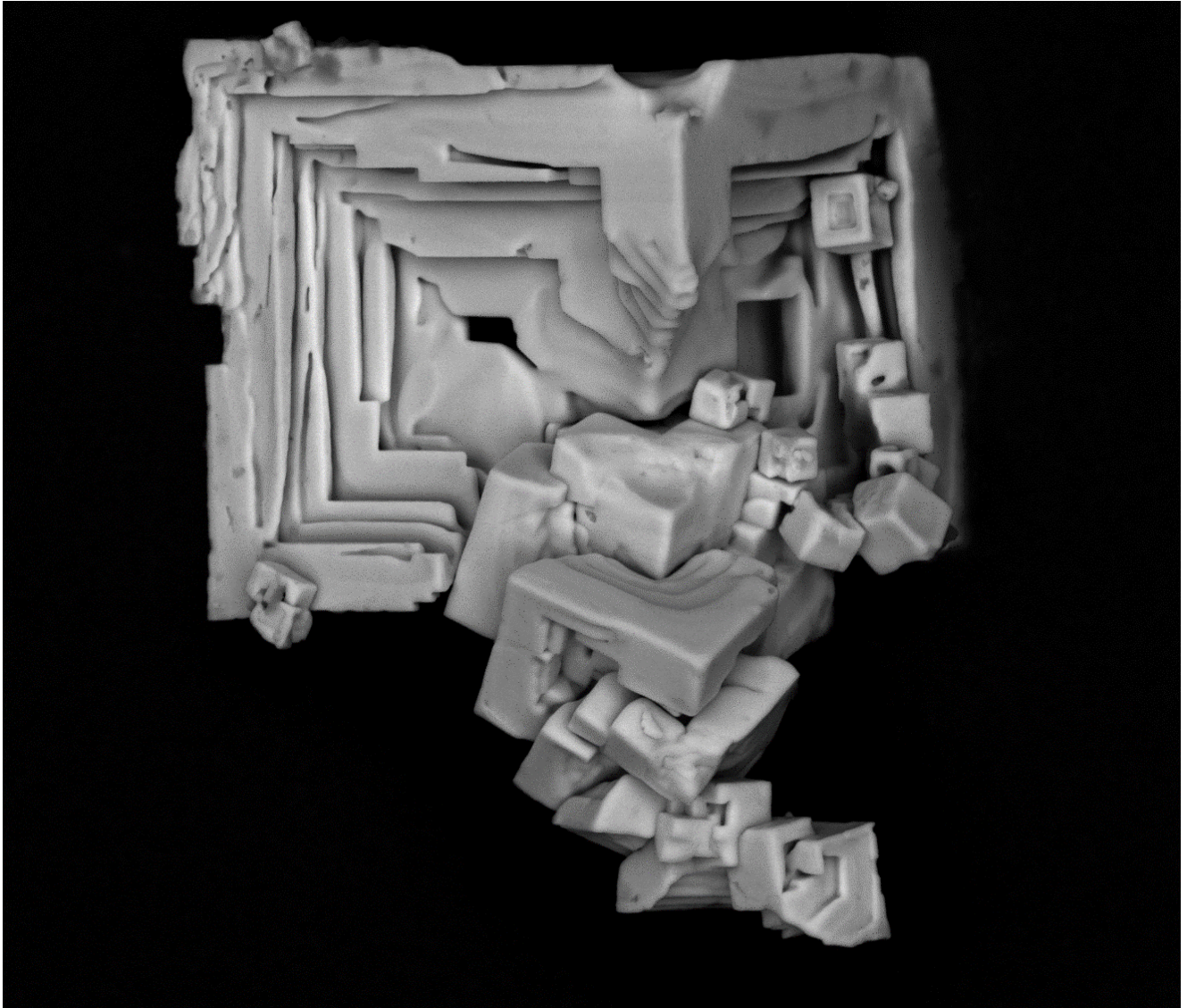


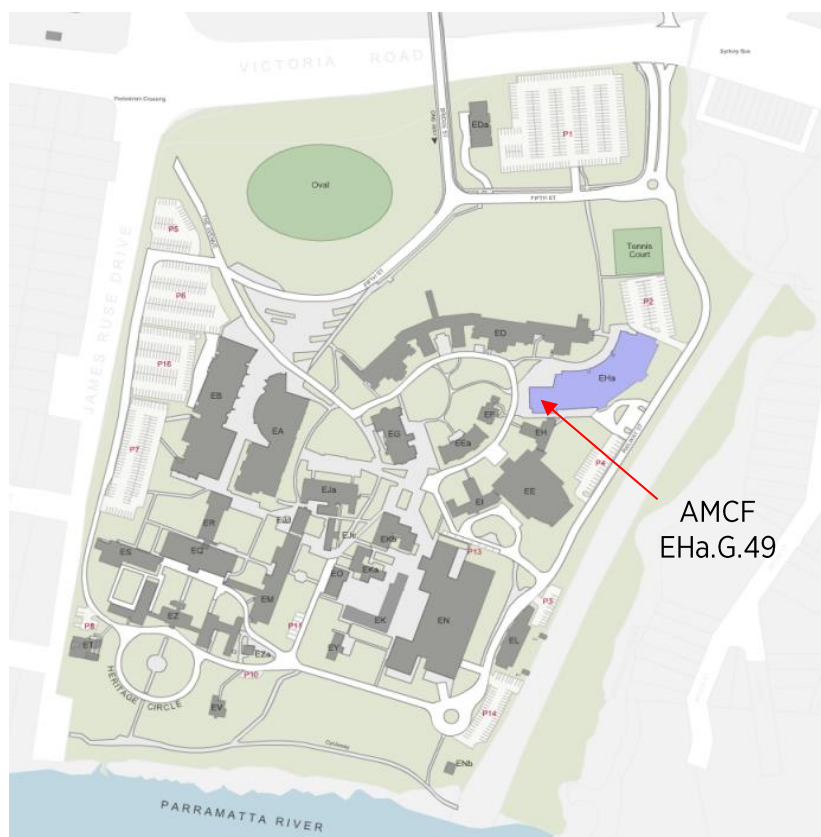
WESTERN SYDNEY
UNIVERSITY



AMCF

Advanced Materials Characterisation Facility

Newsletter: December 2022



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Front Cover Image:

A backscattered SEM image of potassium iodide crystals from Masters student Kenny Zhang, taken by Daniel Fanna on a Hitachi TM4000 SEM (mag x1000, 15 kV, uncoated high vacuum).

Back Cover Image:

A pseudo coloured X-ray map (XRM) of cement concrete sample with gel reaction zone from AMCF user Brendan Boyd-Weetman collected on our Jeol 8600 probe by Richard Wuhler.

10th Edition Newsletter, December 2022

Editors: Daniel Fanna, Laurel George and Richard Wuhler

The AMCF is a part of the:

Research Infrastructure

Research Services

Office of the Deputy Vice-Chancellor (Research, Enterprise and International)



FROM THE FACILITY RESEARCH MANAGER

By the time you receive this newsletter, we will be a couple weeks from Christmas and the end of another year. What happened to 2022? It feels like a big blur with many things happening.

This year began with many users trying to catch up on their incomplete analysis that was disrupted by COVID restrictions through 2020/2021. At the beginning of the year, the AMC Facility initially had many researchers and academics utilising our instrumentation. Over the last 4 months though, we have seen a rapid increase in the number of HDR's requiring access and training. This is great to see. The facility already has several dozen bookings for January and February 2023.

