

ANSTO-HZB Neutron School

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Book of Abstracts

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A structural study on the cation disorder of Zinc – group-IV – nitrides (group-IV elements = Si, Ge, Sn)

Author(s): Zhenyu Wang¹

Co-author(s): Joachim Breternitz¹; Susan Schorr¹

¹ Helmholtz-Zentrum Berlin für Materialien und Energie

Zinc-group IV-nitrides (ZnIVN₂, with IV=Si, Ge, Sn) are currently being considered as promising candidates for photovoltaic absorber materials in thin film solar cells, since they consist of abundant elements and provide an excellent tunability of the band gap energy.[1] The latter is mainly achievable through two effects: alloying of different group IV elements,[2] and through different cation distributions.[1] Especially this second mechanism is of great interest since it would allow a rather unique band gap tuning mechanism, making this class of materials quite distinct.

In case of a statistic cation distribution the material adopts the hexagonal wurtzite-type structure (space group *P63mc*) with the cations occupying the Wyckoff position *2b*. A cation ordering introduces a symmetry reduction, thus the material with a complete ordered arrangement of cations crystallizes in the orthorhombic β -NaFeO₂-type structure (space group *Pna21*) where the cations occupy two distinct *4a* Wyckoff positions.[3,4]

The aim of our investigations are structure-property relations in Zn – group-IV – nitrides, especially variations of the band gap energy *E_g* in dependence on the cation distribution in the orthorhombic crystal structure. Since Zn²⁺ and Ge⁴⁺ are isoelectronic, they are merely indistinguishable from each other using conventional X-ray diffraction, but well distinguishable using neutron diffraction (*b*Zn = 5.68 fm, *b*Ge = 8.185 fm, *b*Sn = 6.225 fm).[5] Additionally we found in our systematic study on powder samples which we grow by ammonolysis from oxide precursors, that already Zn_{2-x}GeO_{4-x}3yN_{2y} oxide nitrides, which are an intermediate product in the synthesis of ZnGeN₂, show the orthorhombic β -NaFeO₂-type structure. This raises an additionally question about the anion distribution on the two different *4b* anion positions in the crystal structure. Oxygen and nitrogen are light, electronic similar elements, neutron diffraction gives the opportunity to distinguish these both elements in Rietveld data analysis clarifying the anion distribution in the crystal structure.

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Additive manufacturing of high strength aluminium alloys

Abirami Babu¹

¹ Monash University

Corresponding Author(s): abirami.babu@monash.edu

Introduction/Purpose:

Selective laser melting is a form of additive manufacturing technique that uses to laser source to melt and fuse powders, layer by layer, to form a final component. It is particularly arduous to fabricate aluminium through SLM owing to several difficulties and therefore only a very few conventional compositions are currently explored. The main difficulty for processing such alloys included the formation of hot cracks and porosities. The low laser absorption, poor flowability and high laser reflectivity also made the SLM processing of aluminium undesirable.

Methods:

The primary objective of research is to undertake a thermodynamic approach which can assist in developing new Aluminium alloys with high strength that can be produced by Selective Laser Melting. Research was done to minimise the effect of hot cracking by utilising the RDG criterion, along with the addition of high concentration of Zinc and Magnesium, thereby attaining high volume fraction of second phase particles to promote mechanical properties. The new alloys are expected to possess yield strengths of over 600 MPa and a suitable ductility of above 5% which will surpass the properties of existing high strength aluminium alloys whilst also permitting production in net shape.

Results:

New alloys of the Al-Zn-Mg system were successfully printed with low porosities and good mechanical properties. The hardness range of the new alloys were of the order of 180 HV and new phases produced by rapid solidification are explored.

Conclusions:

The structures and phases formed during this process are of utmost interest where the particles formed exhibit a quasi-crystalline structure with unknown properties and demands further examination through advanced diffraction techniques.

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An investigation into specific ion effects of multi-responsive polymers

Author(s): Hayden Robertson¹

Co-author(s): Erica Wanless ; Grant Webber ; Ben Humphreys¹ ; Edwin Johnson ; Andrew Nelson²

¹ *University of Newcastle*

² *ANSTO*

Corresponding Author(s): edwin.johnson@uon.edu.au, andrew.nelson@ansto.gov.au, erica.wanless@newcastle.edu.au, ben.humphreys@uon.edu.au, grant.webber@newcastle.edu.au, hrobertson1@uon.edu.au

Polymer brush coatings have the ability to alter the physicochemical properties of a surface. Multi-responsive polymers are terminally grafted onto a silica surface, where changes in pH, temperature and salt concentration can dramatically alter the system's hydrophobicity and thus adhesion, wettability and lubricity.

This project aims to investigate specific ion effects on thermo-responsive copolymer brushes in mixed salt environments. Various copolymer brushes, such as poly(N-isopropylacrylamide) and poly(oligo(ethylene glycol) methacrylate), will be used to conduct a range of physicochemical experiments as a function of temperature. These will include neutron reflectometry, ellipsometry, X-ray reflectometry, atomic force microscopy (AFM) and quartz crystal microbalance with dissipation monitoring (QCM-D).

