in/from different complex environmental compartments. These devices can be constructed in a variety of ways to cater for the research question of interest. In the examples reported here, plasma polymerization was used to immobilize the Ag-NPs on polyimide tape for XANES analysis and on Si wafers for XPS investigations. The nIDDs were exposed to a range of environmental conditions including a freshwater lake, a marina, freshwater and saltwater sediments, a sewer system and to the atmosphere in a number of cities in Australia, Europe and the US. Exposure time varied from few hours (sewer system) to a few weeks (air exposure). In the technological and environmental compartments the chemical and physical conditions play a dominant role in determining Ag speciation. Complexation of Ag by reduced sulfur groups was the key transformation mechanism but variability existed within various compartments. Further development is ongoing to integrate nIDDs with other devices to expand their use beyond speciation assessment and to NPs other than Ag.

Poster Session 2 - Board: BT-26 / **197**

Some novel imaging and diffraction capabilities on B16 Test Beam Line at Diamond Light Source, UK

Author(s): Mr. LUNT, Alexander[1]

Co-author(s): Dr. DOLBNYA, Igor [2] ; Prof. KORSUNSKY, Alexander [3] ; Dr. SUI, Tan [3] ; Dr. BAIMPAS, Nikolaos [3]

[1] *Department of Engineering Science, University of Oxford*

[2] *Diamond Light Source*

[3] *University of Oxford*

Corresponding Author(s): alexander.lunt@chch.ox.ac.uk

The development of micro- and nano-focusing optics is a key factor for the advancement of capabilities of modern synchrotron radiation beamlines. We present two newly developed micro-focusing optics systems recently commissioned at the B16 Test Beam Line at Diamond Light Source, UK: Compound Refractive Lenses (CRLs) and Kirkpatrick-Baez (KB) mirrors. These setups facilitate studies at the micro- and nano-meter length scale using both monochromatic and polychromatic radiation.
The main emphasis of B16 is placed on combining imaging and diffraction to study complex engineering materials such as alloys, ceramics, tissues and crystal structures. The results of four recent high resolution studies are presented in order to demonstrate the capabilities of the CRL and KB focusing arrangements:

1. Phase composition and residual strain mapping in a veneered zirconia dental prosthesis
2. Nano-scale mapping of lattice strain and orientation inside carbon core SiC fibres 1
3. Development of an iterative algorithm capable of providing quantitative broadband Fresnel phase retrieval under white beam conditions
4. X-ray birefringence imaging to probe orientation properties of molecules and/or bonds in anisotropic solids [2]

References:
1 N. Baimpas, A.J.G. Lunt, I.P. Dolbnya, J. Dluhos & A.M. Korsunsky, Carbon 79 (2014) p. 85-92.
[2] B.A. Palmer, G.R. Edwards-Gau, B.M. Kariuki, K.D.M. Harris, I.P. Dolbnya, S.P. Collins, Science 344, (2014) p. 1013-1016.

Plenary / **4**

The Development of TPS Light Source in Taiwan: Phase-II Commissioning and Future Planning

Dr. LUO, Gwo-Huei[1]

[1] *NSRRC*

Corresponding Author(s): luo@nsrrc.org.tw

The construction of Taiwan Photon Source (TPS) started in 2010 and the first light was emitted from the beam port at the end of 2014. It was a swift record in commissioning two new rings, which took only 3 weeks to have the 150 MeV electron beam ramp to 3 GeV in the booster and store 5 mA beam in the storage ring. The commission of the TPS and fine-tuning the machine were carried out in the first quarter of 2015 and the stored beam has reached 100 mA. The measured key parameters are consistent and matched well with the designed targets. Especially, the emittance value has reached the design goal. In the 2nd and 3rd quarters of 2015, the TPS was shut down to install superconducting RF cavities, insertion devices (IDs), and beamlines. A new double mini-betay lattice is available for commission with the new 2 cavities and 10 IDs. With three sets of double mini-betay IDs installed, the TPS is expected to eventually reach a 500 mA stored beam current. The average brightness produced from the IDs will have a great opportunity to place the TPS at the crest of the synchrotron light community around the world.

Poster Session 1 - Board: EM-19 / **228**

Synthesis and structural characterisation of cadmium dithiocarbamate ionic liquids

Author(s): Ms. MACREADIE, Lauren[1]
Co-author(s): Dr. TURNER, David [1] ; CHESMAN, Anthony [2] ; Prof. BATTEN, Stuart [1]

[1] *Monash University*
[2] *CSIRO*

Corresponding Author(s): lauren.macreadie@monash.edu

Cadmium dithiocarbamate complexes, [Cd(S2CNR2)2], have found application as precursors for cadmium sulfide (CdS) thin film development and subsequent incorporation into photovoltaic devices. However, their dimeric nature limits their solubility in green, organic solvents commonly used in solution deposition routes to thin film formation.1 To increase the solubility of [Cd(S2CNR2)2] complexes, a series of monomeric cadmium dithiocarbamate salts were synthesised and structurally characterised using synchrotron X-ray diffraction. The cadmium dithiocarbamate anions, [Cd(S2CNR2)3]−, are charge balanced by ammonium counter ions which include tetramethylammonium (Me4N), tetrapropylammonium (Pr4N), 1-propyl-3-methylimidazolium (C3mim) and 1-butyl-1-methylpyrrolidinium (C4C1py). The latter two counter ions are known to form ionic liquids, due to their assymmetry and poor crystal packing abilities, and when used allowed the formation of cadmium dithiocarbamate ionic liquids. The C3mim[Cd(S2CNR2)3] compounds were room temperature ionic liquids, while the C4C1py[Cd(S2CNR2)3] compounds were crystalline materials at room temperature and melted at temperatures below 100°C. Investigation of the overall crystal packing arrangement of these structures allowed for better understanding of their thermal properties in the solid state, in particular the formation of ionic liquids using the C3mim and C4C1py cations, in contrast to the tetraalkylammonium cations. All compounds showed a higher solubility in common laboratory solvents and therefore can be deemed as viable precursors towards CdS thin film formation using solution deposition processes.

1. Knapp, C. E.; Carmalt, C. J. Chem. Soc. Rev. 2016.

Biological Systems / 77

XFM mapping of elemental distributions in brain stem sections from multiple sclerosis patients using the BioMaia detector

Prof. PAMPHLETT, Roger[1] ; Prof. LAY, Peter[1] ; Dr. MAK, Rachel[1]

[1] *University of Sydney*

Corresponding Author(s): rachel.mak@sydney.edu.au

Locus ceruleus (LC) neurons supply central nervous system cells with noradrenaline, and damage to the LC has been found in multiple sclerosis (MS) and in neurodegenerative diseases such as Alzheimer's disease. LC neurons selectively accumulate heavy metal toxicants, which could play an important role in the pathogenesis of these diseases. Histochemical studies of brain tissue from MS patients suggest Hg as a potential toxin in the LC, but there may be other metal toxicants present in the LC that cannot be detected histochemically. We therefore used the X-ray Fluorescence Microscopy (XFM) Beamline at the Australian Synchrotron to image the LC in cryo-fixed brain stem sections of MS patients. The 384-element BioMaia detector provided the elemental sensitivity required to map the metal toxicants of interest (such as Hg, Pb, and Cr), as well as lighter elements such as S and Se, whose co-localization with the heavy metals can provide further evidence for the physiological effects of these metals. The spatial resolution of BioMaia (smaller than 1 um) is also important in identifying toxicants in glial cells (such as oligodendrocytes, average diameter 10 um), which are smaller than the LC neurons (average diameter 40 um). We show that in MS (1) a number of different metal toxicants can be found in LC neurons, and (2) glial cells may also contain metal toxicants.

Poster Session 1 - Board: IM-07 / **107**

Updates on the computed tomography experiment at the Medical and Imaging beamline of the Australian Synchrotron

Author(s): Dr. MAKSIMENKO, Anton[1]
Co-author(s): HAUSERMANN, Daniel ; Dr. STEVENSON, Andrew [2] ; Dr. HALL, Chris [1] ; ACRES, Robert [1] ; Dr. LIVINGSTONE, Jayde [1] ; Dr. PELLICCIA, Daniele [3] ; Dr. PEARSON, James [4]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron/ CSIRO*

[3] *RMIT University*

[4] *IMBL / Monash University*

Corresponding Author(s): anton.maksimenko@synchrotron.org.au

The Imaging and Medical Beamline (IMBL) of the Australian Synchrotron (AS) is now becoming one of the most advanced instruments of this type in the world. It is designed to provide a wide variety of imaging techniques including but not limited to the in-line and analyzed phase contrasts, monochromatic and pink beam imaging. Three beamline's enclosures at various distances, when combined with the 25kW superconducting multipole wiggler and double Laue bent monochromator provide the end user a good choice of beam characteristics ranging from the hi-flux for high resolution and size up to huge 48x5cm beam at 134m from the source with the allowed energy range 17-120kEv or pink beam. The wide range of the area detectors allows the computed tomography (CT) to be applied to almost any known X-ray imaging modality. The beamline's data acquisition system is directly linked to the high performance computing cluster. Deep integration of the acquisition, reconstruction and rendering facilities allows one to think of their combination as of a single system with modular architecture. The system is designed for the fully automated experiments with minimal user interaction. It has multiple levels of flexibility allowing quick design and implementation of a new experiment. This report summarizes implemented, designed and planned features of the beamline as applied to the imaging experiments. Some latest outcomes of the CT system are presented with the samples coming of different fields of science: Biology, Geology, Paleontology and Medicine.

Poster Session 2 - Board: BS-06 / **215**

An Atlas of Metal Dependent Histone Deacetylase Expression in the Developing and Adult Mouse Brain

Author(s): Ms. MALIK, Neha[1]
Co-author(s): Dr. VONGSVIVUT, Jitraporn (Pimm) [2] ; Dr. BAMBERY, Keith [2] ; Dr. KARAGIANNIS, Tom [3]

[1] *Baker IDI, Heart and Diabetes Institute*

[2] *Australian Synchrotron*

[3] *Baker IDI Heart and Diabetes Institute*

Corresponding Author(s): nmalik@bakeridi.edu.au

Histone deacetylases (HDACs) are enzymes that transcriptionally alter the chromatin by removing an acetyl group from the ε-amino acid from the lysine residue on the core histone tails. This allows negatively charged DNA to wrap tightly around the histones. Mammalian HDAC classes I, II and IV are categorized as metal dependent enzymes and consist of HDACs 1-11. The deacetylation of histones is commonly linked to gene silencing and is involved in many cellular pathways including apoptosis and cell cycle arrest. An understanding of normal homeostatic levels of HDAC expression is necessary for therapeutics to progress in the field of diseases linked to neurodevelopment and neurodegeneration. In order to elucidate the changes in development between embryonic and adult mouse brain we investigated the expression levels of HDACs 1-11. Firstly, a semi-quantitative method based on immunofluorescence staining was used to examine differences in the endogenous expression levels of the HDACs between E13.5, E14.5 and adult brains. Secondly, utilising focal plane array microspectroscopy (FPA) on the infrared beamline at the Australian Synchrotron, we observed spectral changes in the brain during different stages of development. Combining these experimental techniques our aim is to establish a comprehensive atlas of neurodevelopment focusing on chemical mapping obtained from FPA and the HDAC expression. Our results indicate

high expression levels of HDAC 9 and 11 for all three developmental stages and HDAC 2 for embryonic brain development. Spectral changes attributing to lipid and amino acid composition were altered during different stages of neurodevelopment.

Poster Session 1 - Board: IM-13 / **176**

Three-dimensional Strain State Comparison for CVD-grown Single Crystal Nanodiamonds using Bragg Coherent Diffractive Imaging

Author(s): Mr. MAQBOOL, Muhammad Salman[1]
Co-author(s): Dr. HOXLEY, David [1] ; Mr. PHILLIPS, Nicholas [2] ; Ms. COUGHLAN, Hannah [1] ; Dr. DARMANIN, Connie [3] ; Dr. JOHNSON, Brett [4] ; Dr. HARDER, Ross [5] ; Dr. CLARK, Jesse [6] ; Dr. BALAUR, Eugeniu [1] ; Dr. ABBEY, Brian [1]

[1] *La Trobe University*

[2] *LTU/CXS*

[3] *La Trobe*

[4] *University of Melbourne*

[5] *Advanced Photon Source*

[6] *SLAC National Accelerator Laboratory*

Corresponding Author(s): salman.maqbool87@gmail.com

The unique properties of nanodiamonds make them suitable for use in a wide range of different applications, including as biomarkers for cellular tracking in vivo at the molecular level. The sustained fluorescence of nanodiamonds containing nitrogen-vacancy (N-V) centres is related to their internal structure and strain state. Theoretical studies predict that the location of the N-V centre and the nanodiamonds residual elastic strain state have a major influence on their photoluminescence properties. However, to date there has been no direct measurements made of their spatially resolved deformation fields due to the challenges that such measurements present. Here we apply the recently developed technique of Bragg Coherent Diffractive Imaging (BCDI) to map the three-dimensional deformation field within a single nanodiamond of ˜ 0.5 um diameter. The results indicate that there are high-levels of residual elastic strain already present in the nanodiamond which could have a critical influence on its optical and electronic properties.

Poster Session 2 - Board: BT-30 / **204**

Electrically-cooled HPGe detector for advanced x-ray spectroscopy and imaging

Author(s): Dr. MARIAN, Vlad[1]
Co-author(s): Mr. CLAUSS, Jean [2] ; Dr. PIRARD, Benoit [2] ; Mr. QUIRIN, Pascal [2] ; Mr. FLAMANC, Jeremy [2] ; Dr. LAMPERT, Marie Odile [2]

[1] *Canberra France*

[2] *Canberra*

Corresponding Author(s): vlad.marian@canberra.com

This paper describes a novel High Purity Germanium (HPGe) detector, specifically designed to address the challenges of ultimate x-ray spectroscopy and imaging applications for synchrotrons. It consists of a multichannel HPGe crystal (monolithic or individual elements) providing new and ultimate X-ray energy resolution level especially at high count rates (reaching 190eV at 6kev and 0.1μs shaping time), and high throughput.
The crystals are cooled using a state-of-the-art electrical cryocooler with active vibration cancellation. The use of a cryocooler does not have any negative impact on the detector performance.

Poster Session 2 - Board: IM-06 / **82**

Two-plane holography with customizable references

Author(s): Dr. MARTIN, Andrew[1]
Co-author(s): Dr. D'ALFONSO, Adrian [2] ; Dr. VAN RIESSEN, Grant [3]

[1] *ARC Centre for Excellence for Advanced Molecular Imaging, School of Physics, University of Melbourne*

[2] *The University of Melbourne*

[3] *La Trobe University*

Corresponding Author(s): andrew.martin@unimelb.edu.au

Fourier-transform holography is an established method of high-resolution coherent x-ray imaging, but is limited by the need to fabricate highly specific reference structures. Traditional reference structures must be coplanar with the sample, and are typically fabricated along with the sample. We have recently developed the technique of holography using an arbitrary customizable reference, greatly enhancing the flexibility of experimental geometries and allowing for the reference scatterer to be upstream of the sample. In this way, holography can be offered as a permanent technique provided by a coherent imaging beamline, rather than requiring a sample modification fabricated by the user. We will present the first results obtained at the Soft X-Ray Imaging branchline at the Australian Synchrotron.

Poster Session 1 - Board: BT-37 / **232**

Synchrotron-beam Focal Plane Array (FPA) illumination: Developing fast acquisition, high spatial resolution FT-IR chemical mapping at the IR Microscopy beamline

Author(s): MARTIN, Danielle[1]
Co-author(s): Dr. BAMBERY, Keith [1] ; Dr. VONGSVIVUT, Jitraporn (Pimm) [1] ; Dr. TOBIN, Mark [1]

[1] *Australian Synchrotron*

Corresponding Author(s): danielle.martin@synchrotron.org.au

The IR Microscopy (IRM) beamline at the Australian Synchrotron is used to generate detailed FTIR chemical maps of samples at diffraction-limited spatial resolutions, with high S/N ratios. Using a single element detector and confocal-like apertures to focus the beam at the sample surface, 2D maps at spatial resolutions between 3-5 microns can be measured. This is however time-consuming, with one 50 micron squared map taking 1-2 hours to acquire. How then can sample throughput be improved? FTIR mapping systems using Focal Plane Array (FPA) detectors are capable of covering much greater surface areas at a time; each array pixel can measure a full FTIR spectrum, and the IRM beamline at the Australian Synchrotron is equipped with a 64x64 FPA. The compromise is that a Globar source must be used to evenly illuminate this relatively large detector, greatly reducing spatial resolution. So how then to illuminate a large array with a small, low-emittance SR beam? The IRENI beamline, SRC, extracted 12 IR beams from their source to achieve full FPA illumination across a 96x96 array (1). We extract only one IR beam, therefore such wide field illumination is not possible. Instead this poster outlines a method similar to that used at NSLS (2), where the single beam is split into 4, to successfully illuminate a 16x16 FPA grid. The overall setup and some results are shown.
(1) Nasse et al. Nature methods 8.5 (2011)
(2) Stavitski et al. Analytical chemistry 85.7 (2013)

Plenary / 190

Membrane fusion: a riddle, wrapped in a mystery, inside an enigma

Prof. MARTIN, Jennifer[1]

[1] *University of Queensland*

Corresponding Author(s): j.martin@imb.uq.edu.au

Membrane fusion is a fundamentally important process required for transport of cellular cargo. It is essential - for example - in neurotransmission and blood glucose control.
The 2013 Nobel Prize in Medicine or Physiology was awarded to Rothman, Schekman and Su¨dhof for their discovery of the molecular machinery supporting SNARE-mediated membrane fusion. This machinery is conserved from yeast to humans. Consequently, we know that two protein families are required for every membrane fusion event: (i) SNARE proteins, and (ii) Sec1/Munc18 (SM) proteins.
The SNARE proteins are located on different membranes and zip together in response to specific signals to bring the two membranes into close proximity. Formation of the SNARE protein complex is thought to be essential for providing the energy required for the two membranes to fuse.
The role of the SM proteins has proven much more difficult to define. Some reports describe a positive regulatory role for SM proteins on SNARE complex formation and membrane fusion. Other reports conclude a negative regulatory role.
This presentation explores the molecular basis of SNARE-mediated membrane fusion. A range of complementary biophysical methods were used including synchrotron MX and SAXS, as well as SANS with contrast-matching and chemical cross-linking with mass spectrometry. These technologies have allowed us to probe the atomic interactions and conformational changes that occur in these fascinating yet enigmatic nano-machines.

Poster Session 1 - Board: EM-05 / **92**

The effect of ordering of conductive polymer (pEDOT) on the conductivity in composites and the stage of manufacturing at which ordering occurs

Author(s): Mr. MAYEVSKY, David[1]
Co-author(s): Dr. GARVEY, Chris [2]

[1] *Monash University*

[2] *ANSTO*

Corresponding Author(s): david.mayevsky@monash.edu

Some conducting polymer composites have shown counterintuitive increases in conductivity with increased quantities of incorporated non-conducting polymer (NCP). For example the conductivity of pEDOT, as a function of volume fraction of NCP, paradoxically increases for up to 70% volume fraction of PEG, however this is distinct to what is being observed for pEDOT:gelatin composites which follows percolation theory in its conductivity trend. GIWAXS measurements were made on the SAXS/WAXS beamline at the Australian Synchrotron to investigate the effects of adding varying quantities of NCP on the packing of the conducting polymer in the composite thin films. In-situ GIWAXS was used to explore the stages of pEDOT composite film manufacture at which ordering occurs.

Imaging I / 131

Dynamic study of rising and baking bread dough

Author(s): MAYO, Sherry[1]
Co-author(s): MCCANN, Thu [1] ; DAY, Li [2] ; FAVARO, Jenny [1] ; TUHUMURY, Helen [1] ; Dr. MAKSIMENKO, Anton [3]

[1] *CSIRO*

[2] *AgResearch, Charles Sturt University*

[3] *Australian Synchrotron*

Corresponding Author(s): sherry.mayo@csiro.au

Australia is a major wheat producer for the domestic and international market. Properties of wheat and its suitability for bread-making varies depending on the variety and the region where

it was grown. Bread-making performance can also be significantly affected by dough additives including different salts.
Previous studies have analysed dough structure using micro-CT but few have looked at the dynamics of the complete proofing and baking process in situ. In this study we use the high-speed imaging capability of the Imaging and Medical Beamline to observe the dynamic of rising and baking in a series of bread dough formulations made from high and low protein flour with different salt additives. We were able to observe this process in 16 different samples with scans at 29 time-points for each sample during 2 hours of proofing and around 30 min of baking.
Using Avizo we developed automated scripts for analysis of this huge amount of data to extract features such as void-size and wall thickness. We also have attempted to identify the points at which voids burst and connect with one another.
With this we can discover the effect of different formulations on dough performance. The long term aim of which is to improve formulations to boost the value obtained from Australian flour.