As you read through the newsletter you will see why the year has passed so quickly. Many users have operated a variety of instrumentation (accounting for over 10,000 hours of usage); the number of courses, workshops and masterclasses offered in the second half of the year have increased; we have enjoyed the presence of some international visitors and small tour groups; we have had a number of instrument upgrades; and new software upgrades. Indeed, the AMC Facility, in conjunction with Bruker, have just finished a 3-day workshop on "TOPAS", a profile fitting based software for quantitative phase analysis, microstructure analysis and crystal structure analysis. Well done Daniel for organising!

In the last month we had a couple of new instruments placed in the AMC Facility for demonstrations and these will be installed before Christmas.

The New Year will be busy as we plan to run various introductory workshops on our instruments. The first course/workshop is in February 2023 in conjunction with Netzsch. The course is titled, "Thermal Analysis Using Differential Scanning Calorimetry (DSC)". Further information can be found in this newsletter.

As always, we are happy to show anyone our facility. Do not hesitate to contact us for a walk through our labs.

The AMC Facility will be closed for the Christmas to New Year period from Friday 16th of December (12pm) until Tuesday 3rd of January 2023. No usage of instrumentation and/or bookings will be possible due to the closure. Instruments will either be shut down or placed in standby mode during this period. All instruments should be up and running again by Wednesday 4th of January 2023.

On a final note, I would like to wish everyone a safe and Merry Christmas and Happy New Year. I look forward to seeing everyone in the New Year.

Dr Richard Wuhler
Facility Research Manager,
AMC Facility
06/12/2022

RECENT ACTIVITIES

WSU TOPAS Workshop

The AMCF was delighted to finally see the return to face-to-face workshops, courses and masterclasses this year. This included a workshop co-organised by Bruker, on their TOPAS (Total Pattern Analysis Solutions) X-Ray Diffraction (XRD) software run by preeminent expert Ian Madsen. The 3-day workshop was conducted at the WSU Parramatta South campus from the 21st to the 23rd of November and attracted attendees from several universities, ANSTO and Australian industry giants in mining and construction. Ian's workshop was a level 1 TOPAS beginner course aimed at intermediate XRD users looking to take



Left to right, Richard Wuhrer, Daniel Fanna and Ian Madsen.

the next step in their data processing. It is worth mentioning that TOPAS is an incredibly powerful and versatile software package and the 3-day workshop only allowed the top surface of functionality to be scratched.

Day 1 of the workshop opened with Ian presenting an introduction to TOPAS. This flowed into other topics such as the information content of a powder diffraction pattern, peak profile fitting, crystallite size/strain determination and specimen preparation. Attendees were guided through several tutorials related to single peak and whole pattern convolutions, whole pattern profile fitting models as well as crystallite size and strain analysis.

The second day of the workshop focused on quantitative phase analysis (QPA) of XRD patterns and guided users through several different QPA strategies. These included Rietveld, Partial Or No Known Structure (PONKCS) as well as strategies for quantifying the amorphous content of samples and more. Ian enlightened users to some tips, tricks and pitfalls in QPA including micro-absorption, errors in sample preparation and modelling, and provided information on what to look out for when extracting crystal structures from databases.

On the third day, attendees were introduced to TOPAS's launch mode and jEdit, a free Java-based text editor. Here, Ian guided attendees through setting up input files as well as showing the power of launch mode for processing batch data sets of in-situ non-ambient XRD data. The workshop finished up with an engaging Q&A session where Ian took the time to address queries and provided insightful solutions to specific challenges the audience might have encountered during their own XRD analysis.

We thank Ian for taking the time to run the course. We cannot express enough how invaluable this was for users, industry partners and ourselves. A special mention should be extended to Neil Hughes from Bruker for supporting the event as well as Kim Shermain (Bruker), Hou Ran Low (Bruker) and Daniel Fanna (AMCF) for organisation. If you would like to get the most out of your XRD scans and/or are interested in indexing, QPA, whole pattern decompositions or other TOPAS features, please contact the AMCF team to discuss.