In collaboration with my supervisors, we plan to submit a new Platypus beamline proposal in March, for which I will be the lead experimentalist. The neutron reflectometry results will yield the polymer volume fraction profile normal to the silica substrate, thus clarifying the polymer segment density and the solvent composition as a function of brush height. To complement this, I will be conducting experiments at the University of Newcastle throughout semester 1 in preparation for the planned beamtime later in the year. These experiments will consist of ellipsometry and AFM measurements on the POEGMA polymer brushes that will be used for later beamtime, in order to gain a deeper insight into these coatings as a function of solvent quality which for these polymer brushes is determined by a complex combination of solvent, solute and temperature. Overall these experiments will yield an in-depth understanding of multi-responsive brush systems. They form part of a greater collaborative project between my supervisors, ANSTO and Dr Stuart Prescott at UNSW.

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Controlling digestion kinetics through food microstructure design

Meltem Bayrak¹ ; Amy Logan² ; Charlotte Conn³ ; Juliane Floury⁴

¹ *RMIT University & CSIRO*

² *CSIRO*

³ *RMIT*

⁴ *Agrocampus Ouest*

Corresponding Author(s): amy.logan@csiro.au, juliane.floury@agrocampus-ouest.fr, charlotte.conn@rmit.edu.au, meltem.bayrak@csiro.au

Food is a complex combination of chemically diverse structures, influenced by composition and processing. The nutritional quality of food cannot be solely based on individual contents in nutrients as food structure will strongly modulate the bioaccessibility of nutrients upon digestion. In previous studies, the most common approach for measuring the extent of proteolysis and nutrient uptake was to compare the initial macroscopic features of ingested food to final concentrations in the bloodstream. However, there is limited literature to the support underlying mechanisms of the digestion of food in the stomach and enzyme diffusion in solid food substrates. In the present work, the influence of casein protein gel microstructure on enzymatic digestion will be investigated for the future development of personalised foods. Casein gels with identical composition, but differing by the coagulation mode, will be characterized and submitted to simulated gastric digestion. Small angle neutron scattering (SANS), small angle x-ray scattering (SAXS) and confocal microscopy will be used to study the microstructural changes in gel structure over time. The molecular interactions that occur as a gel network is formed, and subsequently broken down under digestive conditions will be investigated.

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Effect of metallurgical transformations on the evolution of residual stresses and identification of critical deposition parameters in direct laser metal deposition

CHAITANYA VUNDRU¹ ; Wenyi Yan¹ ; Ramesh Singh² ; Shyamprasad Karagadde²

¹ *Monash University*

² *Indian Institute of Technology Bombay*

Corresponding Author(s): chaitanya.vundru@monash.edu

Direct laser metal deposition (DLMD) is a promising additive manufacturing technique which has huge potential in remanufacturing and restoration of high value dies/molds and aerospace components. The residual stresses developed in the material deposited via DLMD plays an important role in the restoration of these components. The service life of the restored component will be compromised if tensile residual stresses are present in the deposited layer. The residual stresses in DLDM originate due to differential thermal expansion/contraction, volumetric dilation and transformation induced plasticity due to martensite formation. The influence of these metallurgical transformations and processing conditions on the resultant residual stresses of DLDM processed components needs to be understood and modeled for sustainable repair. Hence, a finite element model has been developed to capture the coupled effect of thermomechanical and strains due to phase transformations on the evolution of residual stresses in DLDM. In this study, the individual and coupled effects of strains due to volume dilation and transformation induced plasticity on residual stress evolution have been analyzed. It may be noted that the presence of tensile residual stresses in the deposited layer is detrimental as these components are subjected to cyclic thermomechanical loading and can fail under fatigue. Hence, the fully coupled thermomechanical and metallurgical model has been used to obtain optimal deposition parameters to ensure that the longitudinal residual stress are compressive during single layer deposition. Deposition carried out at the optimal process parameters increase the reliability of the restored components.

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Finite Element Approach to Bragg Edge Neutron Strain Tomography

Author(s): Riya Aggarwal¹

Co-author(s): Mike Meylan¹; Christopher Wensrich¹; Bishnu Lamichhane¹

¹ *University of Newcastle*

Corresponding Author(s): christopher.wensrich@newcastle.edu.au, blamichha@gmail.com, mike.meylan@newcastle.edu.au, riya.aggarwal@uon.edu.au

My research is based on the Finite Element approach applied to Bragg edge neutron transmission strain tomography. This method will allow the reconstruction of detailed stress and strain distributions within polycrystalline solids from sets of Bragg-edge strain images by using the time of flight techniques to increase the resolution of the images. Neutron Transmission methods have recently shown promising results in terms of tomographic reconstruction of strain tensor fields within samples. The proposed technique involves reconstruction from sets of Bragg-edge transmission strain images is measured by pixelated time-of-flight neutron detectors at pulsed neutron sources. As opposed to conventional Radon based CT, this revolves around the inversion of the Longitudinal Ray Transform (LRT) which has known issues surrounding uniqueness. In this work, reconstruction is approached via a least squares approach constrained by equilibrium formulated through the finite element method.