Poster Session 1 - Board: BS-07 / **217**

Draft Synchrotron-Fourier transform infrared maps of ovalbumin-induced murine chronic allergic airways disease: Correlation with conventional histology and immunofluorescence

Author(s): Ms. MAZARAKIS, Nadia[1]
Co-author(s): Dr. VONGSVIVUT, Jitraporn (Pimm) [2] ; Dr. BAMBERY, Keith [2] ; Dr. ROYCE, Simon [3] ; Dr. KARAGIANNIS, Tom [1]

[1] *Epigenomic Medicine, Baker IDI Heart and Diabetes Institute*

[2] *Australian Synchrotron*

[3] *Monash University*

Corresponding Author(s): nadia.mazarakis@bakeridi.edu.au

Synchrotron-Fourier transform infrared (FTIR) tissue mapping is yet to be investigated in chronic models of allergic airways diseases. Here, spectra derived from synchrotron-FTIR maps were used to analyse an ovalbumin (OVA)-induced murine chronic allergic airways disease model. Analysis of the chemical maps resulted in distinct clusters and significant changes in the lipid, proteins and nucleic acid regions of the spectra between the saline control and OVA-induced allergic airway response within murine lung tissue samples. These results are supported by structural and biological changes within conventional histological and immunofluorescence methodologies. Future studies will aim to include larger and higher resolution maps to improve clustering and quality of the data produced to elucidate the underlying mechanisms involved in a chronic murine model of OVA-induced allergic airways disease.

Plenary / **45**

Microstructure of High Performance Polymer Electronics

MCNEILL, Chris[1]

[1] *Monash University*

Corresponding Author(s): christopher.mcneill@monash.edu

Conjugated polymers are an interesting class of material whose semiconducting properties enable application in light-emitting diodes, polymer solar cells and organic field-effect transistors (OFETs). The molecular packing and microstructure of conjugated polymer thin films strongly influences the function of such electronic devices. Due to the semicrystalline nature of conjugated polymers, characterisation of the thin film microstructure can be challenging, especially when films less than 100 nm thick are used. For OFETs in particular charge transport is localised to within a ~ 3 nm thick accumulation layer at the film interface, requiring characterisation techniques that are highly surface sensitive. In this presentation I will overview the application of synchrotron-based techniques such as Near-Edge X-ray Absorption Fine-Structure (NEXAFS) spectroscopy and Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) to disclose the microstructural signatures of high performance polymers that enable large-area MHz electronics.

Energy Materials II / 147

Molecular-level understanding of metals in geo-fluids: combination of synchrotron-based XAS and ab initio molecular dynamics

Author(s): Dr. MEI, Yuan[1]
Co-author(s): Dr. LIU, Weihua [1] ; Dr. ETSCHMANN, Barbara [2] ; Prof. BRUGGER, Joël [2] ; Prof. SHERMAN, David [3] ; Dr. TESTEMALE, Denis [4] ; Mr. RAE, Nicholas [5]

[1] *CSIRO*

[2] *Monash University*

[3] *University of Bristol*

[4] *CNRS*

[5] *Australian Synchrotron*

Corresponding Author(s): yuan.mei@csiro.au

Aqueous fluids under wide range of T-P conditions are an essential medium for transporting metals in the Earth's crust. Metals are dissolved by forming complexes with ligands such as chloride and bisulfide, and understanding the nature and thermodynamic properties of these complexes is crucial for predicting solubilities of minerals and the mechanics of ore formation. Synchrotron based in-situ X-ray Absorption Spectroscopy (XAS) can provide insights into the molecular structures and thermodynamic properties of metal complexes in situ up to conditions beyond the critical point of water. With the advance of high-performance computing techniques, ab-initio Molecular Dynamics (MD) provides an independent means to determine the nature and stabilities of metal complexes, and particularly delivers independent crosschecks and reliable molecular models to help interpreting XAS data.
Here we demonstrate our recent studies of combining XAS and ab-initio MD in understanding the speciation, structural properties and thermodynamic stability of Zn(II)-Cl/HS, Pd(II)-Cl/HS, and Pb(II)-Cl complexes. The bond distances, coordination numbers and Debye-Waller factors for these metal complexes obtained from ab-initio MD are broadly consistent with the XAS results. The complex geometries and stoichiometries calculated from MD also agree with the XANES measurements. By combining the results from MD and XAS with existing solubility data, we recalculated the thermodynamic properties of Zn(II)-Cl/HS and Pd(II)-Cl/HS complexes, and predicted the solubilities of zinc and palladium in hydrothermal fluids with improved accuracy and reliability.

Imaging I / 90

Dual Energy X-ray Analysis Using Synchrotron Computed Tomography at 30–100 keV

Author(s): Dr. MIDGLEY, stewart[1]
Co-author(s): Dr. SCHLEICH, Nanette [2] ; Dr. STEVENSON, Andrew [3]

[1] *Adjunct Research Associate*

[2] *Department of Radiation Therapy, University of Otago, Wellington, New Zealand*

[3] *Australian Synchrotron/ CSIRO*

Corresponding Author(s): stewart.midgley@monash.edu

Dual energy X-ray analysis (DEXA) uses computed tomography (CT) measurements at two photon energies to characterise the density and composition of materials. Results are expressed as the electron density (Ne) and fourth statistical moment ($R4$) describing the elemental composition similar to the concept of effective atomic number. The accuracy of the technique was investigated for liquid samples of known density and composition; aqueous ethanol and salt solutions.
CT scans were conducted with near mono-energetic radiation of 30 to 100 keV. The radiation dose delivered by each scan was 4-9 mGy, approximately 50% of that for medical CT. Reconstruction used filtered back projection with a ramp filter to 0.2 mm pixel size. For individual slices the

noise to signal ratio (NSR) was 3.2-8.4%. Analysis used the mean of 40 summed slices with an NSR of 0.8-1.9%.
The measurements were combined to obtain coefficients describing the compositional dependence of elemental cross-sections. DEXA considered all 34 materials and 45 permutations of beam energies separated by 5 keV to 70 keV. The difference between DEXA results and true values improved with wider energy separations reaching approximately 0.5% (one standard deviation) for separations 20 keV or more. Propagation of errors analysis was employed to quantify contributions from random and systematic errors, accounting for the observed accuracy of the technique. The applications for DEXA are sample characterisation and predicting interaction coefficients at other photon energies for attenuation correction and radiation dosimetry calculations.

Poster Session 1 - Board: EE-11 / **173**

Mechanism of Fe(III)-Precipitate Formation and Transformation in Circumneutral Aqueous Solutions in the Presence of Phosphate Under Conditions Relevant to Membrane Bioreactor Wastewater Treatment

Author(s): Dr. MILLER, Christopher[1] ; Mr. WU, Hao[2]
Co-author(s): Dr. IKEDA-OHNO, Atsushi [3] ; Dr. WANG, Yuan [2] ; Prof. WAITE, T. David [2]

[1] *School of Civil and Environmental Engineering, The University of New South Wales*

[2] *The University of New South Wales*

[3] *Helmholtz-Zentrum Dresden-Rossendorf*

Corresponding Author(s): c.miller@unsw.edu.au

The formation of iron-phosphate minerals influences the transport and bioavailability of phosphate in natural systems, despite this importance, understanding of the mechanism and rate of this process is limited. Iron addition is also used to remove phosphorous during municipal wastewater treatment to prevent eutrophication and associated algal blooms in receiving waters. The poor understanding of the kinetics of the interaction between Fe and P and the ability of $Fe^{III}PO_4$(s) formation to compete with rapid Fe(III) hydrolysis to iron oxyhydroxides limits the effective use of this technology, which is one of the few available processes to treat wastewaters to increasingly stringent phosphate discharge limits.
This study has used Fe K-edge and P K-edge X-ray absorption spectroscopy experiments (undertaken at BL17C1 and BL16A1 at NSRRC Taiwan) to determine the composition of the Fe-P species in the sludge formed from Fe- and P-containing solutions under a range of initial Fe-oxidation states, relative Fe and P concentrations and also pH (which strongly influences the rate of Fe(II) oxidation and Fe(III)-precipitation). This data has been interpreted using a linear combination fitting scheme that has been adjusted to fit the sample composition to the Fe XANES and EXAFS as well as the P-XANES simultaneously. Coupling this solid-state chemical composition with the solution phase kinetics derived from standard chemical measurements allows the critical processes in the formation of the desired Fe-PO_4 minerals to be examined.

Imaging II: Sponsored by MASSIVE / 103

Visualising Evolution and Extinction through silicified fossil fruits from Queensland.

Author(s): MILROY, Anita[1]
Co-author(s): Dr. MAKSIMENKO, Anton [2] ; Dr. ROZEFELDS, Andrew [3] ; Dr. HOLMES, Ashley [1]

[1] *Central Queensland University*

[2] *Australian Synchrotron*

[3] *Queensland Museum*

Corresponding Author(s): anita.milroy@cqumail.com, anton.maksimenko@synchrotron.org.au

A recent successful trial using the Imaging and Medical (IMBL) at the Melbourne Synchrotron has revealed the internal anatomy and morphology of rare, three-dimensionally preserved, 30

million year old silicified fruits from Capella, in Central Queensland. These IMBL scans are the first application of this technique to the study of this kind of material. Previous medical CT scanning did not reveal any internal information. During the permineralisation process silicates have replaced the organic material of the fruit and thus biological information (such as DNA) is impossible to obtain. This in turn makes accurate taxonomic classification extremely difficult. Physical sectioning of these rare fossils for visualisation has many risks as it invariably destroys the specimen and is not guaranteed to produce any additional information. However, the current IMBL scans have provided us with accurate, detailed images of the internal reproductive structures of these enigmatic fruits, enabling, for the first time, a direct physical comparison between internal morphologies of extinct and extant rainforest fruits. This extra vital information effectively enables researchers to establish or confirm classifications to appropriate family, genus and species. Accurate species identification will help to advance knowledge of past environments and climates in Australia. Our collaboration specifically aims at combining art, science and technology to explore various approaches in the visualisation of this material, to drive content not only for scientific publication, but for exhibitions in galleries and museums and thereby attract entirely new audiences to this research.

Poster Session 1 - Board: AM-09 / **64**

High temperature structural properties of CrAlTiN coatings from in-situ Synchrotron Radiation X-ray Diffraction

Author(s): Mr. MOHAMMADPOUR, Ehsan[1]
Co-author(s): Dr. JIANG, Zhong-Tao [1] ; Dr. ALTARAWNEH, Mohmmednoor [2] ; Mr. MONDINOS, Nicholas [1] ; DLUGOGORSKI, Bogdan Z. [1]

[1] *School of Engineering & Information Technology, Murdoch University, Murdoch, WA 6150, Australia*

[2] *School of Engineering & Information Technology, Murdoch University, Murdoch, WA 6150, Australia.*

Corresponding Author(s): e.mohammadpour@murdoch.edu.au

This paper describes thermal stability of CrAlTiN hard coatings, deposited by magnetron sputtering technique in temperature range of 25-700 °C. The microstructure and phase combination of coatings were investigated using in situ synchrotron radiation X-ray diffraction (SR-XRD). Rietveld refinement was carried out on the characterisation of SR-XRD spectra to investigate the structure and phase composition of coatings. The SR-XRD analysis demonstrated that CrN is the dominant phase below 700 °C. Solution of Ti and Al in CrN changed the preferential growth orientation of the coating material and indicated the complex structure of the coating in shape of crystalline CrTiAlN solid solution surrounded by amorphous AlN matrix. Domain size and strain of CrN crystallite in both coatings at different temperatures were estimated. The high quality crystalline data obtained from this study provides deeper understanding of the non-structural and thermal stability of CrAlTiN nanocomposite. Obtained data also offers feasibility to simulation mechanical properties at high temperature using computational modelling, such as Density Functional Theory.

Poster Session 1 - Board: BT-27 / **198**

Computing developments and tools supporting beamline science at the Australian Synchrotron

Author(s): MOLL, Andreas[1]
Co-author(s): FELZMANN, Uli [1] ; MUDIE, Nathan [1] ; Dr. JONG, Lenneke [1]

[1] *Australian Synchrotron*

Corresponding Author(s): andreas.moll@synchrotron.org.au

The Scientific Computing and IT group at the Australian Synchrotron develops software tools to support beamline science, maximise the user experience and accelerate the scientific outcomes of their beam time. Our suite of open source tools facilitate better and more streamlined data collection integrated with automatic and real-time processing, the results of which can inform decisions about further data collection during the user's beam time, optimizing the data they can collect at one visit. In addition, we have developed stand-alone data analysis workflow tools

designed for processing and analysis of data, both at the facility and post-experiment at the user's home institute.

Earth and Environment / 11

Oxidative disintigration of greigite (Fe3S4): New insights from XAS

Author(s): Dr. MOON, Ellen[1]
Co-author(s): Dr. MATA, Jitendra [2] ; Prof. BUSH, Richard [1]

[1] *Southern Cross University*

[2] *Bragg Institute, ANSTO*

Corresponding Author(s): ellen.moon@scu.edu.au

Greigite (Fe3S4) is a ferrimagnetic iron sulfide mineral, containing both Fe(II) and Fe(III) centres. There is ongoing debate over the role of greigite in sedimentary settings, especially acid sulfate soils: its partially oxidised nature has traditionally been seen as indicative of a metastable intermediate in low temperature sulfide mineralization, however others have found greigite to be a distinct end-member that forms under partially oxic (or oscillating redox) conditions. From a thermodynamic perspective it should have limited stability with respect to pH and dissolved sulfur activity, yet has been identified in natural sediments of up to a few million years old.
The iron sulfides are an important sink and potential source for metals in contaminated environments. Understanding the oxidative transformation of greigite is vital for understanding contaminant release and sequestration.
We present a study into the oxidation of greigite under aqueous conditions. The effects of solution pH, Cl- and SO42- concentrations are examined with respect to transformation kinetics, mineralogy of the oxidation products, and the relationship between Fe and S oxidation (using X-ray absorption spectroscopy). The results of this study provide new insights into the role and longevity of greigite in natural sediments and will underpin new remediation strategies for acid sulfate soils, while also adding to our understanding of the geochemical cycling of Fe and S.

Poster Session 1 / 152

Study of swift heavy-ion irradiation of amorphous silicon oxynitride films

Author(s): Mr. MOTA SANTIAGO, Pablo[1]
Co-author(s): Mrs. NADZRI, Allina [2] ; Dr. MEDLING, Scott [1] ; SCHAURIES, Daniel [3] ; Dr. KLUTH, Patrick [1]

[1] *Australian National University*

[2] *Australian National University (ANU)*

[3] *ANU*

Corresponding Author(s): pablo.mota@anu.edu.au

In this work we present direct evidence of ion track formation in 1-micron-thick silicon oxynitride films deposited by Plasma Enhanced CVD (PECVD) after irradiation with 185 MeV Au ions at different fluences. Silicon oxynitrides are gradient refractive index materials (GRIN), where its physical properties are linear combination of Si$*{3}N{4}andSiO{2}.Themorphologyoftheiontrackswerestudiedbymeansof Sm rayScattering(SAXS)whilethestructuraldamagewasanalysedbyFourierTransformInfraredSpectroscopy(FTIR).Sw SiO{2}$ is provided.
SAXS measurements of samples irradiated at low fluences average a large number of single tracks providing reliable results about the morphology. Continuous tracks with a core-shell structure were found, a small core (less than 2 nm) surrounded by a thick shell (4-6 nm), presumably with an underdense core and an overdense shell, similar to the results found in a-SiO$*{2}.Onlyslightdifferenceswerefoundforiontracksin LPCVDSi{3}N_{4}$.

Analysis from FTIR measurements yields an ion track radius of 1.8 nm, which closely matches the core size. This is an indication that in amorphous materials most of the radiation damage is produced in the core region.

Imaging II: Sponsored by MASSIVE / 129

Elastic and Inelastic Properties under Simulated Earth's Mantle Conditions in LVPs in Conjunction with Synchrotron Radiation

Dr. MUELLER, Hans J.[1]

[1] *GFZ German Research Centre for Geosciences*

Corresponding Author(s): hjmuel@gfz-potsdam.de

The interpretation of highly resolved seismic data from Earth's deep interior require measurements of the physical properties of Earth's materials under experimental simulated Earth's mantle conditions. More than a decade ago seismic tomography clearly showed subduction of crustal material can reach the core mantle boundary under specific circumstances. That means there is no longer space for the assumption deep mantle rocks might be much less complex than deep crustal rocks known from exhumation processes. Viscosity data of melts measured under in situ high pressure conditions are crucial for the understanding of Earth's lower mantle and the interior of terrestrial and extrasolar Super-Earth planets. Consequently in situ data of the elastic and inelastic properties of complex Earth's materials are of extraordinary importance for the interpretation of geophysical data from great depths of planets. Recent large volume presses provide sample volumes of several cubic millimeters. Ultrasonic interferometry necessarily requires in situ sample deformation measurement by X-radiography. Time-resolved X-radiography makes in situ viscosimetry and even the measurement of elastic and inelastic properties in the seismic frequency range by using the recent deformation technique achievable. This way current geophysical high pressure research is more and more bridging the gap between indoor and outdoor seismology and supplies large ranges of engineering and other material sciences with excellent toolboxes to meet their demands. The paper presents recent techniques of geophysical and general material sciences high pressure LVP in situ conditions research and their results.

Cheiron School Student Presentations / 219

Examination of High Temperature Structural Phase Transformations in Strontium Uranium Oxides Using Synchrotron X-ray Diffraction and Spectroscopy

Author(s): Mr. MURPHY, Gabriel[1]
Co-author(s): Prof. KENNEDY, Brendan [2] ; AVDEEV, Maxim [3] ; ZHANG, Zhaoming [3]

[1] *University of Sydney*

[2] *The University of Sydney*

[3] *ANSTO*

Corresponding Author(s): gmur5714@uni.sydney.edu.au

Interest in nuclear power has recently increased as many argue it will play a pivotal role in the transition away from fossil fuel energy. However, little progress has been made regarding the understanding of the fundamental solid state chemistry of UO2 fuel matrices, the interaction they have with fission daughters such as Sr-90, and the solid-phases that form during operation of reactors. This has resulted in significant challenges for nuclear waste immobilisation methods, currently there are no viable long term solutions for nuclear waste.
Our investigations have revealed SrUO4 exists in two structural types, a metastable rhombohedral (α) and a stable sensitive to oxygen vacancies orthorhombic (β) form. The structural transformation between the polymorphs is unusual and appears to be facilitated by loss of oxygen and subsequent generation of reduced forms of uranium. Once significant oxygen de-occupation has occurred the lattice is able to transform into the orthorhombic β variant but only if significant atmospheric

oxygen is available for reabsorption for it become stoichiometric. Without oxygen reabsorption the material cannot obtain thermodynamic stability, continuing as a high temperature structurally metastable rhombohedral material with extensive oxygen vacancies and unstable forms of uranium. Understanding this process has involved a combination of in situ synchrotron x-ray and neutron diffraction, as well as X-ray absorption spectroscopy under normal and reducing conditions. Uranium demonstrated surprising structural flexibility uranium in controlling oxide lattice reactivity and thermodynamic stabilisation and highlights the importance of ionic conductivity in uranium oxides.

Poster Session 1 - Board: EE-01 / **7**

Characterization of latent and etched ion tracks in apatite by small-angle X-ray scattering (SAXS)

Author(s): Mrs. NADZRI, Allina[1]
Co-author(s): SCHAURIES, Daniel [2] ; Mr. MOTA SANTIAGO, Pablo [3] ; Dr. HAWLEY, Adrian [4] ; Mr. PROFT, Max [1] ; Dr. KLUTH, Patrick [3]

[1] *Australian National University (ANU)*

[2] *ANU*

[3] *Australian National University*

[4] *Australian Synchrotron*

Corresponding Author(s): allina.nadzri@anu.edu.au

Ion tracks consist of narrow (˜10 nm), long (˜10-100 μm) cylindrical defect regions that are left behind by high-velocity heavy ions when they pass through a solids. Such tracks are used for determining the age and thermal history of geological material by studying the number and length distribution of chemically etched tracks that result from spontaneous fission of natural inclusions of uranium in the material. The etching enlarges the original damage area such that the track can be studied using optical microscopy. The present work investigates how differences in the un-etched track morphology translate into etched ion track dimensions, in particular the influence of different mineral compositions and thermal annealing. Apatite samples were irradiated with 185 MeV Au ions to simulate fission tracks. Subsequently, the samples were chemically etched and the resulting track morphology was investigated using synchrotron SAXS and scanning electron microscopy (SEM). Results indicate that the etching process is highly anisotropic, exhibiting hexagonal etch-pits that depend on the mineral composition and track orientation. The annealing kinetics of un-etched tracks in different compositions and orientations of apatite were also investigated using SAXS. The results show a dependence on the orientation of the tracks in the crystal; tracks perpendicular to the apatite c-axis recover faster compared to tracks parallel to the c-axis. These results provide important input to develop an understanding of the correlation of etched and un-etched fission tracks and the use of SAXS as a tool for studying etched tracks.