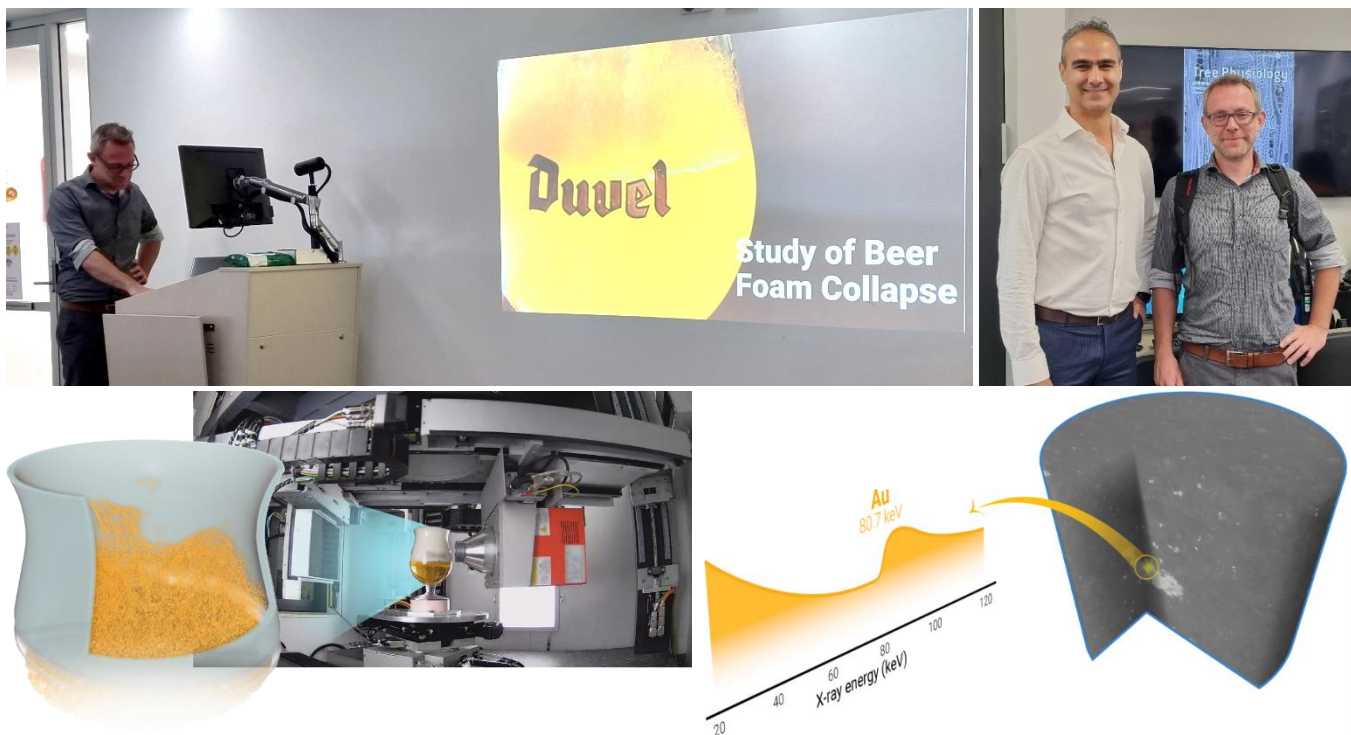


Workshop attendees working their way through TOPAS tutorials under the guidance of Ian Madsen.

TESCAN Micro-CT Lecture

In October we welcomed Frederik Coppens and Kamran Khajepour from TESCANA to give an insightful talk titled 'New dimensions to micro-CT imaging: Fast dynamic CT imaging and spectral CT on TESCANA micro-CT systems'. Micro-CT is a burgeoning field offering insights to specimen characterisation, previously unobtainable.

It was fantastic to see some of the new developments by TESCANA, particularly how the latest micro-CTs are fast to run and have the ability to provide chemical and compositional analysis. We were impressed by some of the outstanding capabilities of the instrument. These included the fast in-situ scanning of beer foam collapse to help better model foam dynamics, creating tastier beer; in-situ fluid permeation through a porous sample; and use of an energy-sensitive photon counting detector to identify gold and other precious elements within an unprocessed rock core.