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Investigating the Expansion Mechanism of Deleterious ASR Gels in Mortars and Concretes.

Author(s): Elsie Nsiah-Baafi¹

Co-author(s): Kirk Vessalas¹; Paul Thomas²; Vute Sirivivatnanon³

¹ *School of Civil and Environmental Engineering, University of Technology Sydney, Australia*

² *School of Mathematical and Physical Sciences, University of Technology Sydney, Australia*

³ *School of Civil and Environmental Engineering, University of Technology Sydney, Australia*

Corresponding Author(s): kirk.vessalas@uts.edu.au, paul.thomas@uts.edu.au, vute.sirivivatnanon@uts.edu.au, elsie.nsiah-baafi@student.uts.edu.au

Alkali silica reaction (ASR) is one of the most recognized chemical reactions leading to distress problems in concretes. Occurring between reactive silica in some aggregates and alkalis of Portland cement, ASR produces an alkali-silica gel that expands in the presence of moisture resulting in cracks and subsequent deterioration of concrete structures. For high profile structures, concrete repair is not an option. These structures are decommissioned and removed from service prematurely, making this reaction very costly and inconvenient.

The severity of ASR is largely dependent on the expansive nature of the ASR gel formed. Consequently, it is pertinent to develop knowledge on the formation and swelling behaviour of ASR gel to aid in a greater understanding of reaction and thus allow for the development of more reliable methods for the prediction and mitigation of ASR. This project proposes to characterise the ASR gel in the concrete matrix by standard laboratory techniques (such as SEM-EDS and vibrational spectroscopy), in conjunction with characterising the water dynamics in situ in mortars containing ASR gels. This will be carried out primarily by determining the mobility of water in the ASR gels using quasi-elastic neutron scattering. The project also aims to investigate the transport of water by characterising the pore size and distribution which may be identified using neutron tomography for large pores and small angle neutron diffraction in the case of the capillary pores. A combination of an in-depth understanding of the character and distribution of the ASR gel, as well as the transport dynamics of ASR reactants in the mortar and concrete environments will provide a foundation for the formation of a consistent risk assessment processes for the use of aggregates in concrete

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Investigation of Magnetic Skyrmions in Multiferroic Materials by Neutrons and Light Scattering

Author(s): Jorge A. Saucedo Flores¹

Co-author(s): Rosanna Rov²; Luis M. Camacho Ealdama²; Gaurav Vats¹; Myung-Geun Han³; Joseph Garlow³; Yimei Zhu³; Elliot Gilbert⁴; Jan Seidel¹; Tilo Soehnel²; Clemens Ulrich¹

¹ *University of New South Wales*

² *University of Auckland*

³ *Brookhaven National Laboratories*

⁴ *ANSTO*

Corresponding Author(s): j.saucedaflores@student.unsw.edu.au

Unconventional topological spin structures such as chiral spin systems, realized in multiferroics or in skyrmion systems offer a plethora of fascinating phenomena for fundamental research and future technological applications [Fert]. A skyrmion is a topologically stable particle-like object comparable to a spin vortex at the nano-scale. These spin rotational bodies have diameters of 10-100 nm and typically form a 2-dimensional hexagonal superstructure perpendicular to an applied external magnetic field [Nagaosa]. Most skyrmion materials formerly discovered such as MnSi are metallic. However, the recently discovered Cu₂OSeO₃ (COSO) is a unique case of a multiferroic material where the skyrmion lattice appears in an insulating system, which opens avenues for controlling the dynamics of skyrmions through the application of an external electric field [Milde, Chacon].

Our research aims to unveil the fundamental magnetic interactions that give rise to magnetic skyrmions, their excitations, and interactions between skyrmions. To fulfil our goals, I work under the supervision of A/Prof. C. Ulrich and in close collaboration with the group of Prof. T. Soehnel at the University of Auckland, which contributes with samples.

Last July, I started my PhD in Physics at the UNSW, and we have obtained our first results using the Small Angle Neutron Scattering technique, on instrument QUOKKA at ANSTO. We have successfully determined the magnetic phase diagram of the helical and skyrmion phases in undoped and Te-doped COSO. Therefore, neutron scattering techniques play a crucial role in my PhD thesis and I would appreciate participating in the HZB Neutron School.