Poster Session 1 - Board: SS-03 / **76**

Mechanical Rubbing Changes the Molecular Packing and Orientation of a Conjugated Semiconducting Polymer

Author(s): Mr. NAHID, Masrur Morshed[1]
Co-author(s): GANN, Eliot [2] ; MCNEILL, Chris [1]

[1] *Monash University*

[2] *Australian Synchrotron*

Corresponding Author(s): masrur.morshed.nahid@monash.edu

In making organic electronics a reality, donor-acceptor based conjugated semiconducting polymers are playing pivotal role. However, the molecular packing, crystallinity and the disorder of the polymer matrix in the thin-films typically result in low charge transport mobilities. To this end, mechanical rubbing with velvet cloths is used to mediate the chain assembly and directional

alignment of the polymer, poly[4-(4,4-dihexadecyl-4H-cyclopenta[1,2-b:5,4-b']-dithiophen-2-yl)-[1,2,5]-thiadiazolo-[3,4-c]-pyridine], (**PCDTPT**). Intrinsic mobility and the charge transport properties of the PCDTPT thin-films are characterized by Organic Field Effect Transistors (**OFETs**), molecular packing and relative crystallinity are probed by the Grazing Incidence Wide-Angle X-ray Scattering (**GIWAXS**) and the surface molecular orientations are probed by the Near Edge X-ray Absorption Fine Structure (**NEXAFS**) spectroscopy. Top-Gated OFET mobility of the spin-coated films is found very high, ˜ 2.8 ± 0.2 cm2/VS. GIWAXS reveals that mechanical rubbing introduces a face-on orientation of the crystallites, a stark contrast to the spin-coated films with edge-on orientation. In both the samples, the pi-pi stacking distance is 0.355 ± 0.005 nm and the alkyl-chain stacking distance is 2.50 ± 0.05 nm. Likewise, C- and N-edge NEXAFS experiments confirm that the crystallites at the top-surfaces of the rubbed-films are indeed packed in a face-on fashion, but they adapt an edge-on orientation in the spin-coated films.

Poster Session 2 - Board: IM-10 / **155**

Embryos in a synchrotron: revealing the internal structure of marsupial embryos and pouch young using synchrotron radiation

Author(s): Ms. NASRULLAH, Qamariya[1]
Co-author(s): SIU, Karen [2] ; Dr. MAKSIMENKO, Anton [2] ; Prof. RENFREE, Marilyn [3] ; Dr. EVANS, Alistair [1]

[1] *Monash University*

[2] *Australian Synchrotron*

[3] *University of Melbourne*

Corresponding Author(s): qamariya.nasrullah@monash.edu

The reconstruction, visualisation and interpretation of anatomy during the development of an embryo present significant difficulties, particularly when dealing with complex 3D structures. Historically, 3D reconstruction of embryonic structures requires alignment of histological slices, a destructive technique with inherent distortion of morphology, or the use of size-limited techniques such as optical projection tomography (OPT). The use of these techniques is highly limited or not possible when mineralised tissues are present. Here we report on the application of contrast-enhanced synchrotron X-ray microCT to investigate the development of teeth in embryos and pouch young of the tammar wallaby *Macropus eugenii*. Using Lugol's iodine as a contrast agent, we can identify key soft tissue and mineralised layers and structures in the developing tooth, including oral epithelium, dental lamina, enamel epithelium, dentine and enamel. We confirmed the identity of the features using comparative histological sections. Staining and X-ray imaging at high resolution enabled the reconstruction of 3D morphology for developing teeth during the entire development sequence from dental lamina and bud stage through to mineralisation and tooth eruption. We reconstructed the 3D position and orientation in the developing jaws of both tooth generations (deciduous and permanent, including vestigial tooth germs) for incisors, premolars and molars. Imaging at 34 keV, just above the K-edge of iodine, significantly improved contrast between iodine-stained tissues and surrounding material. This study demonstrates the major advantages over earlier techniques, making the most of rare specimens in embryonic or later stages of development.

Techniques I / **118**

Live cell nano-imaging free from radiation damage by using X-ray free-electron laser

Author(s): Prof. NISHINO, Yoshinori[1]
Co-author(s): Dr. KIMURA, Takashi [1] ; Dr. JOTI, Yasumasa [2] ; Prof. OSHIMA, Tairo [3] ; Dr. BESSHO, Yoshitaka [4]

[1] *Research Institute for Electronic Science, Hokkaido University*

[2] *Japan Synchrotron Radiation Research Institute*

[3] *Institute of Environmental Microbiology, Kyowa-kako Co. Ltd.*

[4] *Institute of Physics, Academia Sinica*

Corresponding Author(s): yoshinori.nishino@es.hokudai.ac.jp

Coherent diffractive imaging (CDI) is a growing technique in photon science. In CDI, sample images are numerically reconstructed from the coherent diffraction data without the need for objective lenses. CDI is thus advantageous for X-rays, for which high-magnification objective lenses are difficult to fabricate. CDI has been demonstrated to be a powerful tool in visualizing cells and organelles using synchrotron radiation. Emerging X-ray free-electron lasers (XFELs) with femtosecond pulse durations further extends the ability of CDI to achieve spatial resolution beyond the conventional radiation-damage limitation.
We performed live cell nano-imaging using a Japanese XFEL facility, SACLA. We employed pulsed coherent X-ray solution scattering (PCXSS), a form of X-ray CDI, developed by our group [1,2]. A unique feature of PCXSS is to keep solution sample under a controlled environment in micro-liquid enclosure array (MLEA) chips. We succeeded in reconstructing a live cell image from a coherent diffraction pattern recorded with a single XFEL shot [2]. The reconstructed image quantitatively revealed the internal structures, *e.g.* high-image-intensity structure indicative of dense DNA. PCXSS can also be effectively applied to nano-imaging of materials functional in solution.
References:
1 J. Pérez and Y. Nishino, Curr. Opin. Struct. Biol. 22, 670–678 (2012).
[2] T. Kimura *et al.*, Nature Commum. 5, 3052 (2014).

Collaborating with Industry - the perils and the pleasure / 183

The Elements of Industry Engagement

Prof. NOLLER, Barry[1]

[1] *The University of Queensland*

Corresponding Author(s): b.noller@uq.edu.au

Industry engagement offers alternative sources of applied research funding. Because industry and the private sector are culturally-different to both government and the tertiary sector, the challenge is to sell the need for the high investment cost of applied research to deliver the outcome needed by industry within a prescribed framework and time limit. Academic freedom is constrained in the private sector platform by issues of risk from exposure to perceived negative outcomes or liability from the public via the media. Contractual arrangements usually require a defined completion time and a lag time in the release of findings deemed to be sensitive to industry. In extreme situations public release of findings may never be allowed by industry and is a worse-case risk of undertaking this kind of research. The academic freedom of the university environment is offset by research that can be undertaken with industry problems that may allow for extensive data collections at a level of detail beyond what is generally possible with limited resources in the tertiary sector. Against a seemingly daunting task of securing funding from industry is the opportunity to engage in frontier research with industry that can involve fundamental study with sophisticated techniques such as the array of synchrotron radiation-induced spectroscopies now available at the Australian Synchrotron to give explanations at molecular levels in both biotic and abiotic media. Above all else time is required for CEOs to have sufficient trust in the research providers and confidence to approve embarking on innovative research.

Poster Session 1 - Board: SS-01 / **19**

Resolving conflicts in the understanding of molecular adsorption: benzonitrile on Si(001)

Author(s): Dr. O'DONNELL, Kane[1]
Co-author(s): Dr. WARSCHKOW, Oliver [2] ; Dr. THOMSEN, Lars [3] ; Dr. HEDGELAND, Holly [4] ; Dr. SCHOFIELD, Steven [4]

[1] *Curtin University*

[2] *University of Sydney*

[3] *Australian Synchrotron*

[4] *University College London*

Corresponding Author(s): kane.odonnell@curtin.edu.au

Near-Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy is a powerful means of determining the orientation of molecular moieties with respect to a substrate. Still, interpretation is challenging in the case of small molecules on clean semiconductor surfaces. These surfaces are highly reactive and a typical molecule can adsorb in many ways. A classic example is benzonitrile on Si(001) where scanning tunneling microscopy (STM) studies 1 disagree with NEXAFS/photoemission studies [2] despite both being complemented by density functional theory calculations.
Here we show how this confusion arises as a function of molecular coverage. We use the Soft X-ray Spectroscopy beamline at the Australian Synchrotron to study the adsorption of benzonitrile at very low coverages (STM regime) using NEXAFS and photoemission. Using density functional theory to simulate NEXAFS spectra, it can be shown that the low coverage adsorption structure is the cross-row tripod structure found using STM, whereas at higher coverages the surface is increasingly populated by the 2+2 cycloaddition structure with a free-standing phenyl ring. Unlike our previous work with acetophenone [3], it is not possible to induce the free-standing structure with mild annealing. Instead, we observe rapid molecular dissociation confirmed with STM measurements at elevated temperatures.
1 Belcher, et al, JACS 134, 15312 (2012) [2] Rangan, et al, Phys Rev B 71, 165318 (2005) [3] O'Donnell, et al, J Phys Condens Matter 27, 054002 (2015)

Poster Session 2 - Board: BS-08 / **229**

Supramolecular interactions in organoamidoplatinum(II) anticancer compound

Mrs. OJHA, Ruchika[1] ; Prof. BOND, Alan[2] ; Prof. DEACON, Glen[2] ; Prof. JUNK, Peter[3]

[1] *student*

[2] *Monash University*

[3] *James Cook University*

Corresponding Author(s): ruchika.ojha@monash.edu

The investigation of the crystal packing of organoamidoplatinum(II) [Pt(p-YC6F4)NCH2CH2NR'2(py)X] (Y = H, F, Br; R'= Et or Me; X = Cl, Br, I) anticancer compounds show supramolecular interactions in the solid state which include intermolecular H bonding and π-π interactions.
The supramolecular interactions mainly depend on the nature of the alkyl groups (methyl/ethyl) present on the amine N. The crystal packing is similar for the compounds having same alkyl groups if a small substituent (H or F) is in the para position of the polyfluoroaryl ring, but the presence of bulky substituent like Br in the para position of the polyfluoroaryl ring changes the crystal packing. Due to the difference in crystal packing, H-bonding is slightly different for –NEt2 and –NMe2 compounds.
Figure 1. X-ray crystal structure of Pt{(p-HC6F4)NCH2CH2NEt2}Cl(py)] (a) showing asymmetric unit. Hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at the 50% probability level. (b) showing H...F bonding (c) showing unit cell with H-bonding and π-π interactions between the polyfluoroaryl ring planes and between the pyridine planes.

Radiotherapy and Radiobiology / 46

Local and Abscopal Inflammatory Response to Synchrotron Radiation

Author(s): Mr. PALAZZOLO, Jason[1]

Co-author(s): Dr. SPRUNG, Carl [2] ; Prof. MARTIN, Olga [3] ; Dr. FORRESTER, Helen [2] ; Dr. IVASHKEVICH, Alesia [4] ; Dr. SMITH, Andrea [1] ; Dr. STEVENSON, Andrew [5] ; Dr. HALL, Christopher [6] ; Dr. LOBACHEVSKY, Pavel [7] ; Ms. VENTURA, Jessica [1] ; Dr. HAYNES, Nicole [8]

[1] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, VIC, Australia*

[2] *Hudson Institute, Centre for Innate Immunity and Infectious Diseases, Australia & Monash University, Department of Molecular and Translational Sciences, Clayton, VIC, Australia*

[3] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, VIC, Australia & Sir Peter MacCallum Department of Oncology, the University of Melbourne, Melbourne, VIC, Australia & Division of Radiation Oncology and Cancer Imaging, Peter MacCallum Cancer Centre, Melbourne, VIC, Australia*

[4] *Monash University, Department of Molecular and Translational Sciences, Clayton, VIC, Australia & Radiation Oncology, Canberra Hospital, Garran, ACT, Australia*

[5] *CSIRO, Clayton, VIC, Australia & Australian Synchrotron, Clayton, VIC, Australia*

[6] *Australian Synchrotron, Clayton, VIC, Australia*

[7] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, VIC, Australia & Sir Peter MacCallum Department of Oncology, the University of Melbourne, Melbourne, VIC, Australia*

[8] *Cancer Therapeutics Program, Peter MacCallum Cancer Centre, Melbourne, VIC, Australia*

Corresponding Author(s): jason.palazzolo@petermac.org

Microbeam radiation therapy (MRT) is a promising modality for administering synchrotron-generated ionizing radiation (IR). Compared to conventionally used broadbeam (BB) radiation, MRT yields improved therapeutic benefits by preserving healthy tissues whilst selectively ablating tumours. By offering beam precision and reduced radiation scattering, the Australian Synchrotron (AS) is ideal for studying non-targeted effects of radiation, such as the bystander and abscopal effect. To establish whether these non-targeted effects depend on the immune system, C57BL/6 mice were irradiated with BB or MRT at the AS. Mice were exposed to 10Gy or 40Gy peak doses in 8x8mm or 8x1mm areas. Irradiated skin and bystander skin and intestine, were collected at 24h and 96h post-irradiation and processed immunohistochemically for apoptotic events and immune response changes in situ, compared to unirradiated control mice.
Activated macrophages and dendritic cells in irradiated skin increased up to 2.1 fold and up to 1.7 fold in bystander skin. Neutrophils increased up to 0.8 fold in irradiated skin and 2 fold in bystander skin. T-lymphocytes showed no significant changes in the irradiated skin, however, increased 2 fold in bystander skin. Apoptotic cells showed no significant changes across any tissue. Intestinal tissue yielded consistent results to bystander skin. Therefore, following pulsed radiation exposure, there is an innate immune response in IR-targeted mouse skin. Whilst, within bystander tissues, there is a response from innate and adaptive immunity. Future experiments aim to study these immune modulators in immuno-compromised mice.

Collaborating with Industry - the perils and the pleasure / 202

Diving for Dollars – how to succeed in gaining government funding

Corresponding Author(s): buzz@stcaustralia.org

Australia ranks third in the world with respect to excellence in academic research, indicating that Australia is exceptionally pioneering and cutting edge. Many Australian universities rank highly globally for innovation and STEMM, there is an exciting, attainable opportunity to position universities locally, regionally, nationally and internationally as entrepreneurial ecosystem foundations. Achieving this will require focused and sustained initiatives with unique programming that adopts culture change and addressing internal drivers.
The role of the university has evolved beyond simply teaching and research, with many universities striving for strong economic development contributions delivered through entrepreneurship and commercialisation. However, institutional entrepreneurship is difficult to engineer. Successful entrepreneurial universities (whether driven ground-up or engineered top down) typically have a culture that includes a willingness to take risks, shared governance and appropriate reward systems. To ensure that Australia continues to contribute to the world's stock of knowledge we

need to create a supportive environment that nurtures and drives entrepreneurship and innovation. Australia needs to coordinate leadership that inspires and directs a shift in government policy that cuts across education, culture with accessible investment platforms to build a progressive ecosystem.

Poster Session 1 - Board: BT-25 / **196**

Construction status of hard x-ray beamline at PAL-XFEL

Author(s): Dr. PARK, Jaehyun[1]
Co-author(s): Dr. KIM, Sangsoo [2] ; Dr. NAM, Kihyun [2] ; Dr. KIM, Bongsoo [2] ; Prof. KO, In Soo [3]

[1] *Pohang Accelerator Laboratory*

[2] *PAL*

[3] *POSTECH*

Corresponding Author(s): fermi13@postech.ac.kr

Pohang Accelerator Laboratory X-ray Free Electron Laser (PAL-XFEL) is planning to finish the construction by the end of this year. The light source will provide ultra-bright (assuming 1 x 10^{12} photons/pulse at 12.4 KeV) and ultra-short (10-60 femtosecond) X-ray pulses. The HEH2 (Hard x-ray Experimental Hutch 2) is mainly focused on the serial femtosecond crystallography (SFX) for macromolecular systems and coherent diffraction imaging (CDI) for bio specimens and nano structures etc. In this poster, we describe the details of the beamline layout, optical components, focusing optics (Kirkpatrick-Baez mirror and Beryllium CRLs), liquid phase sample injector and other components that will be installed at the HEH2.

Poster Session 2 - Board: BT-08 / **81**

Performance of the PAL-designed all-in-one processor for PSIC or XBPM in Pohang Light Source-II

Author(s): Dr. PARK, Yong Jun[1]
Co-author(s): Dr. KIM, Yongsam [1] ; Mr. RYU, Chun Kil [1] ; Mr. KIM, Jung Su [1] ; Dr. YU, Chungjong [1] ; Mr. SEO, In Deuk [1] ; Mr. LEE, Chae-Soon [1]

[1] *Pohang Accelerator Laboratory*

Corresponding Author(s): pjun@postech.ac.kr

Real-time monitoring of the beam position during whole measurement at synchrotron radiation facility is extremely important, since it is essential to maintain the stability of the X-ray beam on the sample point. When a very fine collimator is used before sample, the stabilization of the beam position in front of the collimator, should result in stabilizing the incident beam. Thus, there are several kind of the beam position feedback systems with the x-ray position monitoring system near sample position.
We developed the 4-channel processor which is adaptable to PSIC(Position Sensitive Ion Chamber) or XBPM (X-ray Beam Position Monitor). This all-in-one processor includes all electric devices (high voltage supply, current amplifier, analog-to-digital converter, etc) for X-ray position measurement. And, it's available for use with rocal mode and remote mode.
The results of 2μm spatial resolution with PSIC is possible to apply as a XBPM for mostab FB (monochromator stabilizer feedback) system. Measured results and several calculated parameters (linear range, spatial resolution, positional uncertainty, etc) will be displayed. Whole data were collected and analyzed at the beamline of Photon Test Facility in PLS-II.

Plenary / **13**

Investigating extreme states of matter by x-ray absorption spectroscopy

Author(s): Dr. PASCARELLI, Sakura[1]

Co-author(s): Dr. MATHON, Olivier [1] ; Dr. KANTOR, Innokenty [1] ; Dr. TORCHIO, Raffaella [1]

[1] *European Synchrotron Radiation Facility*

Corresponding Author(s): sakura@esrf.fr

The last decades have witnessed an unprecedented surge in the study of matter and materials at extreme values of pressure, temperature, and magnetic field. The fundamental importance of this research stems from the fact that such extreme conditions can deeply modify chemical bonds and induce myriad changes in materials. Many breakthroughs have been achieved at synchrotrons worldwide, in fields ranging from Earth and planetary sciences to fundamental physics, chemistry and materials research, and even in the life sciences where questions on life and biological function under extreme conditions have been studied. The European Synchrotron Radiation Facility is approaching the end of the Phase I of its upgrade program. One of the first upgrade beamlines to become operational has been designed to provide state-of-the-art conditions to perform time resolved and extreme conditions x-ray absorption spectroscopy. The strategy exploits the micron size focal spot to reduce the interaction zone, the high flux and the fast acquisition scheme to reduce the interaction time, and ultimately to drastically reduce the energy needed to reach extreme thermodynamical states. Target experiments for the coming years include kinetic studies of chemical reactions at high pressure and temperature, and investigation of extreme states of matter that can be maintained only over very short periods of time. Preliminary data will be shown from the first attempts to probe the electronic and local structure in melts at high pressures and in laser-shocked matter.

Poster Session 2 - Board: BT-28 / **200**

Chemical Speciation Imaging at Environmentally Relevant Concentrations using X-ray Fluorescence Microscopy

Author(s): PATERSON, David[1]
Co-author(s): HOWARD, Daryl [1] ; Dr. DE JONGE, Martin [1] ; Dr. SPIERS, Kathryn [1] ; Dr. RYAN, Chris [2] ; Dr. LOMBI, Enzo [3] ; Dr. KOPITTKE, Peter [4] ; ETSCHMANN, Barbara [5]

[1] *Australian Synchrotron*

[2] *CSIRO*

[3] *University of South Australia*

[4] *The University of Queensland*

[5] *Monash University*

Corresponding Author(s): david.paterson@synchrotron.org.au

X-ray fluorescence microscopy (XFM) can be used for elemental and chemical microanalysis across length scales ranging from millimeter to nanometer. XFM is ideally suited to quantitatively map trace elements within whole plant and other biological specimens, environmental and soil samples. The elemental sensitivity of the X-ray fluorescence probe provides valuable information in a diversity of environmental sciences, and the high penetration of hard X-rays enables measurement of whole cells, tissue sections and a diverse range of environmental samples with a minimum of preparation. Rapid advances in X-ray fluorescence detection methods such as the Maia detector now enable high definition images approaching megapixel per minute rates. The ability to rapidly acquire 2D images enables 3D information such as fluorescence tomography to be obtained in realistic times. Chemical speciation (or valence) imaging (CSI) is a technique where the third dimension is spectroscopic detail. CSI results in an X-ray Absorption Near Edge Structure (XANES) spectra from the X-ray fluorescence signal at each pixel in the spatial image.
CSI has been demonstrated at the Australian Synchrotron XFM beamline with micron resolution and moderate definition (10K pixels) across a diverse range of sciences and applications from environmental chemistry to arsenic toxicity in crop production. Studies probing and optimising the efficiency and sensitivity of CSI to achieve measurements at environmentally relevant concentrations will be presented.

Poster Session 1 - Board: SB-05 / **127**

WHAT CAN YOU DO WITH A β-HELICAL STRUCTURE ?