Clockwise from top left: Frederik giving his talk on the study of beer foam collapse. Kamran (left) and Frederick (right) in the AMCF for a morning tea Q&A post talk. A fast in-situ micro-CT scan of beer foam collapse. Detection of gold within an unprocessed rock core.

Graduations 2022

It's always great to see our research students in their graduation gear, especially when they come to visit us so we can join the celebration. A big congratulations to Tia Richardson on the completion of her Masters of Research.

Tia's research, with supervisors Dr Jason Reynolds and Dr Ian Wright, focused on the analysis of wastewater which runs off mining sites into surrounding water systems. In particular she was interested in the geochemistry of minerals that form in the sediments settling in nearby creek beds. Tia has since been employed by one of our commercial clients, Membraneworks, and regularly visits the facility for characterisation work.

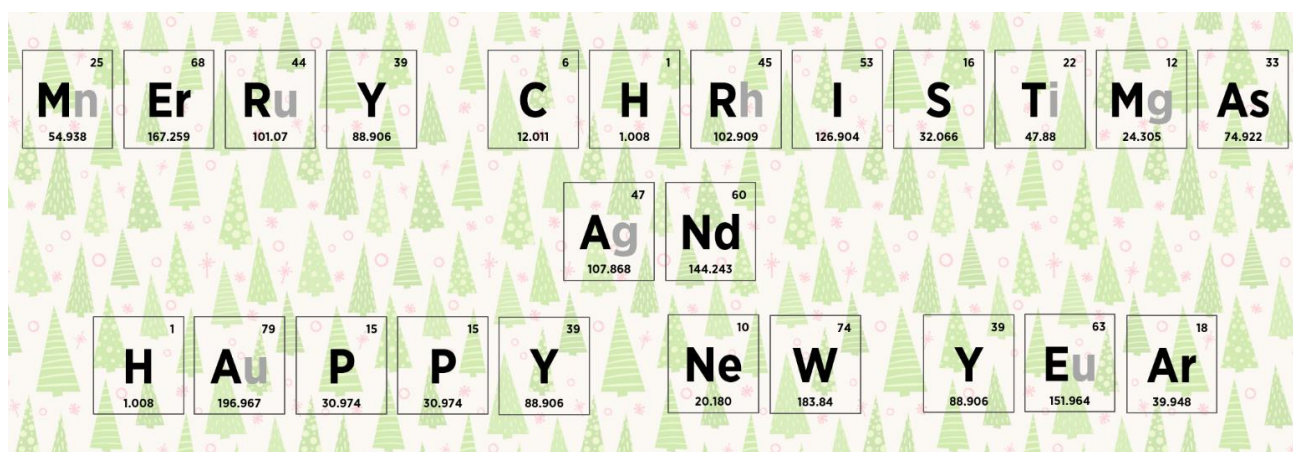


Newly graduated Tia Richardson, with Laurel George, Ric Wuhner and Daniel Fanna

Mandatory Leave and Christmas/New Year Closures

The AMC Facility will be closed for the mandatory Christmas to New Year leave period, from Friday 16th of December (12pm) until Tuesday 3rd of January 2023. Instruments will either be shut down or placed in standby mode during this period, and can therefore not be used/booked. All instruments should be up and running again by Wednesday 4th of January 2023.

- Friday 16th December, 2022: Last day AMCF labs are open for regular use.
- Tuesday 3rd January, 2023: Instrumentation start-up and checks.
- Wednesday 4th January, 2023: AMCF labs open again for regular use.