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Investigation of phonons by neutron scattering in hot carrier solar cell and thermoelectric materials

Author(s): Bharat Thapa¹; Milos Dubajic²; Gavin Conibeer²; Santosh Shrestha²

¹ *UNSW*

² *UNSW Sydney*

Corresponding Author(s): g.conibeer@unsw.edu.au, s.shrestha@unsw.edu.au, m.dubajic@unsw.edu.au, bharat.thapa@unsw.edu.au

Hot carrier solar cells (HCSC) are highly affected by the electron-phonon interaction happening in the hot carrier absorber (HCA) material. Longer carrier (hot electrons and hot holes) times are essential for an HCA to operate with high efficiency. It is considered that phononic properties such as large phonon band gap, low maximum acoustic phonon energy are desirable for an HCA material for HCSC to function at high efficiencies. However, determination of phononic band gap and density of states for most suitable HCA materials have mainly limited to theoretical (for e.g. DFT) calculations so far. Inelastic neutron scattering (INS) can help understand the phonon properties of HCA materials. Further, Brillouin zone mapping of phonons by INS also helps reveal thermal properties such as thermal conductivity which is a metric to characterize a material's thermoelectric application. The HCSC group at SPREE UNSW, which I belong to, is investigating a range of materials such as HfN, ZrN, TiHx, GaAs/AlAs MQW, perovskites for their potential use in HCSC and/or thermoelectrics. Indeed, our group has measured transverse and longitudinal acoustic phonons at significant diffraction planes on selected halide perovskites using SIKA in last January and due to run another set of measurements with TAIPAN in March. The neutron scattering school would help me understand detailed theories and practicalities of the neutron characterizing techniques and help me characterize single crystal perovskites and other potential HCA materials. It will significantly help me with my PhD project.

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MACROMOLECULAR EPOXY STRADDLED ORGANIC RADICALS

Author(s): Jaworski Capricho¹

Co-author(s): Bronwyn Fox¹; Nishar Hameed¹

¹ Swinburne University of Technology

Corresponding Author(s): jcapricho@swin.edu.au, blfox@swin.edu.au

Relying on the delocalized π -electrons as the electroactive element for charge transport, conjugated organic macromolecular backbones enhanced with chemical dopants have been in the forefront of many contemporary conductive devices. Material design out of persistent organic radical based on nitroxide moiety that can facilitate electric conduction without metal ions and π -electron overlap is a radical alternative for conjugated polymers. When in large densities on a polymer backbone, electron movement is brought about not by leveraging on the overlapping of π -orbitals but by the radical to radical hopping of monovalent electrons. When an organic radical polymer with pendant nitroxide groups possessing a conductivity value of 20 S m⁻¹ has been demonstrated, it catalysed renewed interest in radical chemistry that can encroach the realm reserved for traditional conjugated polymers. [2] However, such polymeric designs have not been reported so far for epoxy-based thermosets, although, multifarious contrivances with conductive epoxy matrices have been developed. [3]–[5] An epoxy monomer with organic free radical unit based on 4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl was synthesized and characterized. The chemical structure of this epoxy monomer was confirmed with FTIR, UV-VIS and 1H-NMR. The molecular weight was obtained after analysis using UPLC-MS as the [M+1]⁺ base ion. Electron paramagnetic resonance spectroscopy revealed persistent organic radical character even after chemical modification. DSC analysis of cured polymer samples using an amine based crosslinker exhibited comparable glass transition temperature with DGEBA resin. The electrochemical properties of this material will be investigated and the potential for electronic devices will be explored.

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Measurement of Residual Stresses for Development of Ultrasonic Measurement Techniques

James Hughes¹ ; Andrei Kotousov¹

¹ *The University of Adelaide*

Corresponding Author(s): a1669202@adelaide.edu.au, andrei.kotousov@adelaide.edu.au

The characterisation of residual stresses is of great importance in aerospace, railway, and mechanical engineering industries. Current methods for residual stress determination, such as hole-drilling or sectioning, are destructive in nature and therefore cannot be readily applied in-situ. Alternative methods, such as neutron scattering, require the use of highly specialised equipment which is not typically available. Therefore, there is a need to investigate alternative residual stress measurement techniques that are cost effective, accurate, and can be applied in-situ.

The current project is focused on promising stress measurement techniques which exploit the properties of guided waves. Measurement of stresses can be achieved through the utilisation of a range of phenomena, for example, the acoustoelastic effect or the rate of accumulation of higher order harmonics. The acoustoelastic effect has received considerable attention in recent years in regards to measurement of applied stresses, however, harmonic generation has received considerably less attention due to experimental difficulties.

In order to advance the field of ultrasonic stress measurements, it is important to accurately determine the residual stresses in the metallic samples which are used for ultrasonic testing. Residual stress measurements made using state of the art neutron scattering techniques could be used as a baseline to compare results gained through ultrasonic guided wave testing, and to validate the new ultrasonic methodologies developed.

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Metallurgical changes and mechanical properties of laser clad rail components

Olivia Kendall^{None}

Corresponding Author(s): olivia.kendall@monash.edu

High load bearing railways are relied upon as a main method of iron ore and coal transportation in Australia, however require ongoing maintenance and expenditure due to rapid rail degradation. These loading conditions are unique to our region and there is limited published research on this subject worldwide.

Increased axial loading, speed and haulage frequency promote wear and rolling contact fatigue between the wheel and railhead, facilitating plastic deformation, material loss and crack propagation before failure.