Author(s): Dr. PAXMAN, Jason[1]
Co-author(s): Dr. LO, Alvin [2] ; Dr. PANJIKAR, Santosh [3] ; Dr. MORIEL, Danilo [2] ; Dr. GEE, Christine [3] ; Prof. SCHEMBRI [2] ; Dr. HERAS, Begoña [1]

[1] *Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, VIC*

[2] *Australian Infectious Diseases Research Centre, School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane QLD*

[3] *Macromolecular Crystallography, Australian Synchrotron, Clayton, VIC*

Corresponding Author(s): j.paxman@latrobe.edu.au

Autotransporter (AT) proteins are important virulence factors and constitute the largest family of secreted and outer membrane proteins in Gram-negative bacteria. Despite their importance in bacterial pathogenesis there are only 12 structures of AT α-domains in the PDB and their mechanisms of action are poorly understood. Most structurally determined AT α-domains were found to be built upon right-handed β-helical structures. Our crystal structure of Antigen 43a from uropathogenic Escherichia coli (UPEC) showed that two self-associating interfaces along with bending of the β-helical structure were critical for dimerization, which in turn promotes UPEC aggregation and biofilm formation. Using the MX beamlines at the Australian Synchrotron along with some assistance from an Australian Synchrotron fellowship we have determined the structures of two new AT α-domains; UpaB and TibA from UPEC and enterotoxigenic E. coli (ETEC) respectively. These new structures demonstrate the large plasticity in their β-helical scaffolds that along with further modifications, allow these proteins with the same basic architecture to promote different functions in pathogenesis. The UpaB structure revealed unique extensions of the β-strands at the centre of the β-helix that gives rise to a 'belly' domain. In contrast, TibA forms a long narrow twisted β-helix that allows for extensive interactions to occur between neighbouring monomers. Unusually TibA is also glycosylated by an associated glycosyltransferase TibC. I will discuss how these different structures and modifications facilitate interactions with their newly identified protein binding targets and how this affects their role in bacterial pathogenesis.

Poster Session 1 - Board: RR-01 / **27**

Development of an image guidance protocol for MRT at IMBL

Author(s): Dr. PELLICCIA, Daniele[1]
Co-author(s): Dr. LIVINGSTONE, Jayde [2] ; Dr. POOLE, Christopher [3] ; HAUSERMANN, Daniel ; CROSBIE, Jeff [3]

[1] *RMIT University*

[2] *Australian Synchrotron*

[3] *University of Melbourne*

Corresponding Author(s): daniele.pelliccia@rmit.edu.au

Synchrotron microbeam radiation therapy (MRT) is a novel, preclinical form of radiotherapy that shows promise of providing a major advance in cancer control if successfully translated to clinical practice. To generate MRT, the synchrotron beam is segmented by a collimator into a lattice of microbeams, usually 25-50 μm wide. The beams have minimal divergence and are spaced at regular intervals of 200-400 μm. Typical radiation doses are 300-1000 Gy in the peaks, and 5-20 Gy in the valleys. This dose is delivered in milliseconds. We describe the developments in image guidance for the MRT station for preclinical small animal trials at the Imaging and Medical Beamline (IMBL). Image guidance is required to guarantee precise control of the radiation field to accurately deliver the prescribed dose to the target and not to surrounding structures. A valid protocol must be able to generate live images of the patient and register these with existing treatment plan. The double Laue monochromator at IMBL allows for a 20 mm displacement between the monochromatic beam and the pink beam. Either beam can be selected by moving a slit. In-vacuo filtering is chosen to select the treatment beam with mean energy of 95 keV. The monochromator is aligned to select an imaging energy of 50 keV. After imaging the sample and the relevant beam line components are translated into the treatment beam without changing the

beam filtration or the monochromator settings. Experimental results of such an image guidance procedure will be presented.

Poster Session 1 - Board: AM-19 / **154**

Heteroleptic Iron(III) {Quinolylsalicylaldimine/Thiosemicarbazone-salicylaldimine} Complexes: Spin crossover, intermolecular structural and solvation features, magnetism and Mössbauer spectra

Author(s): Dr. PHONSRI, Wasinee[1]
Co-author(s): Prof. MURRAY, Keith [1] ; Dr. MOUBARAKI, Boujemaa [1] ; Prof. JAMESON, Guy [2]

[1] *Monash University*

[2] *University of Otago*

Corresponding Author(s): wasinee.phonsri@monash.edu

The relationship between intermolecular interactions and spin-crossover features such as the abruptness of the spin transition and cooperativity, in crystalline complexes of iron(II) and iron(III), is of much current interest.1 We were particularly interested to make heteroleptic complexes of Hqsal and H2thsa ligands (where Hqsal = quinolylsalicylaldimine2 and H2thsa = thiosemicarbazone-salicylaldiminate3) for the first time, to explore the intermolecular interactions when two different ligands are present around each Fe(III) centre. A family of neutral, heteroleptic iron(III) complexes, [Fe(qsal)(thsa)]•solvent, is presented where solvent is 0.4BuOH, 0.5MeCN, 0.5THF, as well as two polymorphs of solvent free compounds i.e.[Fe(qsal)(thsa)]. We describe a fascinating array of intermolecular interactions occurring in the various crystals, all containing two distinct Fe sites, including similarities and differences and the importance of a void in the lattice structure wherein solvate molecules sit (or do not sit, in [Fe(qsal)(thsa)] polymorphs), and how these all relate to differences in spin states of neighbouring [Fe(qsal)(thsa)] molecules i.e. HS-HS and spin crossover HS-HS to HS-LS. Supporting information and insights are provided by TGA, PXRD and Mössbauer spectral data.

Beamline updates / **106**

LASER PHOTOLYSIS ON THE THZ BEAMLINE AT THE AUSTRALIAN SYNCHROTRON

Author(s): PLATHE, Ruth[1]
Co-author(s): Dr. APPADOO, Dominique [2]

[1] *Australian Synchrotron*

[2] *The Australian Synchrotron*

Corresponding Author(s): ruth.plathe@synchrotron.org.au

Laser photolysis is a new capability that is presently being added to the THz/Far-IR beamline. This technique will allow our users to perform pioneering spectroscopic studies at ultra-high spectral resolution on gaseous molecules of astrophysical interest; it will also enable our users to study photochemical changes in condensed-phase, solid and biological systems after or during laser irradiation.1[2]
The addition of lasers will also allow a host of sunlight driven reactions to be studied, providing a source of radicals such as OH or halogens.[3]
We currently have to two lasers: A 40 W cw CO2 laser from Monash University, operating at 10.6 μm, and, a 10 Hz pulsed 480 mJ Nd:Yag Surelite Continuum laser from La Trobe University, operating at 1064, 532, 355 and 266 nm A photolysis gas cell is also available for use. It is suitable for creating steady-state chemical populations with the laser, which can then be probed by the Synchrotron source. We are the only THz beamline with these capabilities.
REFERENCES 1 J Nishii et al, “Photochemical reactions in GeO2-SiO2 glasses induced by ultraviolet irradiation: Comparision between Hg lamp and excimer laser” Physical Review B 52.3 (1995): 1661. [2] Kaiser, Ralf I., et al. “Untangling the chemical evolution of Titan’s atmosphere

and surface–from homogeneous to heterogeneous chemistry." Faraday discussions 147 (2010): 429-478. [3] W.J.R. French, "Hydroxyl Airglow Temperatures above Davis Station, Antarctica", University of Tasmania, Australian Antarctic Division (2002)

Poster Session 1 - Board: EM-09 / **126**

Formation of CeO2 in CeTiO2 catalyst studied by the in situ XANES

Dr. POO-ARPORN, Yingyot[1]

[1] *Synchrotron Light Research Institute*

Corresponding Author(s): yingyot@slri.or.th

Cerium-doped titanium dioxide was prepared by a sol-gel method using Titanium(IV)-isopropoxide and Ce(NO3)3•6H2O as the Ti and Ce precursors. X-ray absorption near edge structure (XANES) measurement was performed on the time-resolved XAS (Bonn-SUT-SLRI) beamline at Synchrotron Light Research Institute, Thailand. The beamline employs an energy dispersive monochromator and the position sensitive detector to record an XANES spectrum. For as prepared Ce/TiO2, XANES spectra show mainly the characteristic peaks due to the Ce3+. To monitor transition mechanism between Ce3+ and Ce4+ in Ce/TiO2, the in situ XANES measurements were performed. Ce L3-edge XANES spectra were recorded in 5 K intervals from 573 K to 823 K. Each spectrum was recorded at 250 ms with the averaging of 10 scans. At temperature lower than 763, there was no significant changes of whiteline peak. Two peaks corresponding to the CeO2 were clearly observed at 808 K. Although the calcinations temperature was increased to 823 K, there was no significant change in Ce L3-edge XANES spectra. This result indicated the sufficient temperature for CeO2 formation.

Radiotherapy and Radiobiology / **115**

The Eclipse^{TM} treatment planning system for microbeam radiotherapy trials at the Australian Synchrotron

Author(s): Dr. POOLE, Christopher[1]
Co-author(s): Prof. ROGERS, Peter [2] ; Prof. CROSBIE, Jeffrey [1]

[1] *School of Applied Sciences, RMIT University, Melbourne, VIC 3001, Australia*

[2] *University of Melbourne Department of O&G, and Royal Women's Hospital, Parkville, VIC 3052, Australia*

Corresponding Author(s): christopher.poole@rmit.edu.au

Before clinical trials of synchrotron microbeam radiotherapy (MRT) on humans can occur, a computerised treatment planning system (TPS) to calculate the dose distribution in the patient must be developed and validated. To satisfy this requirement, we use a research licenced version of the Eclipse^{TM} TPS from Varian Medical Systems. This research license allows for customised dose calculation algorithms to be integrated with the clinical work-flows in Eclipse^{TM} that are typical to modern radiotherapy.

Our treatment planning system is designed for the dynamic MRT modality that has been developed for the Imaging and Medical Beamline. It uses a pencil beam convolution algorithm for dose calculation, and allows for the design of customised conformal masks. For the treatment itself, the white beam is collimated to a 30 mm wide and 1 mm high field which illuminates the MRT collimator, which in turn produces 50 um wide vertical microbeams separated at 400 um center-to-center. The sample and a mask is then dynamically swept through this array of microbeams, producing a dose of radiation in the sample that is conformal to the mask aperture. Dose calculation considers the sample geometry derived from conventional CT data, custom bolus structures, conformal masks, and multiple fields. Beam configurations and sample stage motions are limited so as to reflect the actual limits on the beamline. We have compared the output from the MRT TPS to measurements on the beamline, and documented our experiences in using it for planning the delivery of known doses to samples.

Beamline updates / 150

Chemical Crystallography at the Australian Synchrotron MX Beamlines

Author(s): Dr. PRICE, Jason[1]
Co-author(s): CARADOC-DAVIES, Tom [2] ; Dr. HARROP, Stephen [1] ; Dr. ARAGAO, David [1] ; Dr. RIBOLDI-TUNNICLIFFE, Alan [1] ; ERIKSSON, Daniel [1] ; Dr. PANJIKAR, Santosh [1] ; Dr. WILLIAMSON, Rachel [1]

[1] *Australian Synchrotron*

[2] *Australian Synchrotron.*

Corresponding Author(s): jason.price@synchrotron.org.au

The single crystal diffraction beamlines, Macromolecular Crystallography 1 and 2 (MX1 and MX2) serve a wide range of experimental conditions and sample types. While the bulk of the beamtime is allocated to the structural biology community there is a very active and successful chemical crystallography community that gains substantial befit from the use of synchrotron radiation. I will highlight some of the fine work that has been carried out by this field as well as exploring beamline development projects that are of significance to this community. In particular the successful deployment of the mini-kappa goniometer on MX1 allowing convenient full sphere collections of low symmetry structures, and feedback on the testing of the Dectris, Eiger detector that was tested on MX2.

Biological Systems / 169

Amyloid Fibril Morphology: Relevance to Disease and Materials Science

Author(s): Dr. REYNOLDS, Nicholas[1]
Co-author(s): Dr. LARA, Cecile [2] ; Dr. BERRYMAN, Joshua [3] ; Prof. ZHANG, Afang [4] ; Prof. MEZZENGA, Raffaele [2]

[1] *Swinburne University of Technology*

[2] *ETH Zurich*

[3] *The University of Luxembourg*

[4] *Shanghai University*

Corresponding Author(s): nreynolds@swin.edu.au

Amyloid fibrils are implicated in over 20 neurodegenerative diseases. The mechanisms of fibril structuring and formation are not only of medical and biological importance but are also relevant for material science and nanotechnologies due to the unique structural and physical properties of amyloids. We found that hen egg white lysozyme (HEWL), homologous to the disease-related human lysozyme, can form left-handed giant amyloid ribbons, closing into nanotubes. To obtain an improved understanding of the molecular processes that underpin fibril assembly we identified an amyloidogenic peptide from HEWL and with a combination of nanoscale analytical techniques we were able to follow its assembly. These results will improve our understanding of structure-function relationships of amyloids in relation to neurodegenerative disease and materials science.
Using matrix-assisted laser desorption ionization mass spectrometry analysis, we identified a peptide sequence, which drives amyloid formation in HEWL, namely the ILQINS hexapeptide. By combining atomic force microscopy, circular dichroism and synchrotron based small angle X-ray scattering, we found that this fragment, also forms amyloid fibril structures, with rapid assembly kinetics. Additionally, all fibrillar structures formed possessed an unexpected right-handed twist, a rare chirality within the corpus of amyloid experimental observations. We confirm by wide-angle X-ray scattering and molecular dynamics simulations that these fibrils are composed of conventional left-handed β-sheets, but that packing stresses between adjacent sheets created this unusual chirality. We also show that the right-handed fibrils represent a metastable state present before the formation of β-sheet-based microcrystals.

Poster Session 2 - Board: IM-14 / **178**

Synchrotron scanning fundamentally changing how dinosaurs and other vertebrates can be both studied and "excavated" from embedding rock.

Author(s): Dr. RICH, Tom[1]
Co-author(s): Dr. SIU, Karen [2] ; Dr. MAKSIMENKO, Anton [2] ; Dr. KUNDRAT, Martin [3] ; Dr. ACRES, Robert [2] ; Dr. EVANS, Alistair [4]

[1] *Museum Victoria*

[2] *Australian Synchrotron*

[3] *University of Uppsala, Sweden*

[4] *Monash University*

Corresponding Author(s): trich@museum.vic.gov.au

Scanning of the small dinosaur Leaellynasaura amicagraphica at the Australian Synchrotron is making possible the eventual reconstruction of its entire skeleton. Embedded in extremely hard rock, its bones are simply too fragile to ever physically extract from rock. However, by making a 3D rapid prototype print of the scanned bones, it will be possible to reconstruct a skeletal mount for study and display. Currently disarticulated, it will be possible to reconstruct the skull by manipulation of 3D rapid prototypes of the various preserved components.
Microscanning of tiny teeth of mammals contemporaneous with Leaellynsaura and other South Polar dinosaurs dinosaurs has permitted production of 3D rapid prototype prints X10 natural size, facilitating both their study and exhibition. Particularly critical, such scans have also made possible precise measuring of fossils still partially embedded in the rock.
The same scan data have been used for non-destructive histological investigations of the internal structure of mammalian teeth - specimens so rare that such investigation was previously impossible.
From the perspective of a vertebrate palaeontologist, the technological advance most sought is the advancement of methods to automatically differentiate between fossils and rock automatically. At present, manual processing of literally thousands of slices is often required simply because the density contrast between fossils and the surrounding rock is not great enough with current techniques to automate this critical step. The 3D prints currently produced in this laborious way provide a unique understanding of the morphology, not possible using any other known technique.

Poster Session 1 - Board: SB-01 / **61**

Structura Insights into the pro-apoptotic protein Bax

Author(s): Dr. ROBIN, Adeline[1]
Co-author(s): Dr. CZABOTAR, Peter [1] ; Prof. COLMAN, Peter [1]

[1] *WEHI*

Corresponding Author(s): robin@wehi.edu.au

Programmed cell death, AKA apoptosis, is a biological mechanism by which dangerous cells, such as cancer cells, are killed. Commitment to this process is governed by the Bcl-2 family of proteins, which respond to cellular stresses. The proteins within this family share 1 to 4 Bcl-2 Homology domains (BH1 to BH4) and can be divided in three sub-categories according to their function. One subgroup, the BH3-only proteins, is upregulated upon cellular stresses and initiate apoptosis through interactions with other Bcl-2 family members. Another subgroup, the pro-apoptotic Bax or Bak proteins, are the effectors of apoptosis: upon activation these proteins oligomerize at the mitochondrial outer membrane and provoke its permeabilization. The resulting release of cytochrome c and other pro-apoptotic proteins leads to cell death.
The BH3-only proteins Bim and Bid can directly activate Bax or Bak. Recently the structure of the BidBH3 in complex with the hydrophobic groove of Bax enlightened how BH3-only proteins activate the Bax protein. [Czabotar, Westphal et al., Cell, 2013, 152, 519-531.] We have now crystallized new forms of Bax: 1- Novel structures of full length monomeric Bax and P168G

mutant of Bax show the hydrophobic groove of Bax occupied by the trans-membrane helix 9 of Bax. 2- BimBH3:Bax complexes structures help us to understand the specifics of the BimBH3 peptide binding to the hydrophobic groove of Bax.
These new structures reveal further insights into key interactions that initiate Bax activation.

Poster Session 1 - Board: EE-03 / **32**

From molecules to minerals: Resolving fast mineral formation processes in aquatic systems using energy dispersive XAS

Author(s): ROSE, Andrew[1]
Co-author(s): AVARO, Jonathan [2]

[1] *Southern Cross University*

[2] *Southern Cross Geoscience, Southern Cross University*

Corresponding Author(s): andrew.rose@scu.edu.au

While the formation and transformation of many minerals has been relatively well studied empirically at a macromolecular scale, the precise mechanisms by which minerals form and transform at the molecular level remain poorly described. Time-resolved X-ray absorption spectroscopy (XAS) allows observation of changes in the local coordination environment of molecules involved in the very early stages of mineral formation in aquatic systems, and thus has the potential to provide detailed information on the mechanisms involved. We attempted to use energy dispersive XAS at the ODE beamline of the Synchrotron SOLEIL to study the formation of strontium carbonate and iron oxyhydroxide minerals. Employing a Quantum ULTRA detector and a Biologic XFM stopped-flow device permitted time resolution as short as 50 μs, thereby offering the possibility to observe the very first steps in the mineral formation process. Despite numerous technical difficulties, we were able to collect high quality XAS data (including EXAFS) at very short timescales for both mineral systems. While the technical issues meant that the data collected were not able to provide unequivocal evidence for particular mechanisms, our results provide several new insights into the processes that govern mineral formation in aquatic systems and confirm the potential for this technique to be used on such systems in future.

Techniques II / 21

Technique for the Identification of Phases and Phase Transformations in In Situ Diffraction Data

Author(s): Dr. ROWLES, Matthew[1]
Co-author(s): Dr. SHEPPARD, Drew [1] ; Dr. HUMPHRIES, Terry [1] ; Prof. BUCKLEY, Craig [1]

[1] *Curtin University*

Corresponding Author(s): matthew.rowles@curtin.edu.au

In situ X-ray diffraction is a common technique for observing and determining structural transitions in crystalline materials with changes in temperature, pH, pressure, or some other driving force. In the analysis of metal hydride systems, there can be structural transitions composed of multiple phases forming and decomposing simultaneously. These patterns are often overshadowed by high intensity peaks, leaving the subtle phase transitions undetected by conventional automated techniques. We are developing an automated method based on wavelet peak identification and diffraction pattern derivatives to separate and identify these subtle phase transitions. The method will include peak-to-phase assignment and possibly indexing.

Poster Session 2 - Board: SB-10 / **168**

A Comparison of the Measurement of Protein Solutions on a MetalJet Equipped Laboratory SAXS Instrument and a Synchrotron Beamline

Author(s): Dr. JARRETT, Kevin[1]
Co-author(s): Prof. BUCKLEY, Craig [1] ; Prof. BOND, Charlie [2] ; Mr. KNOTT, Gavin [2] ; LYNGSO, J [3] ; PEDERSON, J. S. [3]

[1] *Curtin University*

[2] *University of Western Australia*

[3] *Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, University of Aarhus, DK-8000 Aarhus, Denmark*

Corresponding Author(s): matthew.rowles@curtin.edu.au

SFPQ is a protein that suppresses tumours in humans. Two samples were prepared from the same batch and frozen until just prior to measurement. Traditionally the investigation of protein solutions has been limited to synchrotron facilities, though more recently instruments making use of microfocus rotating anodes have allowed more measurements to be made in the laboratory. One sample was measured on a Bruker AXS Nanostar using the MetalJet X-Ray source from Excillum, the latest generation of x-ray generators for laboratories. The MetalJet X-Ray source makes use of a pressurised liquid metal anode capable of withstanding a high power electron beam and the resulting x-ray beam is much brighter than conventional sources. The SAXS instrument was further equipped with long Montel multiæayer mirrors and home-built "scatterless" slits. While rotating anode sources often require at least 30 minutes of collection time for scattering curves from weakly scattering biomolecular solutions the MetalJet data presented here were collected in 1 minute. While this is still significantly longer than what is required at synchrotron facilities it represents a major improvement on current generation laboratory instruments. The new SAXS facilities in Western Australia will provide the user community with access to a larger range of experiments and also help in generating preliminary data for experiments that specifically require synchrotron access.

Imaging I / 41

Tomography at the Australian Synchrotron XFM beamline

Author(s): Dr. RUBEN, Gary[1]
Co-author(s): Dr. DE JONGE, Martin [2] ; MAYO, Sherry [3] ; Dr. RYAN, Chris [3]

[1] *CSIRO, Australian Synchrotron*

[2] *Australian Synchrotron*

[3] *CSIRO*

Corresponding Author(s): gary.ruben@csiro.au

The X-ray Fluorescence Microscopy (XFM) beamline at the Australian Synchrotron is host to the Maia x-ray fluorescence detector, developed by CSIRO and BNL 1. The Maia's large collection area and optimised photon event processing combine to achieve high sensitivity and photon count rates, enabling rapid, microscale mapping of trace metals in a variety of specimen types from biological to mineralogical [2].
High pixel rates can be used to measure large specimens at high definition or to exploit extra information using multi-scan techniques such as X-ray Fluorescence Computed Tomography (XFCT), resulting in elemental maps of 2d slices and / or 3d volumes. Recent upgrades to the Maia detector and scanning stages have led to dramatic improvement of beamline capability. Here we report on recent upgrades to the beamline, and outline a workflow that will enable rapid processing of elemental-specific tomographic data. We describe some of the benefits and disadvantages of measuring hydrated vs freeze-dried specimens.
A persistent desire to map low-Z elements (e.g., P & S, but also K & Ca) in larger specimens leads to the issue of self absorption [3]. We discuss local progress towards developing self-absorption corrections and their inclusion in the anticipated data pipeline.
1 R Kirkham et al. AIP Conf. Proc. 1234, 240 (2010) [2] CG Ryan et al., J. Phys.: Conf. Ser. 499, 012002 (2014) [3] MD de Jonge, S Vogt, Curr. Op. in Struct. Biol. 20/5, 606 (2010)

Advanced Materials I / 193

Unraveling how electronic and spin structures control macroscopic properties of manganite ultra-thin films

Dr. RUSYDI, Andrivo[1]

[1] *National University of Singapore*

Corresponding Author(s): phyandri@nus.edu.sg

Perovskite manganites exhibit fascinating transport and magnetic properties. With the development of thin film technologies, more exotic properties have been observed in doped-manganites over a wide range of temperatures. Unraveling the interplay of spin, charge and orbital degrees of freedom that drives exotic, macroscopic properties is therefore crucial for the understanding of strongly correlated electron systems. Using a combination of transport, spectroscopic ellipsometry, X-ray absorption spectroscopy and X-ray magnetic circular dichroism, we observe two concomitant electronic and magnetic phases (insulating paramagnetic phase for T˜195 K and insulating cantedferromagnetic for T˜140 K) with an intermediate metal-like state in ultra-thin La0.7Sr0.3MnO3 (LSMO) film on DyScO3 substrate. Surprisingly, the O2p-Mn3d hybridization strength reduces with decreasing temperature, driving the system more insulating and ferromagnetic. The Jahn–Teller effect weakens markedly within the intermediate temperature range, making the system more metal-like. We also apply this comprehensive method to a LSMO film on SrTiO3 substrate. We find strong electron-electron and electron-hole interactions manifested in Wannier-like exciton and high-energy resonant excitons in SrTiO3 strongly influences physical properties. I will introduce fascinating phenomena of high-energy optical conductivity in correlated electron system, using the case of LaAlO3SrTiO3 heterostructure in which different mechanisms for the polarization divergence compensation in insulating and conducting interfaces are found.

Poster Session 2 - Board: BT-34 / **216**

Co-Flow: A sheath flow sample environment for biological solution X-ray scattering at the Australian Synchrotron.

Author(s): Dr. RYAN, Tim[1]
Co-author(s): Dr. HAWLEY, Adrian [1] ; Dr. COWIESON, Nathan [1] ; Dr. MUDIE, Stephen [1] ; Dr. KIRBY, Nigel [1]

[1] *Australian Synchrotron*

Corresponding Author(s): tim.ryan@synchrotron.org.au

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 there are currently significant limitations, particularly in regards to the susceptibility of biomolecules to radiation damage and sample consumption that limit the utility of the technique to the wider protein community. We believe that this degree of radiation damage is in part due to the fluidics of the flow in the capillary, which causes a very slow moving boundary of material that is highly susceptible to beam damage near the edges of the capillary. We have sought to remove this factor from the measurement of the protein samples by adopting a sheath flow sample environment, termed Co-Flow. In this approach, the protein sample is introduced into the centre of a sheath fluid, which acts as a barrier between the sample and the capillary wall, abrogating the slow moving fluid boundary. In practice, this approach allows sensitive protein solutions to be exposed to at least 10 fold greater flux. Further the biomolecule samples do not come into contact with the capillary at all, and hence do not stick. These advantages enhance the use of SAXS at the australian synchrtron particularly for susceptible protein samples.

Poster Session 1 - Board: BT-01 / **24**

VIRTUALISATION OF BEAMLINE CONTROL SYSTEMS

Author(s): SAMARDZIC-BOBAN, Vesna[1]
Co-author(s): MUDIE, Stephen [1] ; KIRBY, Nigel [1] ; FELZMANN, Uli [1] ; HOBBS, Nicholas [1]

[1] *Australian Synchrotron*

Corresponding Author(s): vesna.samardzic-boban@synchrotron.org.au, stephen.mudie@synchrotron.org.au, nigel.kirby@synchrotron.org.au

Virtualisation technologies have been introduced to control systems at the Australian Synchrotron (AS) and results of recent virtualisation on a couple of beamlines are presented here. Reasoning and motivation for having beamline Virtual IOCs (Input Output Controller's) are: replacement of aging computers with physical ones is becoming expensive, desire for reduction of computing infrastructure complexity, invest and build on new technologies that are scalable/ upgradable (currently VMware vSphere architecture/stack has four virtual machine hosts), need to reduce maintenance and replacement effort, increase reliability and reduce beamline down time. Good progress and positive results using virtualisation technologies for beamline control systems has been experienced. No issues with deployed Virtual IOCs were found so far. In the future we recommend to virtualise all soft IOCs across the beamlines wherever performance allows. Small and Wide Angle X-ray Scattering (SAXS/WAXS) beamline has almost all of the control systems virtualised. Both Photon Delivery System (PDS) and End Station soft IOCs have been virtualised. Only three IOCs – Data Acquisition IOC (running on VxWorks Operating System) and two Pilatus detector controllers (SUSE linux). They will remain running on these due to tight Real Time (RT) requirements. Infra Red (IR) Microscope and Far IR beamline control systems have also been virtualised.

Poster Session 1 - Board: IM-09 / **138**

Synchrotron X-ray Tomographic characterisation of titanium parts fabricated by additive manufacturing

Author(s): Ms. SCARLETT, Nicola[1]
Co-author(s): MAYO, Sherry [1] ; Mr. TYSON, Peter [1] ; Mr. FRASER, Darren [1]

[1] *CSIRO*

Corresponding Author(s): nicola.scarlett@csiro.au

Additive manufacturing technologies are applicable to a wide range of materials (polymers, ceramics, metals) and provide unprecedented design freedom and rapid prototyping opportunities. Synchrotron X-ray tomography (SXRT) has been applied to the study of titanium parts fabricated by additive manufacturing (AM). The AM method employed here was the Arcam EBM® (electron beam melting) process which uses powdered titanium alloy, Ti64 (Ti alloy with approximately 6%Al and 6%V) as the feed and an electron beam for the sintering/welding. The experiment was conducted on the Imaging and Medical Beamline (IMBL) of the Australian Synchrotron. The samples considered here represent a selection of simple and complex shapes with a variety of internal morphologies. They were chosen to investigate (i) the effect of build direction and complexity of design on the surface morphology and final dimensions of the pieces and (ii) the location and nature of any defects within the pieces. Such information combined with detailed knowledge of the process conditions can contribute to understanding the interplay between design and manufacturing strategy. This fundamental knowledge may subsequently be incorporated into process modelling, prediction of properties and the development of robust build protocols for the production of defect free parts.

Surface Science / 70

Formation and characterisation of a silicon terminated (100) diamond surface

Author(s): Mr. SCHENK, Alex[1]
Co-author(s): Mr. SEAR, Michael [1] ; Dr. TADICH, Anton [2] ; Dr. STACEY, Alastair [3] ; Dr. PAKES, Chris [1]

[1] *La Trobe University*

[2] *Australian Synchrotron*

[3] *Univeristy of Melbourne*

Corresponding Author(s): a.schenk@latrobe.edu.au

Over the past decade, the interest in diamond materials science, in particular diamond surface science, has grown dramatically. The interest in the surface comes about due to the wide range of properties which the surface can exhibit upon a simple change in the terminating species. The functionalised surfaces of diamond, in particular the oxygen and hydrogen terminations, have provided a route to the realisation of a number of device applications for high power, high frequency components and for biosensing.
A newly emerging generation of diamond device architectures incorporate nitrogen vacancy (NV) centers, which in bulk diamond show properties which are of interest for nano-magnetometry, quantum information processing and as biological tracers. However, the development of future devices permitting the detection of single electron spin requires that a NV center be placed within nanometers of the surface. This environment has undesirable effects on the paramagnetic NV- state, as existing surface terminations either quench the fluorescence of the NV center by interfering with the NV- state, or produce randomly oriented surface spins which limit the sensitivity of the NV—state. There is therefore a need for an alternative surface termination which will address these limitations. Presented here are the results of a series of synchrotron experiments in which a novel silicon terminated (100) diamond surface has been developed, which has some potential as a suitable termination for shallow NV center applications.

Poster Session 2 - Board: BT-36 / **230**

The Laboratories at the Australian Synchrotron - Information for Users

Mrs. SCOTT, Clare[1]

[1] *Australian Synchrotron*

Corresponding Author(s): clare.scott@synchrotron.org.au

Many users of the Australian Synchrotron will have samples requiring final preparation at the synchrotron prior to or during their beam-time. At the synchrotron there are several laboratories available to users in which to undertake this work. The labs are stocked with basic chemical and consumable supplies as well as general laboratory equipment such as balances, ovens, fridges and freezers. Fume cupboards for working with hazardous substances and bio-safety cabinets for working with bio-hazardous material are available in some of the labs and a glove-box for working with oxygen sensitive materials is also available.
Access to the laboratories is dependent on approval by the beam line scientist reviewing the user's Experimental Authorisation, followed by attendance at an induction session for the appropriate lab. The induction sessions are held daily and further information regarding inductions or items available in the laboratories can be obtained by contacting the Laboratory Coordinator.

Poster Session 2 - Board: AM-18 / **153**

Spin Crossover in Iron(II) Imidazolylmethylene-aryl amine Complexes: Tuning by the substituent group on the ligand

Author(s): Ms. SERTPHON, Darunee[1]
Co-author(s): Dr. JAMES HARDING, David [2] ; Dr. HARDING, Phimphaka [2] ; Prof. MURRAY, Keith S. [1] ; Dr. MOUBARAKI, Boujemaa [1] ; Dr. NEVILLE, Suzanne M. [3] ; Dr. LIU, Lujia [4] ; Dr. TELFER, Shane G. [4]

[1] *School of Chemistry, Monash University, Clayton, Melbourne, Victoria, 3800, Australia*

[2] *Molecular Technology Research Unit Cell, Walailak University, Thasala, Nakhon Si Thammarat, 80161, Thailand*

[3] *School of Chemistry, The University of Sydney, Sydney, 2006 Australia*

[4] *MacDiarmid Institute for Advanced Materials and Nanotechnology, Institute of Fundamental Sciences, Massey University, Palmerston North, New Zealand*

Corresponding Author(s): sdarunee3@gmail.com

The new ligands imidazol-4-ylmethylene-aryl amine (4-imaAr; Ar = Bp, Fl) have been prepared by reaction of the aryl amine with imidazole-4-carboxaldehyde.[1,2] Reaction of the ligands with [Fe(H2O)6][ClO4]2 in MeOH or EtOH yields the complexes, [Fe(4-imaBp)3][ClO4]2·EtOH 1, [Fe(4-imaBp)3][ClO4]2·2MeOH 2, [Fe(4-imaFl)3][ClO4]2 3, and [Fe(4-imaFl)3][ClO4]2·3H2O 4. X-ray crystallographic studies reveal strong C-H···π and hydrogen bonding interactions or π-π interactions leading to high cooperativity. SQUID magnetic susceptibility studies show that spin crossover varies from gradual to abrupt with the spin transition occurring at temperatures from ca. 150 to 400 K. The substituent groups on the 4-ima ligand significantly impact the spin crossover characteristics.

Poster Session 1 - Board: RR-05 / **167**

Effects of monochromatic synchrotron X-rays irradiation on functionalised gold nanoparticles treated prostate cancer cells

Author(s): Mr. SHUKLA, Ravi[1]
Co-author(s): Mr. TELUKUTLA, Srinivasa Reddy [2] ; CROSBIE, Jeff [3] ; Dr. HALL, Chris [4]

[1] *School of Applied Sciences, RMIT University*

[2] *RMIT University*

[3] *University of Melbourne*

[4] *Australian Synchrotron*

Corresponding Author(s): ravi.shukla@rmit.edu.au

The concept of using gold nanoparticles for enhancement of radiation therapy appears to be promising approach for improved cancer treatment. As gold is an excellent absorber of X-rays, the cells loaded with gold nanoparticles receive higher dose when compared to the untreated cells. This improved radio sensitization effect allows enhanced radiation induced cell death and minimises the dose of radiation treatment there by reducing adverse side effects of cancer. Recently, we have shown that epigallocatechin-gallate (EGCg) functionalized gold nanoparticles, selectively bind with excellent affinity to Laminin67R receptors, which are over expressed in prostate cancer cells thus allowing the targeted delivery of nanoparticles to the cancer cells. In this study, we propose to investigate the radio (X-ray irradiation, 0-12 Gy) sensitizing effect of functionalised gold nano particles on prostate cancer cells (PC-3) using clonogenic survival assays. The data from the clonogenic assays will not only enhance our understanding on role of EGCG led targeted mechanism in gold nanoparticles and monochromatic X-ray mediated cancer cell death. But it also demonstrates the efficiency of EGCG stabilised gold nanoparticles in X-ray does enhancement selectively in cancer cells.
References

1. Shukla, R. et al Laminin receptor specific therapeutic gold nanoparticles (198AuNP-EGCg) show efficacy in treating prostate cancer. Proc. Natl. Acad. Sci. U.S.A. 2012, 109 (31), 12426−31.

2. Hainfeld, J. F. et al Radiotherapy enhancement with gold nanoparticles. J. Pharm. Pharmacol. 2008, 60 (8), 977−85.

Poster Session 1 - Board: BS-03 / **36**

Age Related Differences in the Collagen Structure and Strength of Pericardium

Author(s): Ms. SIZELAND, Katie[1]
Co-author(s): Ms. WELLS, Hannah [1] ; Mr. HIGGINS, John [2] ; Mrs. CUNANAN, Crystal [3] ; Dr. KIRBY, Nigel [4] ; Dr. HAWLEY, Adrian [4] ; Dr. MUDIE, Stephen [4] ; Prof. HAVERKAMP, Richard [5]

[1] *Massey University*

[2] *Southern Lights Biomaterials*

[3] *Boston Scientific*

[4] *Australian Synchrotron*

[5] *Massey Univeristy*

Corresponding Author(s): k.h.sizeland@massey.ac.nz

Heart valve leaflets can be replaced using bioengineered leaflets from bovine pericardium tissue. The strength and thickness of the material is of crucial importance for both the percutaneous delivery of the leaflet replacement and the long life in service that is required of the biomaterial. Neonatal pericardium is thinner than adult pericardium giving it a physical advantage for heart valve leaflet production but any differences in the strength of the tissues remains unknown. Small angle X-ray scattering was used to characterise the collagen structure of adult and neonatal pericardium and results were compared with the mechanical properties. When compared with adult pericardium, neonatal pericardium was found to have a higher degree of alignment (neonatal OI = 0.78, adult OI = 0.62), a higher elastic modulus (neonatal elastic modulus = 83.7 MPa, adult elastic modulus = 19.1 MPa), and a higher normalised ultimate tensile strength (neonatal tensile strength = 32.9 MPa, adult tensile strength = 33.5 MPa). This research shows that the higher alignment of the collagen fibrils provides the structural foundation for the superior strength of the neonatal pericardium. The physical properties of neonatal pericardium indicate it would be a suitable material for the heart valve leaflet replacements.

Advanced Materials II / 15

New Insight into the Metal-to-Insulator Transition in Vanadium Dioxide.

Prof. SMITH, Kevin[1]

[1] *University of Auckland*

Corresponding Author(s): kevin.smith@auckland.ac.nz

The metal-insulator transition (MIT) in VO2 is of both fundamental and technical interest, the former due to important questions about its origins, and the latter due to possible applications in electronic devices such as ultrafast optical switches and field effect transistors. In bulk VO2, a large structural distortion accompanies the conductivity transition from the metallic (rutile) to the insulating (monoclinic) phase, which is known to impose a significant bottleneck on the timescale of the transition. Recently, the ability to control the transition temperature of the MIT in VO2 through nanoscale engineering via mechanical stress has heralded renewed interest in the potential application of VO2 as a novel functional material. I will present the results of photoemission, x-ray emission, resonant inelastic x-ray scattering, x-ray absorption, low energy electron microscopy, and photoelectron microscopy studies of the MIT in strained VO2 thin films. Our results reveal that the MIT may be driven towards a purely electronic transition, (i.e. one which does not involve a structural transition), by the application of mechanical strain. Our measurements have important implications for novel functional material engineering of VO2, suggesting a route towards circumventing the structural bottleneck in the ultrafast timescale of the MIT.

Poster Session 2 - Board: RR-06 / **206**

Evaluating the biological response of aggressive glioma cell lines to synchrotron microbeam radiotherapy compared to broad-beam irradiation

Author(s): Mr. SMYTH, Lloyd[1]
Co-author(s): Dr. CROSBIE, Jeff [2] ; Dr. DONOGHUE, Jacqueline [3] ; Prof. ROGERS, Peter [4]

[1] *University of Melbourne, Epworth HealthCare*

[2] *RMIT*

[3] *Hudson Institute of Medical Research*

[4] *University of Melbourne*

Corresponding Author(s): lsmyth@student.unimelb.edu.au

Background: Diffuse Intrinsic Pontine Glioma (DIPG) is an aggressive and infiltrative tumour of the brain-stem and is amongst the most lethal brain tumours affecting children. Current treatment options are largely ineffective with less than 10% of DIPG patients surviving to 2 years. Synchrotron Microbeam Radiotherapy (MRT) is a promising pre-clinical therapy which could drastically improve the prognosis of patients with DIPG by allowing much higher radiation doses to be delivered to the tumour without an increase in brain-stem toxicity.
Aim: To compare the response of DIPG cell lines to MRT versus conventional broad-beam (BB) radiotherapy using assays for sphere-forming capacity, cell-cycle and apoptosis, and to determine biologically equivalent MRT and BB doses.
Method: Three DIPG cell-lines were irradiated using MRT and BB. Cells were irradiated as single cells in 2mL tubes in two experimental sessions: July 2015 at the Australia Synchrotron (MRT) and October 2015 at the Walter and Eliza Hall Insititue (BB). MRT doses were 0Gy, 112Gy, 250Gy, 560Gy and 1180Gy and BB doses were 0Gy, 5.0Gy, 7.7Gy, 9.3Gy and 12Gy. Triplicates were used. After irradiation we performed cell-cycle and apoptosis assays and assessed cells for sphere-forming capacity.
Conclusion: Using DIPG cell lines, novel in MRT research, we determined biologically equivalent BB and MRT doses. Results will be used to inform future in-vivo experiments on DIPG-bearing rodents.

Poster Session 1 - Board: AM-23 / **182**

XAS Studies of Mixed Main Group Tin Cluster Materials

Author(s): Mr. ALLISON, Morgan[1]
Co-author(s): Dr. SOEHNEL, Tilo [2] ; Dr. LING, Chris [1] ; Dr. STUART, Glen [3]

[1] *The University of Sydney*

[2] *The University of Auckland*

[3] *The University of New South Wales at the Australian Defence Force Academy*

Corresponding Author(s): t.soehnel@auckland.ac.nz

Layered oxide materials that combine unusual intermetallic architectures and transition metal oxides similar to naturally occurring mineral architectures are promising candidates for the study of strongly correlated-electron systems. One of the key benefits of systems that contain naturally occurring mineral structures is they provide a widely characterized platform to stabilize new architectures such as intermetallic clusters that prove otherwise highly unstable in isolation. The parent compound for this study, Fe4Si2Sn7O16 1, provides a novel situation in oxide compounds. It is described as a layered composite of FeSn6 oxide clusters and Sn-doped Fayalite-type within the one structure resulting in two nearly perfectly 2D oxide systems. To date, all reported tin oxide clusters have been shown to be electron precise, i.e. they follow the 18 valence electron rule. Whilst several attempts have been made to produce electron rich cluster materials in the tin oxide system, only the incorporation of highly stable “natural ligand layers” such as Fayalite has allowed for the stabilization of electron-rich 3d-transition metal clusters. In this presentation we will describe the experimental results of combined Mössbauer/XAS studies that have led to the discovery of the first 19-electron cluster found in the tin system.
1 T. Söhnel, P. Böttcher, W. Reichelt, F.E. Wagner; Z. Anorg. Allg. Chem. 624, 708 (1998).