Surface engineering based maintenance strategies can be applied to improve the wear and fatigue resistance of rails. Laser cladding is an additive manufacturing process which employs a laser beam to metallurgically bond a layer of metallic powder to the substrate. This allows deposition of a material with superior tribological properties to protect the underlying bulk rail and increase the service life.

This project intends to systematically compare the effect of laser cladding of wear resistant alloys 410L, SS420, 415 and Stellite 6 on heavy-haul hypereutectoid rail steel by characterising the microstructure and the wear and fatigue properties after testing using a twin disc rolling tribometer to simulate in-field forces.

The laser cladding process results in high residual stresses due thermal expansion coefficient mismatch between the cladding and substrate, solidification shrinkage and localised high temperature

inputs into the heat affected zones. Therefore, neutron diffraction analysis can provide in-depth internal residual stress measurements which will be used to refine the laser cladding process.

The critical combination of residual stresses and rail-wheel contact stresses will lead to fracture or complete failure. Accurate evaluation and measurement of residual stresses using neutron diffraction is beneficial in the prediction of fatigue life.

The outcomes of this research will be used to establish new cladding alloys and optimised processing parameters for laser cladding rail repairs and to develop economical maintenance strategies.

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Multimodular interactions in TRIM21-mediated ubiquitination

Zuzanna Pietras¹ ; Maria Sunnerhagen¹ ; Cy Jeffries² ; Anthony Duff³ ; Kathleen Wood⁴ ; Francesca Caporaletti⁵

¹ *Linköping University*

² *EMBL Hamburg*

³ *ANSTO*

⁴ *Australian Nuclear Science and Technology Organisation*

⁵ *ILL*

Corresponding Author(s): anthony.duff@ansto.gov.au, zuzanna.pietras@liu.se, kwo@ansto.gov.au

The process of ubiquitination, leading to protein destruction via the proteasome, is tightly controlled by E1, E2 and E3 enzymes in a cascade of reactions. Multimodular protein complexes are critical in this process. In particular, E2-E3 complexes hold critical roles as both molecular matchmakers and catalysts, by bringing together the correctly activated ubiquitin with the appropriate substrates. The RING, B-box and coiled-coil (RBCC) domains of the disease-related TRIM proteins jointly form a multimodular platform.

We found that the TRIM21-coiled-coil houses the epitope targeted in fetal heart block, and that patient epitopes in the RING impair ubiquitination. Our preliminary results suggest that the TRIM21 coiled-coil region plays an activating role in TRIM21-mediated ubiquitination, similar to the helical E2-activating region in the unrelated but multimodular E3 gp78. Emerging visualization of TRIM assemblies have been obtained by crystallography and/or SAXS, and an inhibitory role of the B-box in TRIM21 has been proposed. Still, how TRIM multimodularity regulates ubiquitination is poorly understood.

We aim to describe the structural envelope of the TRIM21-E2-Ub complex by tailored SANS experiment exploiting alternate deuteration of the TRIM21 and E2-Ub. SANS data will together with our NMR, crystallography and SAXS data enable us to derive a complete model for the active TRIM21-RBCC-E2-Ub multimodular assembly, which will serve as a basis for the design of novel therapeutic strategies. This project is in collaboration with ANSTO National Deuteration Facility and QUOKKA beamline.

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Porosity and pore size distribution of flyash/slag based geopolymer using small angle neutron scattering

Tran Huyen Vu¹

¹ *PhD candidate, UTS*

Corresponding Author(s): tran.h.vu-1@student.uts.edu.au

The project at UTS involves chloride induced steel reinforcement corrosion in geopolymers. Chloride ions penetrate into ordinary Portland cement (OPC) concrete mostly by diffusion but capillary absorption and permeation are other mechanisms. All these mechanisms involve transport of chloride ions (0.368 nanometer diameter) through macro pores, micro pores down to 10 nanometer size. Below about 10 nanometer size pores the transport of chloride ions is unlikely.

In geopolymer concrete, however, the size of pores formed and the pore size distribution can be different to OPC concrete because of different chemical gels that are formed and hence changing the tortuosity. Hence evaluating the porosity, pore characteristics (e.g. tortuosity) and pore size distribution of geopolymers is vital for the use of this material for aggressive environments with regard to reinforcement corrosion. Methods such as MIP and VPV have limitations due to high pressure requirements in forcing mercury into concrete specimens (in MIP) and achieving sufficient level of vacuum (VPV).

My experimental program relies on accurate porosity and pore size distribution measurements of geopolymers using techniques such as Neutron scattering, MIP, VPV and Nitrogen adsorption. Other tests include chloride diffusion and corrosion rate of reinforcement of many geopolymer concrete mixes made from a one part geopolymer, where the binder consists of fly ash and slag.