Advanced Materials II / 180

Synthesis and Characterisation of (M1-xFex)2SnO4 (M = Mn, Co, Zn) ternary transition metal-tin-oxygen spinel systems

Author(s): Dr. SOEHNEL, Tilo[1]

Co-author(s): Mr. LEUNG, Cory [1] ; Ms. VYBORNA, Natalija [1] ; Mr. ALLISON, Morgan [2] ; Prof. LING, Chris [2] ; Prof. STEWART, Glen [3]

[1] *The University of Auckland*

[2] *The University of Sydney*

[3] *The University of New South Wales*

Corresponding Author(s): t.soehnel@auckland.ac.nz

Mixed transition-metal oxide (MTMO) spinels including Mn and Zn-metal containing stannate phases have promising material properties and are known for the ability to tailor particular features for different uses. They are currently being explored as possible alternative substrates in many emerging high-tech applications such as electrode materials in lithium-ion batteries and as conducting oxides in gas detector sensors. The project aims to study the crystal and magnetic structures of iron and tin containing quaternary stannate to produce the novel spinel structures (M1-xFex)2SnO4 (M = Mn, Zn and $0 \leq x \leq 1$). Synchrotron X-ray and neutron powder diffraction, Mn and Fe K-edge XANES, Mössbauer, IR and UV-Vis spectroscopy data, magnetic measurements and SEM/EDX have been performed on the (M1-xFex)2SnO4 systems to find out the exact mechanism of Fe substitution, how much Fe and in what oxidation state is substituted and the effects upon the crystal and magnetic structure. For the range of (Zn1-xFex)2SnO4 spinels, initial results support the hypothesis that there is more than one doping mechanism, which is dependent upon the amount of Fe that is doped. Diffraction results and Mössbauer data indicate that an enrichment of Fe relative to Sn is evident in the Fe-rich structures, which might be due to Fe replacing Zn followed by Sn as more Fe becomes present in the system.

Poster Session 2 / **50**

Pore microstructure variation in gradient consolidation of Pearl River Delta saturated clay

Author(s): Dr. SONG, Jing[1]
Co-author(s): Dr. YANG, Sam [2]

[1] *Sun Yat-sen University*

[2] *CSIRO, Manufacturing Flagship*

Corresponding Author(s): songj5@mail.sysu.edu.cn, sam.yang@csiro.au

Clayed soils have been widely used in engineering foundation treatment in the coastal field to solve the issues of creep problems, the deformation, and strength of drainage consolidation. The microstructure porosities and pore size distribution of the clayey soil in the Pearl River Delta were studied by techniques of SEM and pressure gradient method. The loading was investigated based on the stress to improve the efficiency of saturated clayed soil foundation treatment. The effect of stress distribution on mechanical properties in the consolidation process was also investigated through the rate of anisotropy characteristics in the same full of saturated soft clay. It was found that small pores were increased with increasing loading of clay samples. Large pores with diameter of over 4 μm were obviously decreased with increasing loadings because of the squeeze effection which generated much more smaller pores. And the maximum principal stress and pore size with short axis angle were reduced. Furthermore, on the horizontal profile of samples, the round-like pores were abundant, but the direction was not obvious. While on the vertical profile, the pores were relatively flat with low abundance and the obvious direction. All of these indicated that the isotropic characteristic of clayed soil was gradually appeared with increasing pressure gradient. So the stress change in the consolidation process of the saturated soft clay is important in engineering which would be performed step by step based on the stress to improve the efficiency of saturated soft clay foundation treatment.

Poster Session 1 - Board: AM-21 / **172**

Time-resolved phase evolution during creation of nanoporous Cu current collectors by a dealloying approch

Author(s): Ms. SONG, Tingting[1]

Co-author(s): Dr. YAN, Ming [2] ; WEBSTER, Nathan [3] ; Dr. STYLES, Mark [4] ; Dr. KIMPTON, Justin [5] ; Prof. QIAN, Ma [1]

[1] *RMIT University*

[2] *South University of Science and Technology of China*

[3] *CSIRO*

[4] *CSIRO Manufacturing Flagship*

[5] *Australian Synchrotron*

Corresponding Author(s): s3466383@student.rmit.edu.au

Dealloying is used to fabricate nanoporous metals, and is a process where less noble components (e.g. Al) in the precursor (e.g. AlCu) are dissolved, leaving the nobler elements (e.g. Cu) to a nanoporous structure. Nanoporous Cu is desired in lithium-ion batteries as current collectors, which can provide large surface area for active materials. From the perspective of phase evolution, it was reported that only Al-rich phase (e.g. fcc -Al(Cu), tetragonal Al2Cu) can be dealloyed completely to form fcc Cu, but not Cu-rich phase (e.g. monoclinic AlCu, cubic Al4Cu9) placing limitations in creating nanoporous Cu.
To further understand it, we carried out in-situ and ex-situ dealloying experimentation at synchrotron powder diffraction beamline. We selected two two-phase Al-Cu precursors (at.%): Al55Cu45 (Al2Cu and AlCu) and Al45Cu45 (AlCu and Al4Cu9) alloys. The time-resolved phase evolution results showed that, in all three cases, the dealloying of two phases started in sequences with the formation of Cu. The dealloying of the relatively Al-rich phase (e.g. AlCu in Al45Cu55) started preferentially and subsequently it would promote the dealloying of relatively Cu-rich phase (e.g. Al4Cu9 in Al45Cu55). This study improves the understanding of dealloying of AlCu and demonstrates the capability of creating more nanoporous copper via multiphase precursor designing.

Poster Session 1 - Board: BT-35 / **223**

Neutron and infrared spectroscopy: Complimentary tools for vibrational studies.

Dr. STAMPFL, Anton[1]

[1] *Australian Nuclear Science and Technology Organisation*

Corresponding Author(s): aps@ansto.gov.au

A low energy band pass neutron spectrometer that operates in the range of $\sim 50-1200\,\mathrm{cm}^{-1}$ has very recently been commissioned and first experiments run at the OPAL reactor. The so-called Beryllium-filter spectrometer is predominantly used to obtain vibrational density of states spectra from those materials that contain hydrogen, thus making this instrument especially important in the chemical, biological, geological and environmental sciences. In many aspects a neutron spectrum obtained using the Beryllium-filter spectrometer is very similar to spectra obtained in the far-infrared or terahertz regime making neutron spectroscopy a complementary technique to other spectroscopies such as photon (electromagnetic radiation)-based techniques. The neutron's properties are unique amongst other fundamental probes like light, such as outstanding materials penetrability, isotopic sensitivity, magnetic sensitivity and lack of vibrational selection rules. A number of interesting examples are presented that highlight the capabilities and complementarity of vibrational neutron spectroscopy.

Poster Session 1 - Board: AM-25 / **218**

Controlling the Host-Guest Chemistry of a [Fe4L4]8+ Tetrahedral Cage via Ligand Design

Author(s): Mr. STANILAND, Robert[1]
Co-author(s): Prof. KRUGER, Paul [1]

[1] *University of Canterbury*

Corresponding Author(s): robert.staniland@pg.canterbury.ac.nz

A pair of related [Fe4L4]8+ tetrahedral cages were synthesised differing only in the electronic nature of the face-capping ligand. Cage **1** is comprised of four ligands containing a central triazine ring, whilst cage **2** is analogous utilising a benzene core. The cages were structurally characterised using X-ray crystallography performed at the Australian Synchrotron, which showed the cages to be flexible and adaptable. Solution based host-guest interactions were investigated by NMR spectroscopy, revealing that the cages are discriminating and selective in their host-guest behaviour.

Poster Session 1 - Board: IM-01 / **23**

Quantitative characterisation of the white/ pink X-ray beam at the Australian Synchrotron Imaging & Medical Beamline (IMBL)

Author(s): Dr. STEVENSON, Andrew[1]
Co-author(s): Dr. CROSBIE, Jeff [2] ; Dr. HALL, Chris [3] ; HAUSERMANN, Daniel ; Dr. LYE, Jessica [4]

[1] *Australian Synchrotron/ CSIRO*

[2] *RMIT University*

[3] *Australian Synchrotron*

[4] *ARPANSA*

Corresponding Author(s): andrew.stevenson@synchrotron.org.au

A critical phase for any synchrotron beamline involves detailed testing, characterization and commissioning; this is especially true of a beamline as complex as the Imaging & Medical Beamline (IMBL) [1-3]. IMBL staff and expert users have been performing precise experiments aimed at quantitative characterization of the primary white/ pink X-ray beam, with particular emphasis placed on the wiggler insertion devices (IDs), the primary-slit system and any *in-vacuo*/ *ex-vacuo* filters.
We will describe our findings from these studies. Such results will benefit future IMBL users, especially those for whom detailed knowledge of the X-ray beam spectrum (or "quality") and flux density is important. This information is critical for radiotherapy/ radiobiology users, who need to know (to <5%) what X-ray dose/ dose rate is being delivered to their samples.
We account for various correction factors associated with ionization-chamber dosimetry, e.g. recombination, electron loss. A new and innovative approach is developed, which provides confirmation of key parameter values such as the magnetic field in the wiggler and the effective thickness of key filters. IMBL commenced operation in December, 2008 with an Advanced Photon Source wiggler. A superconducting multi-pole wiggler was installed and operational in January, 2013. Results are presented for both of these IDs.
1 – A. W. Stevenson, et al., *J.Synch.Rad.*, **17**, 75-80 (2010). [2] – A. W. Stevenson, et al., *J.Synch.Rad.*, **19**, 728-750 (2012). [3] – J. C. Crosbie, et al., *Med.Phys.*, **40**, 062103 (9pp) (2013).

Poster Session 2 - Board: SB-06 / **134**

STRUCTURAL CHARACTERISATION OF THE RETROMER COMPLEX AND ASSOCIATED SORTING NEXINS

Author(s): Dr. SUZANNE, Norwood[1]
Co-author(s): Dr. LENEVA, Natalya [1] ; Dr. GHAI, Rajesh [2] ; Dr. COWIESON, Nathan [3] ; Dr. DUFF, Anthony [4] ; Dr. WOOD, Kathleen [4] ; Dr. COLLINS, Brett [5]

[1] *University of Queensland*

[2] *UNSW*

[3] *Australian Synchrotron*

[4] *ANSTO*

[5] *The University of Queensland*

Corresponding Author(s): s.norwood@uq.edu.au

Retromer is a protein complex that plays a central role in endosomal traffficking. Recently, retromer dysfunction has been linked to several neurological disorders including Alzheimer's and Parkinson's diseases. The classical mammalian retromer complex consists of a heterotrimeric cargo recognition sub-complex (VPS26, VPS29 and VPS35) associated with a dimer of proteins from the SNX–BAR sorting nexin family that drives membrane deformation and tubulation. By recruiting the cargo-selective sub- complex to the forming tubules, the SNX–BAR coat complex mediates the retrograde transport of proteins from endosomes to the trans-Golgi network. Recent studies, however, have highlighted the functional diversity of retromer and identification of new interacting proteins has revealed that the role of retromer extends to aspects of endosome-to-plasma membrane sorting and regulation of signalling events. Emerging evidence indicates that cargo specificity is mediated by specific sorting nexins. These include SNX3, involved in the trafficking of the Wntless/MIG-14 protein, and SNX27, a PX-FERM protein that mediates the retrieval of the β2-adrenergic receptor. We have acquired crystallographic and small angle scattering data to determine how the core cargo recognition sub-complex assembles and to characterise the retromer-associated sorting nexins. We are using this structural information in combination with biochemical and biological studies in a synergistic approach to understand retromer-mediated endosomal protein sorting. The retromer complex is conserved across all eukaryotes and we are also currently exploring the structure and function of these proteins in zebrafish and *Chaetomium thermophilum*.

Poster Session 2 - Board: SS-06 / **125**

Creating a Stable Oxide at the Surface of Black Phosphorus

Author(s): Dr. TADICH, Anton[1]
Co-author(s): Dr. EDMONDS, Mark [2] ; Dr. O'DONNELL, Kane [3] ; Dr. ANGELO, Ziletti [4] ; Dr. ALEXANDRA, Carvalho [5] ; Prof. FUHRER, Michael [2]

[1] *Australian Synchrotron*

[2] *Monash University*

[3] *Curtin University*

[4] *Boston University*

[5] *National University of Singapore*

Corresponding Author(s): anton.tadich@synchrotron.org.au

The stability of the surface of in-situ cleaved bulk black phosphorus single crystals upon exposure to atmosphere is investigated using high-resolution synchrotron x-ray photoelectron spectroscopy and atomic force microscopy. We demonstrate that after 2 days exposure to atmosphere a stable 0.35nm thick phosphorus oxide forms at the surface of the black phosphorus. Three types of local phosphorus−oxygen environments are identified, and it is found that the majority of the oxide consists of phosphorus pentoxide (P2O5), which represents the most thermodynamically favourable oxidation pathway. The work function increases from 3.9 eV for as-cleaved black phosphorus to 4.0eV after formation of the 0.35 nm thick oxide, with the phosphorus core levels shifting by less than 0.1 eV. These results indicate minimal charge transfer between the oxide and the underlying black phosphorus layers.We conclude that the native oxide formed on black phosphorus is a stable passivation layer with minimal effect on the doping of black phosphorus. The native oxide is also potentially attractive for the subsequent deposition of additional dielectric layers in order to fabricate metal-oxide-semiconductor field-effect structures

Poster Session 2 - Board: EE-08 / **98**

XANES Study of Fe and Ti cations in Blue Sapphires

Author(s): Dr. WONGKOKUA, Wiwat[1] ; Dr. THAMMAJAK, Nirawat[2]
Co-author(s): Ms. WONGRAWANG, Patcharee [1]

[1] *Kasetsart University*

[2] *Synchrotron Light Research Institute (SLRI), Thailand*

Corresponding Author(s): n.thammajak@gmail.com

X-ray absorption near-edge spectroscopy (XANES) can be used to study oxidation state of dilute system such as transition-metal defect in solid-state samples. In blue sapphire, Fe and Ti are key elements that caused the blue colour. Inter-valence charge transfer (IVCT) between Fe2+ and Ti4+ has been proposed to describe the optical colour's origin. However, existence of the divalent iron cations has not been thoroughly investigated. Fluorescent XANES is therefore employed to study K-edge absorptions of Fe and Ti cations in various blue sapphire samples, including, natural, synthetic, diffused and heat-treated sapphires. All the samples showed Fe absorption edge at 7124 eV, corresponding to Fe3+ state; and Ti at 4984 eV, corresponding to Ti4+. Fe, Ti, and other metal cations in the samples were determined qualitatively by synchrotron X-ray fluorescence spectroscopy (XRF) before the XANES experiments.

Poster Session 2 - Board: IM-02 / **38**

A Feasibility Study of X-Ray Phase-Contrast Mammographic Tomography at the IMBL of the Australian Synchrotron

Author(s): Dr. NESTERETS, Yakov[1]
Co-author(s): Dr. GUREYEV, Timur [2] ; Dr. TROMBA, Giuliana [3] ; Dr. MAYO, Sheridan [1] ; Dr. STEVENSON, Andrew [1] ; Mr. THOMPSON, Darren [1] ; Dr. JEREMY, Brown [4] ; KITCHEN, Marcus [4] ; Dr. PAVLOV, Konstantin [5] ; Dr. LOCKIE, Darren [6] ; Dr. BRUN, Francesco [3]

[1] *CSIRO*

[2] *ARC Centre of Excellence in Advanced Molecular Imaging*

[3] *Elettra-Sincrotrone*

[4] *Monash University*

[5] *University of New England*

[6] *Maroondah BreastScreen*

Corresponding Author(s): darren.thompson@csiro.au

We present the results of our recent experiment at the Imaging and Medical beamline of the Australian synchrotron intended to contribute to the development and implementation of low-dose, high-sensitivity 3D mammographic phase-contrast imaging, initially at synchrotrons and subsequently in hospitals and medical imaging clinics. We have tested, quantified, evaluated and optimised the effect of such imaging parameters as X-ray energy, source size, detector resolution, sample-to-detector distance, scanning and processing strategies in the case of propagation-based phase-contrast CT, using a plastic phantom simulating relevant breast tissue characteristics. The data are collected using a Hamamatsu CMOS Flat Panel Sensor, utilised in partial scan mode, with the pixel size 100μm $\times$ 100μm. Analysis of the data revealed the presence of propagation-based phase contrast and demonstrated significant improvement of the quality of phase-contrast CT imaging, compared to conventional (absorption-based) CT, at medically acceptable radiation doses.

Poster Session 2 - Board: BT-16 / **151**

Quick AS NEXAFS Tool (QANT): A program for NEXAFS loading and analysis developed at the Australian Synchrotron

Author(s): Dr. THOMSEN, Lars[1]
Co-author(s): GANN, Eliot [1] ; MCNEILL, Chris [2] ; Dr. TADICH, Anton [1] ; COWIE, Bruce [3]

[1] *Australian Synchrotron*

[2] *Monash University*

[3] *Australian Synchrotron.*

Corresponding Author(s): lars.thomsen@synchrotron.org.au

An analysis program for Near Edge X-ray Absorption Fine Structure (NEXAFS) spectra has been developed and implemented at the Soft X-ray beamline of the Australian Synchrotron.

The program allows for rapid viewing of corrected data channels, including normalizations to a standard, double normalizations where the standard itself has an undesired spectral response, and background subtraction. The program performs compositional analysis and peak fitting and includes common calculations such as the average tilt angle of molecules with respect to the surface, and the determination of the complex index of refraction. These functionalities make common data manipulations done with NEXAFS data quick and straightforward. It greatly increases the throughput of NEXAFS analysis, allowing routine analysis to occur as data is collected.

Poster Session 1 - Board: AM-07 / **43**

Phase transformations of a desert sand to a calcia magnesia aluminosilicate (CMAS) deposit: a Synchrotron powder diffraction study

Author(s): Mr. ZONNEVELDT, Matthew[1]
Co-author(s): Dr. THORNTON, John [1] ; Dr. WOOD, Chris [1] ; Mr. SESSO, Mitchell [2] ; Dr. KIMPTON, Justin [3]

[1] *DSTO*

[2] *Swinburne University*

[3] *Australian Synchrotron*

Corresponding Author(s): john.thornton@dsto.defence.gov.au

Thermal barrier coatings (TBC) are porous layers designed to insulate and protect turbine blade and vanes from the hot and oxidising gases in gas turbine engines. Dust or volcanic ash particles ingested by the engine can melt and form calcia-magnesia-alumino-silicate (CMAS) deposits on the TBC. During further engine operation the molten deposits can infiltrate the porous TBC and chemically interact. On engine shut-down the CMAS solidifies to create a TBC that is less porous and compliant and prone to delaminate as the engine cools down. Without TBCs, the blades and vanes need to be replaced pre-maturely, increasing costs.
To investigate the chemical processes of CMAS formation and CMAS+TBC interaction, we performed a synchrotron powder diffraction study on oxide-mineral rich desert sand and standard TBC zirconia powder. One set of diffraction patterns were collected in real time as a sample was heated and cooled through the range of 25-1400°C while in the diffractometer. These patterns were compared to powder mixtures previously heated in a furnace at 1100 and 1300°C for 4hrs. The results indicated the temperatures at which the desert sand underwent transformations. They also showed that the sand can react with the TBC zirconia to form zircon (ZrSiO4) and increase the amount of monoclinic zirconia. TBCs are manufactured to consist of tetragonal zirconia as coatings made from monoclinic zirconia break apart on thermal cycling. Overall the diffraction study helped to further define the mechanisms by which CMAS attacks TBC.

Biological Systems / **175**

Single Contact ATR Mapping of Soft Materials by Synchrotron FTIR

Author(s): Dr. TOBIN, Mark[1]
Co-author(s): Dr. BAMBERY, Keith [1] ; Dr. VONGSVIVUT, Jitraporn (Pimm) [1]

[1] *Australian Synchrotron*

Corresponding Author(s): mark.tobin@synchrotron.org.au

Attenuated Total Reflection (ATR) is a sampling method frequently used for FTIR microanalysis of samples which cannot be prepared as thin sections for transmission analysis. Generally, an ATR prism is attached to the front of the microscope objective and 2D mapping achieved by repeated contacts with the ATR crystal. The method is more suited to harder materials, since the multiple ATR contacts may lead to damage of softer materials. We have developed ATR devices for the purpose of analysing softer materials, where only gentle contact can be made with

the sample surface, in which the ATR crystal is attached to the microscope stage rather than the objective. Firstly, a modified micro-compression cell, in which a ZnSe ATR prism is brought gradually into contact with the surface of the sample, has been used to study the hydration water in chitosan-hyaluronic acid model biolubricant, as a function of pressure. As part of a study of the resistance of insect wings to biofilm formation, this ZnSe ATR has also been used to map the surface of structured fatty acid films being studied as an analogue to the dragonfly wing epicuticle, revealing the relative peak position of νCH2 absorption of a textured stearic acid film on graphite. More recently, an ATR device which employs more precise piezoelectric sample alignment and ATR contact control has been developed for further analysis of soft materials.