Using facilities available at ANSTO, geopolymer specimens of geopolymer mortar and concrete will be tested for porosity and pore size distribution. Mortar and concrete cylinders of 50mm diameter and 100mm height and slices of 5mm thick and 50mm diameter cut from these cylinders will be tested. The ANSTO instruments used will be as follows:

1. Quokka small angle Neutron Scattering/Bilby small angle Neutron Scattering: Pores in the range of 1-10 nanometer.
2. Dingo Neutron Imaging
3. Kookaburra ultra small angle Neutron Scattering

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Properties of palladium hydride formed above the thermodynamic critical point

Samaneh Sadat Setayandeh¹ ; Evan Gray¹ ; Jim Webb¹

¹ *Queensland Micro- and Nanotechnology Centre, Griffith University*

Corresponding Author(s): e.gray@griffith.edu.au, jim.webb7@gmail.com, samaneh.setayandeh@griffithuni.edu.au

PdH_x where 0 < x < 1 may be formed by exposing clean Pd metal to H₂ gas or by electrolytic charging. At room temperature (RT), 1 bar H₂ gas pressure suffices to achieve x=0.7, although at least 10 kilobar is required to approach x=1 at RT. At 300°C, just above the critical point (T_{crit} = 291 ± 2°C; p_{crit} = 19.7 ± 0.2 atm H₂), about 100 bar is necessary to attain x=0.6. B-PdH_x formed above the critical point is interesting because it is relatively dislocation-free. This is expected from the absence of pressure hysteresis and was demonstrated by electron microscopy, which revealed the formation of dislocations at RT as the pure B-phase transformed to alpha phase. The nature of conventionally formed PdH_x at RT and below is well understood in terms of octahedral (oct) interstitial. At elevated temperatures, however, the state of H (D) in Pd has always been controversial. It has been concluded from neutron diffraction studies performed at ANSTO that significant tetrahedral (tet) D occupancy occurs at 300°C. Tetrahedral occupancy is also claimed to be observed in nanoscopic PdH_{0.363} at 300 K. Tetrahedral occupancy is supported by ab-initio calculations, which show that H in the tet site is in a virtual bound state, whereas D and T are in bound states, owing to their progressively lower zero-point energies. A question therefore arises as to the H(D) occupancy in B-phase samples that have been slowly cooled or quenched to RT from above the critical point, and whether the tet occupancy is additional or alternative to oct occupancy.

Here a careful survey is reported, by high-resolution gravimetry, of the pressure-composition behaviour of PdH_x formed above the critical point and cooled to RT, to determine if this preparation leads to extra hydrogen absorption compared to passage through the two-phase region at RT.

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Residual strain distribution in cold-sprayed copper 3D-printed parts

Author(s): Rebecca Adamson¹

Co-author(s): Andrew Duguid²; Krishnan Kannoorpatti¹; Rebecca Murray¹; Vladimir Luzin³

¹ Charles Darwin University

² SPEE3D

³ ANSTO

Corresponding Author(s): rebecca.murray@cdu.edu.au, krishnan.kannoorpatti@cdu.edu.au, vll@ansto.gov.au, rebecca.adamson@cdu.edu.au, andrew.duguid@spee3d.com

The Advanced Manufacturing Alliance (AMA) at Charles Darwin University makes 3D metal printed parts in complex shapes using a unique cold-spray based technique on the world's first LightSPEE3D printer. However, the cold-spray 3D printing method creates different, and undesirable, residual stresses from other novel and traditional manufacturing techniques due to the high plastic deformation of metal particles on impact and the complex machine paths of the LightSPEE3D that allow the process to build freeform three-dimensional components. AMA's first experiment at the ANSTO diffractometer KOWARI measured residual strain in bulk cold-sprayed copper parts. The neutron diffraction technique was required to measure strain inside these components due to their size.

The AMA team scanned the residual strains in three copper parts of different geometries printed using the LightSPEE3D, a cylinder, a hexagonal prism and a funnel-like sample. The results showed that the residual strains were far lower than expected. One possible explanation for this could be that the residual strains are getting annealed during material deposition due to thermal input from the sprayed particles. An alternative explanation is that the residual strains may be expressed as micro-strains across individual grains, which are much smaller than the 1mm voxel size. If high micro-strains are averaged to give a macro-strain, future work with reduced voxel size could complement the macro technique to better understand the results.

AMA will continue to carry out further experiments at ANSTO to build on the initial work and further characterise cold-sprayed components made from copper, aluminium, aluminium bronze and stainless steel. The findings from these will be complemented by a range of other destructive and non-destructive testing methods and enable validation of an individual NDT-based quality certification method for one-off and custom metal components manufactured using the LightSPEE3D.