Poster Session 1 - Board: IM-15 / **224**

Simultaneous Recovery of Sample And Coherence Information in Coherent Diffractive Imaging

Author(s): Mr. TRAN, Giang[1]
Co-author(s): Dr. VAN RIESSEN, Grant [1] ; Prof. PEELE, Andrew [2]

[1] *La Trobe University*

[2] *Australian Synchrotron*

Corresponding Author(s): trannhangiang@gmail.com

Abstract: Coherent diffractive imaging (CDI) is a powerful method whereby the transmission function of an object can be recovered using certain, typically, iterative algorithms. Recently, it has been shown that CDI not only works well with coherent illumination but also with partially coherent illumination. In this work, we use simulated results to demonstrate successful retrieval simultaneously of an object's transmission function and of the characteristic coherence properties of the illuminating wavefield without a priori knowledge. Our approach is based on using a comprehensive modal model of the illuminating beam such that the free parameters representing the coherence properties can be fit during the recovery process.

Poster Session 2 / 12

Formation of surface U(V) by reduction of Ca-U-Carbonate complexes with nanoscale zero-valent iron

Author(s): Mr. TSAREV, Sergey[1]
Co-author(s): Dr. COLLINS, Richard [2] ; Prof. WAITE, David [1]

[1] *UNSW*

[2] *The University of New South Wales*

Corresponding Author(s): s.tsarev@student.unsw.edu.au

While nanoscale zero-valent iron (nZVI) has the potential to be used as a permeable reactive barrier for the remediation of uranium-contaminated groundwaters, there remains some uncertainty regarding the processes of uranium immobilization and the nature of the precipitated phase(s). In this study the reduction of aqueous Ca-U(VI)-carbonate complexes by fresh, aged and corroded nZVI particles representing particles with three types of oxide shells were investigated at circumneutral pH. XAS, XPS and kinetic studies were applied to obtain information about the structural and chemical composition of the uranium–containing reaction products. Kinetic experiments demonstrated quick uranium removal by all types of nanoparticles with the uranium removal rate proportional to the extent of iron oxide layer formaton indicating that the first stage is sorption onto iron oxide (magnetite) surface sites, followed by reduction by the zero-valent iron core. The final oxidation state of uranium depended on the mass ratio between iron and uranium. At 1:1 mass ratio uranium formed nanosized uraninite particles, while surface U(V) complexes were formed at higher iron loadings. U(VI)CaCO3 complexes were reduced more slowly than binary U(VI)CO3 complexes. We observed that the formation of U(V) complexes occurred only in presence of carbonate, which can be attributed to the stabilisation of surface U(V) by carbonate. Based on U and Fe EXAFS results structures for the U(V) complexes were proposed.

Soft Matter / 3

Exploring the *in meso* crystallization mechanism by using synchrotron Small Angle X-ray Scattering

Author(s): Ms. VAN 'T HAG, Leonie[1] ; Dr. KNOBLICH, Konstantin[2] ; Dr. SEABROOK, Shane[3]
Co-author(s): Dr. CONN, Charlotte [4] ; Dr. KIRBY, Nigel [5] ; Dr. MUDIE, Stephen [5] ; Dr. LI, Xu [6] ; Dr. GRAS, Sally [6] ; Dr. CALL, Matthew [7] ; Dr. CALL, Melissa [8] ; Prof. DRUMMOND, Calum [9]

[1] *University of Melbourne / CSIRO*

[2] *Structural Biology Division, The Walter and Eliza Hall Institute of Medical Research*

[3] *CSIRO Manufacturing Flagship*

[4] *RMIT*

[5] *Australian Synchrotron*

[6] *The University of Melbourne*

[7] *Walter and Eliza Hall Institute*

[8] *The Walter and Eliza Hall Institute*

[9] *School of Applied Sciences, College of Science, Engineering and Health, RMIT University*

Corresponding Author(s): leonie.vanthag@csiro.au

Recently, the development of a novel *in meso* crystallization method has facilitated the structural determination of several biologically relevant membrane proteins (MPs). However, *in meso* crystallization remains poorly understood as MPs are difficult to express and handle. An improved understanding of this technique can lead to an improved success rate and facilitate the structural determination of more MPs. These structures are important for rational drug design and designing new treatments for a wide range of diseases. Bicontinuous cubic phases are the most commonly used lipid phases for *in meso* crystallization. The proposed mechanism states that the membrane protein or peptide is initially uniformly dispersed in the cubic phase but that crystals grow from a local lamellar phase which acts as a conduit between the crystal and the bulk cubic phase. However, there is very limited experimental evidence for this theory. In this work we have explored this by characterizing the lipid mesophase microenvironment by using synchrotron Small Angle X-ray Scattering with a micro-sized beam during crystal growth of the DAP12-TM peptide of which the structure was recently solved. Crystal growth was indeed found to occur from the cubic mesophase, and a highly-oriented local lamellar phase was observed consistent with the co-location of the lamellar phase at a crystal face supporting the proposed mechanism for in meso crystallization. A new observation of this study is that some crystals may give rise to diffraction at wide angles which is of potential use in locating these crystals.

Poster Session 1 - Board: RR-07 / **208**

Synchroton Broad Beam and MRT radiation induces DNA damage in normal mouse tissues distant from the irradiated volume

Author(s): Mrs. VENTURA, Jessica[1]
Co-author(s): Dr. FORRESTER, Helen [2] ; Dr. SPRUNG, Carl . N [2] ; Dr. IVASHKEVICH, Alesia [3] ; Dr. SMITH, Andrea [4] ; Dr. STEVENSON, Andrew. W [5] ; Dr. HALL, Christopher [6] ; Mr. PALAZZOLO, Jason. S [4] ; Mrs. BEST, Nickala [4] ; Mr. MASON, Joel [4] ; Mr. NTARGARAS, Andreas [7] ; Mr. KOTSARIS, Vasilis [7] ; Dr. GEORGAKILAS, Alexandros. G [7] ; Dr. LOBACHEVSKY, Pavel [8] ; Prof. MARTIN, Olga . A [9]

[1] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, Australia; Royal Women's Hospital, Parkville, Australia*

[2] *Centre for Innate Immunity and Infectious Diseases, MIMR-PHI Institute, Monash University, Clayton, Australia*

[3] *Centre for Innate Immunity and Infectious Diseases, MIMR-PHI Institute, Monash University, Clayton, Australia; Radiation Oncology, Canberra Hospital, Garran, Australia*

[4] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, Australia*

[5] *CSIRO, Clayton, Australia;Australian Synchrotron, Clayton, Australia*

[6] *Australian Synchrotron, Clayton, Australia*

[7] *Department of Physics, National Technical University of Athens, Athens, Greece*

[8] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, VIC, Australia ;Sir Peter MacCallum Department of Oncology, the University of Melbourne, Melbourne, VIC, Australia*

[9] *Molecular Radiation Biology Laboratory, Peter MacCallum Cancer Centre, Melbourne, Australia; Sir Peter MacCallum Department of Oncology, The University of Melbourne, Melbourne, Australia; Division of Radiation Oncology and Cancer Imaging, Peter MacCallum Cancer Centre, Melbourne, Australia*

Corresponding Author(s): venturaj@student.unimelb.edu.au

Microbeam radiation therapy (MRT) is a novel, preclinical modality; with a unique ability to generate less radiation damage to neighbouring normal tissues, while providing efficient ablation to the tumour mass; compared to the conventionally used Broad Beam (BB) modality. A comprehensive investigation on the mechanisms and side effects of these modalities has currently not been established. Here we compared the radiation-induced bystander effect (RIBE) of BB and MRT irradiation, generated by the Imaging and Medical Beamline at the Australian Synchrotron in C57BL/6 mice. Animals were irradiated with 10Gy or 40Gy peak dose of BB or MRT, in an 8x8, 8x1 and 2x2mm area on the right hind leg, using an X-ray beam with a dose rate of 49Gy/sec and constant current of 200mA. At 24 and 96hrs post-irradiation, we collected irradiated skin and an assortment of unirradiated tissue; these were processed for DSB detection, using the gammaH2AX assay. For both modalities the levels of gammaH2AX foci in unirradiated tissues of irradiated mice, varied in comparison to irradiated animals. Overall, MRT and BB induced an elevated gammaH2AX response at 10Gy, while inhibiting this response at 40Gy. Oxidative clustered DNA lesions (OCDL) in tissues were measured using constant field gel electrophoresis, where genomic DNA was treated with purine, pyrimidine and abasic site-specific enzymes. We found a marked increase of OCDLs in a variety of unirradiated tissues. We will discuss the role of irradiated volume, dose, and beam modality in the manifestation of the in-vivo RIBE.

Poster Session 1 - Board: SM-03 / **221**

Applications of Synchrotron FT-IR secondary structure determination using the amide III region to protein based bioplastics

Author(s): Dr. BIER, Jim[1]
Co-author(s): Dr. VERBEEK, Johan [2] ; Dr. LAY, Mark [2]

[1] *Aduro Biopolymers and University of Waikato*

[2] *University of Waikato*

Corresponding Author(s): jverbeek@waikato.ac.nz

Bulk proteinaceous feedstocks used for bioplastic production are often insoluble and may already be denatured but retain some secondary structural features. The amide I region is commonly used for secondary structure estimation, but can be subject to interference from processing aids used to convert proteins into thermoplastics. The amide III region is much weaker but also sensitive to secondary structure change.

Synchrotron IR sources give a very good signal to noise ratio at small spatial resolutions enabling analysis of the amide III region. A method of estimating relative changes in secondary structure using the inverted second derivative has been developed to overcome the influence of subjective baseline corrections across the multiple spectra collected in spatial maps or time resolved heating experiments. In the context of dried blood as a proteinaceous feedstock, this method successfully predicts a much higher β-sheet content and reduced α-helical content in blood that has been thermally denatured and aggregated than for lyophilised BSA or spray dried haemoglobin, which retain more of their native structure.

Mapping secondary structure distribution in bioplastics made from these proteins showed significant structural rearrangement after extrusion. Even with plasticisers, conformational change towards increased ordered structure occurred at typical processing temperatures, not just on cooling from the melt. The rapidity with which good quality, high signal-to-noise spectra can be collected, suggests kinetic data could also be obtained.

Poster Session 2 - Board: BS-02 / **22**

Mechanistic insights into H9c2 differentiation of myoblasts to cardiac myocytes and skeletal muscle

Author(s): Ms. VERVERIS, Katherine[1]
Co-author(s): Dr. VONGSVIVUT, Pimm [2] ; Dr. BAMBURY, Keith [3] ; Dr. KARAGIANNIS, Tom [4]

[1] *Baker IDI Heart and Diabetes Institute*

[2] *Deakin University*

[3] *3Australian Synchrotron Scientist, Fourier Transform Infrared Spectroscopy Beamline, Australian Synchrotron, Clayton, Victoria, Australia, 3168*

[4] *Epigenomic Medicine, Baker IDI Heart and Diabetes Institute, Melbourne, VIC, Australia*

Corresponding Author(s): katherine.ververis@bakeridi.edu.au

Differentiation of embryonic rat ventricular H9c2 cardiomyoblasts to cardiac myocytes and skeletal muscle has been used widely as a cell culture model system since they were characterised by Kimes and Brandt. The differentiation process and characterisation was further optimised by Mernard. Cardiac myocytes derived from H9c2 myoblasts are widely utilised to investigate cardiac muscle biology and also to study the effects cardiac hypertrophy. The cardiotoxicity as well as the protective effects of various compounds is typically explored in these cells. Despite their widespread use there is still controversy surrounding the nature of cardiac myocytes and skeletal muscle derived from H9c2 cardiomyoblasts. Therefore, we investigated the differentiation process and characterised the expression of various markers by immunofluorescence and infrared microspectroscopy. Our findings indicate that retinoic acid induces differentiation of H9c2 myoblasts to cardiomyocytes in low serum supplemented with retinoic acid. Embryonic myoblasts maintained in DMEM containing 10% FBS were cultured in DMEM containing 1% FBS for seven days resulting in differentiation to skeletal muscle. A seven day culture in low serum media supplemented with 10 nM retinoic acid resulted in differentiation into cardiac myocytes. Immunoflourescence microscopy of MLC[U+2010]2v protein expression (which displays absolute cardiac tissue specificity) indicates overexpression of the protein in retinoic acid treated cells. Further, we explored chemical and elemental maps of the three different cell types and show significant spectral changes attributing to their differences. Overall, our findings indicate that the cells are well differentiated morphologically and express certain markers that are typical for each cell type.

Poster Session 2 - Board: EM-06 / **99**

Phase Separation in PEDOT:Gelatin Composites Revealed by Synchrotron-FTIR-based Grazing Incidence Reflection (S-FTIR GIR)

Author(s): Dr. VONGSVIVUT, Jitraporn (Pimm)[1]
Co-author(s): Dr. TOBIN, Mark [1] ; Dr. WINTHER-JENSEN, Bjorn [2]

[1] *Australian Synchrotron*

[2] *Monash University*

Corresponding Author(s): pimm.vongsvivut@synchrotron.org.au

Conducting polymers (CPs) have emerged and been subject of an intense research for a new generation of electronic devices due to their high conductivity and a number of promising optical properties that come with their light-weight, high flexibility, and solution-processible properties, making them versatile for a diverse range of applications. In particular, poly(3,4-ethylenedioxythiophene) (PEDOT) and its composites have been widely studied as a potential new material in bioelectronics and tissue engineering due to their good biocompatibility and excellent chemical stability.

In this study, we investigated the molecular interaction and the distribution of gelatin that was incorporated into PEDOT films *via* vapour phase polymerization at different ratios, using synchrotron-FTIR-based grazing incidence reflection (S-FTIR GIR) technique. While previous cyclic voltammetry studies indicated no change in electrochemical properties of PEDOT in

PEDOT:gelatin composites, S-FTIR GIR maps interestingly revealed the increasing degree of phase separation in the composite domains as the ratio of gelatin increased (Fig.1). This is the first time that the phase separation in PEDOT:gelatin composites was observed and proved experimentally.

Figure 2: Fig.1: Visible images (left) and the corresponding S-FTIR GIR maps (right) of PEDOT:gelatin composites at two different ratios obtained using 15x grazing angle objective. The plot intensity was based on the integrated area of the band centred at 1280 cm-1 (i.e. thiophene ring stretches).

Surface Science / **55**

Reversible intermediate energy state of CVD graphene: A signature of rippling?

Author(s): Mr. WAHAB, Hud[1]
Co-author(s): Dr. TIMMERS, Heiko [1] ; Prof. CADOGAN, John (Sean) M. [1] ; Prof. MERTINS, Hans-Christoph [2] ; Mr. HAVERKAMP, Robert [2]

[1] *UNSW Canberra*

[2] *UAS Muenster, Germany*

Corresponding Author(s): hudwahab@gmail.com

The application of graphene in device technologies will require that the electronic band-structure of different graphene materials is measured in detail and that graphene-substrate interactions are well understood. Both, the degree of sp2-hybridisation and the electronic band-structure can be directly probed with NEXAFS. Furthermore the technique enables detailed studies of structural changes at the graphene surface and at its substrate interface.
Our NEXAFS studies at the Australian Synchrotron have produced new evidence for a contentious state in graphene near 288 eV. This resonance has been intermittently observed before by others and it is often referred to as an 'interlayer state' due to a perceived analogy with graphite.
For CVD-graphene synthesized on copper we see a pronounced anisotropy for this state and derive an excitation energy of 288.3 eV and a partial overlap with an isotropic contaminating resonance. After annealing and keeping the graphene in ultra-high vacuum, the NEXAFS signature of the 288.3 eV state only gradually appears and builds-up over several hours. This signature can be removed again by renewed annealing. The reversible phenomenon may thus relate to residual lattice mismatch between the graphene and the copper substrate. Associated stress may gradually be relaxed through the rippling of the graphene layer. Tilting angles of >20° appear possible. The rippling is evidenced in our data by a correlated, reversible non-linearity of the cos-square-theta-dependence of the 285 eV π* resonance of graphene.

Poster Session 1 - Board: EM-01 / **75**

Ferrocene conformers: where DFT calculations meet measurements

Author(s): Prof. WANG, Feng[1]
Co-author(s): Dr. BEST, Stephen [2] ; Prof. CHANTLER, Christopher Thomas [2] ; Mr. ISLAM, Shawkat [3] ; Mr. ISLAM, Taulid [2] ; Dr. APPADOO, Dominique [4]

[1] *Swinburne University of Technology*

[2] *University of Melbourne*

[3] *PhD Candidate*

[4] *The Australian Synchrotron*

Corresponding Author(s): fwang@swin.edu.au

As the most important organometallic sandwich compound in chemistry, ferrocene (Fc, Fe(C5H5)2) can also serve in hydrogenanses as metal catalysis in the interaction with enzyme. As a result, understanding the structural and functional details of the active site of hydrogenases through X-ray crystallography, spectroscopic and computational methods, has been the bottleneck of biomimetic and bioinspired catalysts in chemistry. However, it is important to obtain a good understanding of Fc structure as since its discovery, the heated debate whether the eclipsed (e-Fc) or the staggered (s-Fc) is the most stable structure of Fc continues. The fact that electronic structures and many properties of the Fc conformers are strikingly similar has been a key hurdle to differentiate or separate the configurations from one another, until our recently study which discovered theoretically using DFT calculations that the 400-500 cm-1 region of the infrared (IR) spectra of Fc 1 exhibits the fingerprint conformers, which is seen in an earlier IR experiment of Fc. Such the discovery was later confirmed by IR experimental measurements in a number of solutions. In this presentation, we discuss the design and conduction of a series of new high-resolution IR experiments in the gas-phase and solid phase under various temperatures at the Far-IR beamline of the Australian Synchrotron to study the IR for Fc and deuterated Fc-d10. Preliminary results and analysis will be presented at this meeting.

1. Mohammadi, N.et al, J. Organomet. Chem., 213(2012)51-59.

Poster Session 2 - Board: EE-12 / **209**

Does silver sulfide nanoparticles (Ag2S-NPs) possess risks in soil-plant systems?

Author(s): Dr. WANG, Peng[1]
Co-author(s): Dr. LOMBI, Enzo [2] ; Prof. MENZIES, Neal [1] ; Dr. KOPITTKE, Peter [1]

[1] *The University of Queensland*

[2] *University of South Australia*

Corresponding Author(s): p.wang3@uq.edu.au

Silver nanoparticles (NPs) are used in more consumer products than any other nanomaterial and their release into the environment is unavoidable. Of primary concern is the wastewater stream in which they are transformed to silver sulfide NPs (Ag2S-NPs) before being applied to agricultural soils within biosolids. Once within the soil, it is likely that various soil properties (redox status, pH, and chloride concentration) will influence the stability of these Ag2S-NPs. In the present study, we initially examined (i) the stability and transformation of Ag2S-NPs that actually occur in soils over time at varying redox conditions and pH, and (ii) the effects of the presence of chloride on Ag2S transformation in soils. Given their low solubility and reactivity, it has been suggested that Ag2S-NPs are unlikely to constitute an environmental hazard. However, the assumption in the soil-plant systems has not been tested. Therefore, we also investigated (i) the toxicity of Ag2S-NPs during both short-term (24 h) and longer-term (two weeks) exposure to discern any nano-specific effects, and (ii) the accumulation and speciation of Ag within plant tissues. Our findings have shown that Ag2S-NPs were found to be very stable in soils but only subject to change under high Cl conditions. In addition, Ag2S-NPs exerted toxic effects through their direct accumulation in terrestrial plant tissues. These findings need to be considered to ensure high yield of food crops, and to avoid increasing Ag in the food chain.

Poster Session 1 - Board: AM-03 / **18**

Electric field and stress induced phase transformations in polycrystalline BaTiO3

Author(s): Dr. WANG, Zhiyang[1]
Co-author(s): Dr. WEBBER, Kyle [2] ; DANIELS, John [3]

[1] *School of Materials Science and Engineering, UNSW Australia & The Powder Diffraction Beamline, Australian Synchrotron*

[2] *Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany*

[3] *UNSW*

Corresponding Author(s): zhiyang.wang@synchrotron.org.au

This work presents in situ high-energy synchrotron x-ray diffraction measurements on the polycrystalline BaTiO3 at temperatures above the Curie point (TC) during application of unipolar electric fields and uniaxial compressive stresses. The experimental observations provide insights into the general paraelectric/paraelastic to ferroelectric/ferroelastic phase transition behaviors and have important implications for the future development of high-strain lead-free electromechanical materials. The results show the transitions from the high temperature cubic paraelectric/paraelastic phase to a ferroelectric/ferroelastic tetragonal phase induced by the electric field and compressive stress. In both electrical and mechanical cases, the nature of the observed transitions was influenced by the proximity of the temperature to TC. With increasing temperature above TC, the transition electric field and stress both increased while the rate of transitions tended to decrease. At temperatures just above TC, a nearly saturated domain texture existed within the induced phase at the maximum stress (400 MPa) whereas the resultant tetragonal domain texture at the maximum electric field (4 kV mm–1) was not saturated.

Energy Materials I / **122**

In Situ X-ray Diffraction Investigation of the Evolution of Pb-Oxide/Pb-Sulfate Surface Layers on Pb-Alloy Anodes

Author(s): Dr. CLANCY, Marie[1]
Co-author(s): WEBSTER, Nathan [2] ; Dr. STYLES, Mark [3] ; Prof. BIRBILIS, Nick [1] ; Dr. BETTLES, Colleen [1] ; Dr. CHEN, Miao [2] ; Dr. KIMPTON, Justin [4]

[1] *Monash University*

[2] *CSIRO*

[3] *CSIRO Manufacturing Flagship*

[4] *Australian Synchrotron*

Corresponding Author(s): nathan.webster@csiro.au

This presentation will describe the quantitative measurement, by *in situ* X-ray diffraction (XRD) and subsequent Rietveld-based quantitative phase analysis and thickness calculations, of the evolution of the lead dioxide and lead sulfate surface layers formed on a number of lead alloy anodes under simulated copper electrowinning conditions. A novel electrochemical flow cell is also described. The work is the first truly *in situ* XRD study of the surface layer evolution on lead alloy substrates under cycles of galvanostatic (electrowinning) and potentiodynamic (power interruption) conditions, and as such is of key interest to the metallurgical and lead acid battery communities. In a general sense, the *in situ* results show that the β polymorph of lead dioxide forms immediately on the anode under galvanostatic conditions, and undergoes continued growth until power interruption where it transforms to lead sulfate. The amount of residual lead dioxide increases with the number of cycles due to incomplete conversion to lead sulfate, which affects the electrochemical performance of the alloy. Specific variations in surface layer mineralogy and thickness as a function of cycle number and time are used to explain differences in electrochemical performance across the alloy suite.

Poster Session 1 - Board: EM-13 / **181**

Drying dynamics of blade coated P(NDI2OD-T2) via in situ GIWAXS investigation

Author(s): Mr. WELFORD, Adam[1]
Co-author(s): GANN, Eliot [2]

[1] *Monash University*

[2] *Australian Synchrotron*

Corresponding Author(s): adam.welford@monash.edu

Solution cast, organic field-effect transistors (OFET) have many advantages, such as rapid, large area fabrication, low production cost and flexible substrates making them ideal for specialized applications (ex: flexible displays, radio frequency identification). Suitable fabrication techniques that can readily scale up are therefore essential when looking at future manufacturing scenarios. Blade coating, the act of shearing a solution across a surface to generate a thin film is one such technique that can be adopted.
Film morphology plays a key role in determining the electronic properties of any organic semiconductor system. Understanding the dynamic development of blade coated film morphology is an integral first step to enhancing the electronic properties via processing conditions.
In situ grazing incidence wide angle xray scattering (GIWAXS) allows the morphology dynamics of P(NDI2OD-T2) to be investigated throughout film deposition and crystallization in two common solvents, toluene and xylene. A complex picture of crystallization emerges that illuminates the transitory states and speed at which the transition takes place.

Surface Science / 120

Synchrotron studies of chemotherapy drugs and their interactions; a novel application for graphene?

Prof. WELLS, Justin[1]

[1] *Norwegian University of Science and Technology (NTNU)*

Corresponding Author(s): quantum.wells@gmail.com

Chemotherapy treatment usually involves the delivery of fluorouracil (5-Fu) together with other drugs through central venous catheters. Catheters and their connectors are increasingly treated with silver or argentic alloys/compounds. Complications arising from broken catheters are common, leading to additional suffering for patients and increased medical costs. Here, we use synchrotron techniques (PES and NEXAFS) to uncover a likely cause of such failure. We study the surface chemistry relevant to chemotherapy drug delivery, i.e. between 5-Fu and catheter materials. We show that silver catalytically decomposes 5-Fu, compromising the efficacy of the chemotherapy treatment. Furthermore, HF is released as a product, which will be damaging to both patient and catheter. We demonstrate that graphene surfaces inhibit this undesirable reaction and would offer superior performance as nanoscale coatings in cancer treatment applications.

Energy Materials II / 48

In Operando Structure-property Studies of Advanced Nano Materials for Lithium Batteries

Author(s): Dr. WEN, Wen[1]
Co-author(s): Mrs. GAO, Mei [1] ; Mr. GU, Yueliang [1] ; Dr. ZHANG, Xingmin [1] ; Dr. GAO, Xingyu [1]

[1] *Shanghai Synchrotron Radiation Facility, Shanghai Institute of Applied Physics, Chinese Academy of Sciences*

Corresponding Author(s): wenwen@sinap.ac.cn

Lithium ion battery has wide applications in portable electronics and is one of the most attractive power sources for next generation electric vehicles. Thus, research on new intercalation compounds, which are usually nano-scale mixed metal oxides, is extensively carried out.
In a lithium ion battery, charge transfer can be correlated with redox reactions of cations and this has been extensively investigated. Anions could play a significant role in charge transfer as well, while they are less explored. Researchers have pointed out that oxygen ions in LiCoO[sub][2][sub] and Zn doped LiMn[sub][2][sub]O[sub][4][sub] partially contribute to charge transfer during electrochemical cycling[sup][1,2][sup]. Recently, a reversible oxygen redox chemistry[sup][3][sup] was further observed in Ru doped Li[sub][2][sub]MnO[sub][3][sub]. Combined both redox activities of cations and anions opens doors for further performance optimization, while detailed structure-property mechanisms on how oxygen is involved are poorly understood.

In this presentation, a series of bismuth based nano mixed metal oxides, which could have excellent oxygen ionic mobility were used as electrodes for lithium battery applications. Detailed discharge mechanism was further investigated using a combination of in operando XRD and X-ray Absorption Near edge Structure Analysis (XANES).
References: 1. Ceder, G. *et. al. Nature* **1998**, *392*, 694−696. 2. Wen, W. *et. al. J. Electrochem. Soc.* **2005**, *9*, A1902. 3. Sathiya, M. *et. al. Chem. Mater.* **2013**, *25*, 1121−1131.

Poster Session 2 - Board: AM-26 / **225**

Cu_{5-x}Mn_xSbO₆ Raman and Infrared Spectroscopy Investigations

Author(s): Mr. WILSON, Daniel Jeremy[1]
Co-author(s): Ms. CHANG, Fenfen [2] ; Prof. SMITH, Kevin [3] ; Dr. APPADOO, Dominique [4] ; KANG, Hyung-Been [1] ; Mr. SUZUKI, Furitsu [1] ; Dr. SOEHNEL, Tilo [1] ; Dr. URICH, Clemens [2] ; Mr. GRAHAM, Paul J. [2]

[1] *The University of Auckland*

[2] *The University of New South Wales*

[3] *Univeristy of Auckland*

[4] *The Australian Synchrotron*

Corresponding Author(s): daniel.j.wilson@auckland.ac.nz

The large crystallographic and chemical diversity of copper-based metal oxides is one of their highlighting features and cause for pursuit into copper based material research. An interesting feature seen in copper based metal oxides is the coexistence of different copper oxidation states in different crystallographic positions. This can lead to a mixture of magnetically active Cu2+ and magnetically inactive Cu1+ within the same compound, with different structural motifs. One interesting compound that demonstrates this coexistence of mixed copper oxidation states is Cu5-xMnxSbO6 which crystallises in a modified Delafossite structure type (CuFeO2). Here, the magnetically active brucite-like CuO2 layer was diluted in an ordered fashion with non-magnetic Sb5+. These layers were separated by linearly coordinated, magnetically inactive Cu1+, with two modifications, which depended on the stacking of the layers being ordered or disordered. Additionally, manganese was used as a dopant in order to replace the copper in the octahedral layers.
Previous investigations with solid-state Raman spectroscopy showed a reversible pressure-induced phase transition at room temperature for the ordered modification. This was not observed for the disordered modification. With synchrotron X-ray powder diffraction there was an observed increase in the reflections, attributed to the disordered modification in the ordered modification's diffraction pattern, when substituting manganese into the structure. Therefore, we investigated the nature of this phase transition with Raman and infrared spectroscopy, and how the effect manganese has on the two modifications influences this phase transition.

Poster Session 1 - Board: IM-03 / **51**

A Method for the Simultaneous Collection of the data for X-ray Computed Tomography and X-ray Fluorescence Computed Tomography

Author(s): Mr. WINNETT, Alex[1]
Co-author(s): ACRES, Robert [2] ; Dr. HALL, Chris [2] ; Prof. WANG, Feng [1]

[1] *Swinburne University of Technology*

[2] *Australian Synchrotron*

Corresponding Author(s): 7183895@student.swin.edu.au

This project aims to demonstrate a method for the simultaneous collection of the data for X-ray Computed Tomography (XCT) and X-ray Fluorescence Computed Tomography (XFCT) at the

Imaging and Medical Beamline, in conjunction with Swinburne University of Technology. XCT is known to give high quality morphological images of a specimen, while FXCT potentially provides functional information. Combining these two image methods provides complimentary information and has several advantages, such as reducing the radiation dose a patient would receive if the techniques where collected separately.
Initial testing was conducted on a 4 cm diameter plastic cylinder (the phantom) with along the axial direction that was filled with Iodine solution as the fluorophore. This design emulates a rat head, where the holes represent vessels or tissues stained using Iodine based contrast agents. The beam was modulated using a 5 mm thick aluminium comb with 1 mm wide tines, producing bright and dark regions and resulting in modulation of the fluorescence signal emitted by the fluorophore as the phantom rotated through the pattern, without affecting the XCT reconstruction. We hypothesise that this modulated fluorescence signal can then be reconstructed to prove spatial knowledge of the fluorophore.
Results from preliminary experiments that demonstrate the feasibility of this experimental approach will be presented.

Earth and Environment / 47

Iron and phosphorus speciation in Fe-conditioned membrane bioreactor activated sludge

Author(s): Mr. WU, Hao[1]
Co-author(s): Prof. WAITE, David [1] ; Dr. WANG, Yuan [1] ; Dr. IKEDA-OHNO, Atsushi [2] ; Dr. MILLER, Christopher [1]

[1] *University of New South Wales*

[2] *Helmholtz-Zentrum Dresden-Rossendorf*

Corresponding Author(s): 05.wu.hao@gmail.com

Iron dosing of membrane bioreactors (MBRs) is widely used as a means of meeting effluent phosphorus targets but there is limited understanding of the nature of iron and phosphorus-containing solids that are formed within the bioreactor (an important issue in view of the increasing interest in recovering phosphorus from wastewaters). Of particular challenge is the complexity of the MBR system and the variety of reactions that can occur on addition of iron salts to a membrane bioreactor. In this study, the performances of pilot scale MBRs with dosing of ferrous salts were monitored for a period of seven months. The distributions of Fe and P-species in the Fe-conditioned sludges were determined using X-ray absorption spectroscopy at the Fe K-edge and the P K-edge. Regardless of whether iron was dosed to the anoxic or membrane chambers, iron present in the sludges was consistently in the +III oxidation state. Fitting of the Fe K-edge EXAFS spectra showed that an Fe(III)-phosphate species was the main Fe species present in both cases with the remaining fraction dominated by lepidocrocite (γ-FeOOH) and ferrihydrite (am-FeOOH). P speciation revealed by the P K-edge XANES spectra suggested that both co-precipitation (present as strengite or an amorphous ferric hydroxyl phosphate analogue of strengite) and adsorption of phosphorus by iron oxyhydroxide mineral phase contribute to removal of phosphorus from the MBR supernatant. Organic P was also an important component of the residual P pool in the sludges

Poster Session 2 - Board: SB-04 / **121**

The x-ray crystal structure of microplasmin with a small-molecular active site inhibitor PSI-112

Author(s): Mr. WU, Jason[1]
Co-author(s): Dr. HIDAKA, Koushi [2] ; Mrs. JEEVARAJAH, Davadharshini [1] ; Dr. TSUDA, Yuko [3] ; Dr. WHISSTOCK, James [4] ; Dr. LAW, Ruby [1]

[1] *Department of Biochemistry and Molecular Biology, Monash University, Clayton, VIC 3800, Australia*

[2] *Center for Frontier Research in Medicinal Science, Kyoto Pharmaceutical University, Yamashina-Ku, Kyoto 607-8412, Japan*

[3] *Faculty of Pharmaceutical Sciences, Kobe Gakuin University, Kobe, Japan*

[4] *Department of Biochemistry and Molecular Biology, Monash University, Clayton, VIC 3800, Australia; ARC Centre of Excellence in Structural and Functional Microbial Genomics, Monash University, Clayton, VIC 3800, Australia*

Corresponding Author(s): guojie.wu@monash.edu

Plasmin (Plm) is the active form of the zymogen plasminogen (Plg), a serine protease which plays a key role in the fibrinolytic system and several other physiological activities. Physiologically, Plg/Plm activity is regulated by specific inhibitors and activators, making it an attractive therapeutic target for both traumatic bleeding and thrombotic diseases. Here we report the first crystal structure of microplasmin (the catalytic domain of Plm) in complex with a small-molecular active site inhibitor PSI-112 which is highly specific for Plm with IC50 of 0.22 μM. The crystal structure has been determined to 1.62Å, and the inhibitor binds to the substrate binding pocket with extensive additional subsite interactions. This structure may be helpful in developing a more Plm specific inhibitor as a new anti-fibrinolytic agent used to reduce bleeding complications in cardiac surgery or liver transplantation.

Poster Session 1 - Board: BT-13 / **119**

Advanced Micro-crystallography Single Crystal X-ray Diffraction Beamline at TPS

Author(s): Dr. WU, LAI-CHIN[1]
Co-author(s): Dr. JEY-JAU, Lee [1]

[1] *NSRRC*

Corresponding Author(s): wu.lc@nsrrc.org.tw

Molecular and crystal structure are basic but always the key to understand physical and chemical properties. A dedicated small-molecule single-crystal X-ray diffraction beamline is therefore scheduled on phase-II beamline construction at Taiwan Photon Source. Undulator will be used as X-ray source to generate high brilliance X-ray. The energy of this beam line is tunable within 8-32 keV depending on requirement. Monochromatic mode and pink beam mode both will be available at this beamline for different purpose. The monochromatic beam mode will be selected by Double Crystal Monochromator (DCM) and the pink beam mode (with bandwidth ˜ 3 % or less) will be selected by Double Multilayer Monochromator (DMM). Two pairs of focusing mirrors (HFM and VFM) will be used to focus the beam size down to few microns in diameter at sample position. The end-stations will equip with four-axis diffractometer for data collection.
This beamline is designed for advanced crystallographic purpose, which is not only dedicated to structure determination which cannot or very difficult to be done by using in-house diffractometer, but also to determine structure at non-ambient conditions and advanced studies. The techniques used at this beamline will cover (1) Time-resolved dynamic structural study (2) Laue crystallography (3) High pressure single crystal crystallography (4) Photo-induced excited state structural study (5) Ultra-high resolution charge density analysis (6) Resonance diffraction (7) Single crystal gas/solvent absorption-desorption (8) Micro-crystal and large porous structure determination.

Poster Session 1 - Board: BT-03 / **49**

Macquarie University-Australian Synchrotron D-DIA apparatus

Author(s): Dr. WYKES, Jeremy[1]
Co-author(s): Dr. RUSHMER, Tracy [2] ; Dr. CLARK, Simon [2] ; Dr. KAPPEN, Peter [3]

[1] *Macquarie University & Australian Synchrotron*

[2] *Macquarie University*

[3] *Australian Synchrotron*

Corresponding Author(s): jeremy.wykes@mq.edu.au

The recent development of the deformation-DIA (D-DIA) cubic-cell multi-anvil apparatus permits dynamic experiments investigating the rheological properties (measuring stress and strain) of materials at high pressures and temperatures, previously unattainable in deformation apparatus. A D-DIA apparatus is currently being commissioned on the XAS beamline at the Australian Synchrotron. The system consists of a four post frame with a 250-ton hydraulic cylinder pressurising the D-DIA module. Pressure control in the main- and differential rams is via an EPICS PID control loop where pressure is monitored by pressure transducers and varied by stepper-motor driven pressure generators. The sample is heated via a graphite resistance furnace. Temperature is monitored by a Pt-Rh or W-Re thermocouple and controlled via a Eurotherm PID controller. Positioning in the beam is achieved by mounting the press on an ADC X-Y-Z-rotation stage, the whole assembly weighing >3 tons. A particular constraint of of operating the D-DIA apparatus at the AS is that it must be completely removable from the XAS Hutch C end station. The system has been modularised to facilitate convenient movement.
The MQ-AS D-DIA system is capable of exerting hydrostatic pressures of ˜10 GPa and temperatures to ˜1600 K. When commissioning is complete the apparatus will be capable of radiographic imaging and energy dispersive or angle dispersive XRD. Initial experiments will investigate metal-silicate migration and the rheology of mantle mineral assemblages.

Techniques I / 25

DCM characterization of material micro-structures with multi-energy synchrotron X-ray CT

Dr. YANG, Sam[1]

[1] *CSIRO*

Corresponding Author(s): sam.yang@csiro.au

Quantitative and sample-non-destructive (SND) characterization of 3D microscopic composition distribution in materials is important in a broad range of R&D disciplines. The X-ray CT and image threshold segmentation approach has been widely used. Nevertheless, it imposes a length-scale cut-off at the X-ray CT resolution limit, which would limit its usefulness for materials with multi-length-scale structures beyond the CT imaging resolution range.
By integrating statistical physics and synchrotron-based multi-energy quantitative X-ray CT, the data-constrained modelling (DCM) method (http://en.wikipedia.org/wiki/Data_constrained_modelling) can explicitly reconstructs material microscopic distributions of materials in 3D which incorporates fine spatial structures below X-ray CT image resolution as voxel compositional partial volumes. Consequently, the fine length-scale information below the image pixel size is preserved. Such true micro-structure analysis enables more accurate modelling of material properties. The DCM methodology and its applications will be presented in relation to advanced materials science, oil & gas reservoir characterizations, and micro-structre-based material properties modelling.

Poster Session 1 - Board: IM-05 / **58**

Single-shot elemental contrast imaging using PiXirad photon counting detector

Author(s): Ms. YOKHANA, Viona Shlemoon Khames[1]
Co-author(s): Ms. ARHATARI, Benedicta D. [1] ; Mr. ABBEY, Brian [1]

[1] *La trobe university*

Corresponding Author(s): viona@uod.ac

Image detection of an elemental interest in compound samples has a specific interest in many research applications. Pixirad is a new X-ray imaging system, based on chromatic photon counting technology. The detector has a capability to count x-ray photons transmitted through the object and produce an image corresponding to the chosen energy thresholds at one exposure. Combined with wide broadband polychromatic sources, pixirad makes it possible to produce elemental

contrast imaging from a single measurement. The technique operates in full-field imaging mode and uses two energy bandwidths before and after an absorption edge of an element of interest to attain its elemental distribution. In addition to the use of this detector, a three dimensional imaging of a soft tissue will also be applied.

Poster Session 2 - Board: BT-02 / **39**

Small angle X-ray scattering beamline development at SSRF

Author(s): Dr. ZENG, Jianrong[1]
Co-author(s): Dr. TIAN, Feng [1] ; Dr. LI, Xiuhong [1] ; Dr. WANG, Yuzhu [1] ; Dr. YANG, Chunming [1] ; Mr. ZHOU, Ping [1] ; Dr. HUA, Wenqiang [1] ; Dr. LI, Xiaoyun [1] ; Dr. LIN, Jinyou [1] ; Mr. MIAO, Xiaran [1] ; Mrs. HONG, Chunxia [1] ; Prof. WANG, Jie [1] ; Prof. BIAN, Fenggang [1]

[1] *Shanghai Institute of Applied Physics, Chinese Academy of Sciences*

Corresponding Author(s): zengjianrong@sinap.ac.cn

BL16B1 at Shanghai Synchrotron Radiation Facility (SSRF) is a dedicated small angle X-ray scattering (SAXS) beamline in studying the micro structure and dynamic processes of polymers, nanomaterials, mesoporous materials, colloids, liquid crystals, metal materials, etc. Bending magnet is used as the photon source delivering X-rays of 5˜20 keV. After a recent upgrade, the beam is focused to a size about 0.4 mm (H) × 0.5 mm (V) with a flux about 3 × 1011 phs/s @ 10 keV @ 240 mA. SAXS in the q range of 0.03 ˜3.6 nm-1 and wide angle X-ray scattering (WAXS) in the q range of 4.5˜33 nm-1 are the basic and most used experimental modes. Absolute intensity for SAXS can be calibrated using glass carbon or pure water. Measurements in continuous q range of 0.03˜3.6 nm-1 can be carried out in the added simultaneous SAXS/WAXS mode. Grazing incidence SAXS and anomalous SAXS can also be performed. Support laboratories with kinds of conventional instruments for sample preparation and some in-situ devices for heating, shearing, stretching and helium atmosphere protection are available for end users. The beamline control system has been integated into an EPICS platform in Linux operation system, which is convenient for communication among the devices. In the past year, about 120 proposals were approved and over 4500 hours were allocated, bringing a feedback of over 100 SCI indexed publications.

Collaborating with Industry - the perils and the pleasure / 201

Discussion Panel