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Spontaneous Ferroelectric-Relaxor Transition in (Bi_{1/2}Na_{1/2})TiO₃-12BaTiO₃ Piezoceramics and Role of Point Defects

Xi Shi¹; Nitish Kumar^{None}; Mark Hoffman^{None}

¹ unsw

Corresponding Author(s): xi.shi@unsw.edu.au

Using temperature-dependent X-ray diffraction, Raman spectroscopy and dielectric measurement, the (0.88Bi_{1/2}Na_{1/2})TiO₃-0.12BaTiO₃ (BNT-12BT) solid solution is shown to exhibit a spontaneous ferroelectric to relaxor (FE-R) transition at 200 °C during heating, a behavior similar to BKT ((Bi_{1/2}K_{1/2})TiO₃) or PST (Pb(Sc_{1/2}Ta_{1/2})O₃). The microscopic mechanisms responsible for stabilization of ferroelectric phase on adding BT to relaxor BNT have been discussed. Further, point defects were intentionally introduced using nonstoichiometry. It is found that on addition of excess bismuth in BNT-12BT, the concentration of oxygen vacancies reduces, which is accompanied by a reduction in FE-R transition temperature (149.1 °C). On the other hand, a bismuth deficiency resulted in a higher oxygen vacancy concentration and FE-R temperature (225.7 °C). Finally, electric field-temperature (E-T) phase diagrams have been constructed, which summarise the evolution of polar nanoregions (PNRs) with temperature and electric field, and demonstrate the role of oxygen vacancies.

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Structure Investigation of protonated molybdenum oxides: Towards ultrafast and high energy proton batteries

Author(s): Haocheng Guo¹

Co-author(s): Neeraj Sharma² ; Chuan Zhao³

¹ *university of new south wales*

² *UNSW*

³ *University of New South Wales*

Corresponding Author(s): chuan.zhao@unsw.edu.au, haocheng.guo@student.unsw.edu.au, neeraj.sharma@unsw.edu.au

It is always challenging to develop battery-materials also possessing high rate-capability and cycle life like supercapacitors. Recently, new lights might be shed by findings of proton-intercalative materials, where a new proton-battery chemistry can be then established. Utilizing protons as charge-carriers, batteries could require no diffusion for charge-transfer, thus capable to bear a high rate while maintain decent capacity. Additionally, built on the most abundant element in earth-crust, proton-battery also holds bright prospects in scalable energy storage and renewable energy conversion.

Our project concerns developing novel bronze-forming metal oxide as electrodes for proton battery. Now we are focusing on α -MoO₃ as it presents advantages: 1. A high capacity up to 372 mAh g⁻¹ can be delivered with decent voltage, 2. The semi-conductive nature of formed bronzes further facilitate the high rate-capability, 3. Long cycling life due to the reasonable stability. Moreover, the mechanisms how lattice-oxygens mediate proton transfers inside oxides can be gradually deciphered, thus better guiding future materials development. Our preliminary results show the electrochemical properties and reversibility of the anode, but the exact structures at different stages and how they evolve need further in-depth investigation.

Through neutron-based techniques, one of the only several approaches capable to directly probe hydrogen activity, we wish to investigate the mechanism of electrode (de)protonation and to evaluate whether it is a pure (de)hydrogenation or via co-(de)hydration (if yes, how much the degree). We wish to obtain structure information of anode in important stages. These will build up an unparalleled picture of function with which we can further build the mechanism of proton battery.

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Studying the dynamics of reaction-induced porosity in nickel-iron sulphide ore minerals

Muhammet Kartal¹ ; Fang Xia¹ ; David Ralph¹ ; Jitendra Mata²

¹ *Murdoch University*

² *ANSTO*

Corresponding Author(s): jtm@ansto.gov.au, d.ralph@murdoch.edu.au, fang.xia@murdoch.edu.au, muhammet.kartal@murdoch.edu.au

Porosity generation and further evolution are common features of mineral-fluid reactions forming secondary mineral/s on the outer surface of the primary mineral. Such reaction-induced porosity is dynamic and can be a transient feature or can survive geological time¹. Evolution of such porosity during and after mineral-fluid reactions is still poorly understood. Understanding the reaction-induced porosity is important because porosity is contributing to rock permeability which controls the hydrothermal fluids flowing in the crust to form ore deposit; and porosity generation is essential for the emerging greener in situ recovery of base metals from ore deposit without traditional mining.

To fill this knowledge gap, a quantitative understanding of reaction-induced porosity is essential. The key parameters are total porosity, pore size distribution, specific surface area, open-closed pore ratio which can be obtained from USANS/SANS measurement, as been demonstrated in the proof

of concept study of sulphide minerals[2]. Combining such information with experimental results about textural properties such as pore geometry/size distribution/connectivity as well as chemical composition, phase structure, crystal orientation during initial pore formation, and pore coarsening at later stages allow us to evaluate the dynamics of reaction-induced porosity.

To this end, we propose to study the porosity evolution in the replacement of pentlandite by violarite as a model mineral replacement reaction. This is because (i) economically pentlandite and violarite are the major nickel sulphides contributing ~60% of the world's total nickel production[3], and Australia holds the highest nickel resources in the world at 19 million MT (~24.3 %), is the fifth-largest nickel producer in the world[4], (ii) scientifically the reaction-induced porosity is important for understanding the mineralisation in/around nickel deposits and the reactivity during hydrometallurgical processes[5].

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Synthesis and reaction mechanisms of plasmonic sodium tungsten bronze nanoparticles

Author(s): Levi Tegg¹

Co-author(s): Dylan Cuskelly²; Erich Kisi²; Vicki J. Keast¹

¹ School of Mathematical and Physical Sciences, University of Newcastle

² School of Engineering, University of Newcastle

Corresponding Author(s): vicki.keast@newcastle.edu.au, levi.tegg@uon.edu.au

The sodium tungsten bronzes (Na_xWO_3 , $0 \leq x \leq 1$) are sub-stoichiometric insertion compounds, with a perovskite-like unit cell and a Na:W ratio of x . They have recently gained interest as a novel material platform for nanophotonics due to their tunable, low-loss plasmon resonances and their high chemical stability. Our group has reported bulk-scale nanoparticle fabrication using a furnace-assisted technique, but the reaction kinetics and mechanisms leading to Na_xWO_3 synthesis are not well understood, and further reductions in nanoparticle size would be ideal. Many plasmonics-enhanced devices benefit from very small nanoparticles, so understanding the factors which drive or inhibit grain growth during sintering are essential. Here, we discuss potential reaction mechanisms for Na_xWO_3 synthesis using ex-situ X-ray diffraction data and calculated results from density functional theory. We have found that compounds in the $\text{Na}_2\text{WO}_4:\text{WO}_3$ binary appear as secondary phases when the firing parameters are suboptimal, and that the firing temperature which gives the highest reaction yield varies with the x , similar to the variation in the $\text{Na}_2\text{WO}_4:\text{WO}_3$ liquidus. This poster will also include experimental results from electron energy-loss spectroscopy (EELS), supported by simulated responses. We show that Na_xWO_3 exhibits nanoparticle plasmon resonances which are tunable not only by geometry, but also by composition by varying x . These tunable optical properties, combined with their low preparation cost and high chemical stability, makes these materials attractive for applications in solar-control filtering and large-scale plasmonic photocatalysis.

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The Effect of Temperature and Pressure on Functional Materials

Gemma Turner¹

¹ *The University of Western Australia*

Corresponding Author(s): gemma.turner@research.uwa.edu.au

Functional materials are essential components in a wide range of technologies and devices, from quantum computers to invisibility cloaks. Magnetic, optical and electronic properties are native to a broad range of organic and inorganic materials, and can be induced in materials without native functionality by guest adsorption or by an external stimulus (e.g. light, temperature or pressure).

In most cases, these materials are crystalline or polycrystalline due to the requirement of ordering or long-range interactions for holistic functionality. As such, scattering techniques can be used to examine their structure-property relationships. An understanding of these relationships is required to optimise the functional property of a material for a given application.

Here, powder and single crystal X-ray crystallography at extreme conditions is used to examine the structure of a range of crystalline functional materials at variable temperature and pressure in relation to their functional property. Initial work has used variable-temperature high-pressure experiments to trap the spin states of a spin crossover Fe(II) Hofmann framework, allowing the structural changes arising solely from the spin-transition to be identified. This work provides an insight into the true structural mechanism of SCO, without accompanying thermal or barometric effects. Current work is focussed on the pressure-dependent fluorescent behaviour of a set of organic luminogens, which may be applied to OLED displays. In the future, diffraction techniques will be used to study the crystal and magnetic structure of magnetic materials, as well as the structural and mechanical behaviour of functional porous materials under pressure.

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ULTRASHORT SELF-ASSEMBLING PEPTIDES AS ANTIMICROBIAL AGENTS: INTERACTIONS WITH MODEL MEMBRANES

Author(s): Priscila Cardoso¹

Co-author(s): Gary Bryant²; Charlotte Conn³; Celine Valery³; Meikle Thomas³

¹ *Royal Melbourne Institute of Technology (RMIT)*

² *Centre for Molecular and Nanoscale Physics, School of Applied Sciences, RMIT University*

³ *RMIT*

Corresponding Author(s): celine.valery@rmit.edu.au, thomas.meikle@rmit.edu.au, cardosopriscila18@gmail.com, charlotte.conn@rmit.edu.au, gary.bryant@rmit.edu.au

Research on novel antimicrobial therapies is a high priority both at national and global level, given the recent WHO data on antibiotic resistance (1). Recent work has demonstrated that ultrashort peptide sequences can display anti-microbial activity (2,3). We hypothesized that novel families of antimicrobial agents can be designed from small self-assembling peptide building blocks. Through the investigation of de novo peptide self-assembling mechanism and interactions with model lipid phases, we intend to optimise the peptide sequences towards novel antimicrobial formulations and biomaterials.

We designed two peptide family sets: i) 3-5 amino-acid peptides inspired from Battacin (4) and ii) 2-5 amino acid peptides selected through a bottom-up design approach. In this research, we use small angle X-ray scattering, X-ray reflectometry and neutron scattering, amongst other techniques, to investigate de novo peptide self-assembly into nanostructures and the peptide antimicrobial mechanism of action. The mechanism of action of antimicrobial peptides (AMPs) is believed to result from an interaction between the peptide and the microbial lipid bilayers, leading to a loss of structural integrity of the microbial cell membrane (3,5). This project investigates the peptide interactions with model lipid membranes of different compositions.

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