UPCOMING EVENTS

NETZSCH thermal analysis workshops

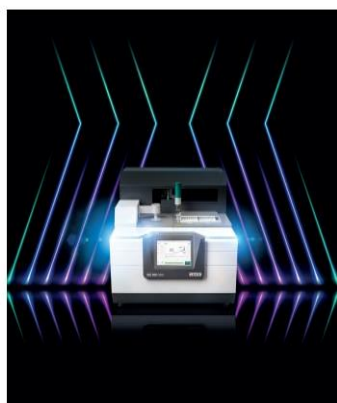
NETZSCH Australia will be running two Sydney based workshops in February 2023:

- Thermal analysis using Differential Scanning Calorimetry at WSU on the 6th of February 2023.
- Workshop: Introduction to Rheology & Rheology testing at UNSW on the 7th of February 2023.

Tickets are expected to sell fast. Please contact Andrew Gillen (Andrew.Gillen@netzsch.com) or Gisele Dickson (gisele.dickinson@netzsch.com) from NETZSCH Australia if you are interested.

Workshop: Thermal Analysis Using Differential Scanning Calorimetry (DSC)

Hosted by NETZSCH Analyzing & Testing



Monday,
February 6, 2023
Sydney¹⁾

Thursday,
February 9, 2023
Melbourne²⁾

Workshop: Introduction to Rheology & Rheological Testing

Hosted by NETZSCH Analyzing & Testing



Tuesday,
February 7, 2023
Sydney¹⁾

Friday,
February 10, 2023
Melbourne²⁾

Conferences to keep an eye on in 2023

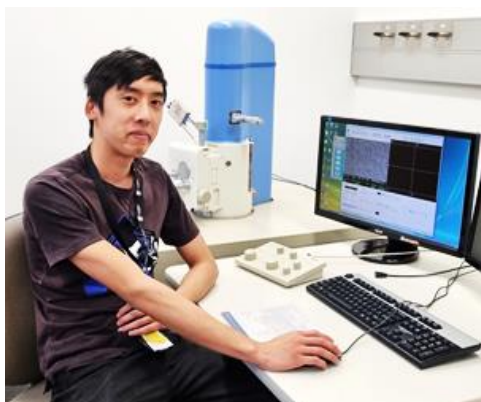
- The 27th Australian Conference on Microscope and Microanalysis (ACMM) will be held in Perth, January 2023. <https://acmm27.org/>
- The 26th Congress and General Assembly of the International Union of Crystallography (IUCr) will be hosted in the Melbourne Convention & Exhibition Centre, August 2023. <https://iucr2023.org/>



26TH CONGRESS AND GENERAL
ASSEMBLY OF THE INTERNATIONAL
UNION OF **CRYSTALLOGRAPHY**
22-29 August 2023
Melbourne Convention and Exhibition Centre
www.iucr2023.org

RESEARCHERS AT THE AMCF

Kenneth Zhang
School of Science



RESEARCH

Masters of Research student Kenneth Zhang has been synthesising Iron(II) metallocenesupramolecular compounds with various ligands and other transition metals, to explore the spin crossover phenomenon. This sensation is the ability for a compound to reversibly switch and stabilise between two spin states; high and low spin. Incorporating this phenomenon into coordination compounds with a large void space has many potential applications.

IMPACT

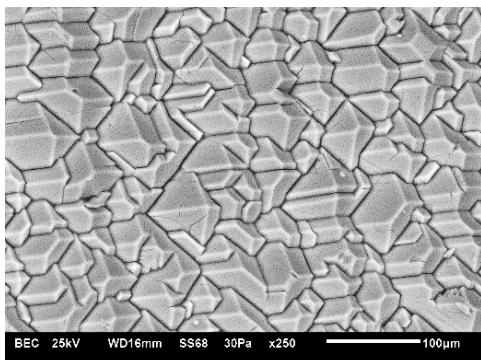
The ability of a material to be bistable in two different states enables for a variety of applications. These compounds can be utilised in drug delivery with the ability of encapsulating and releasing molecules. Additionally, these complexes may have applications in nanotechnology for data storage due to its differing magnetic properties

SUPERVISORS

Dr Feng Li, Dr Jason Reynolds and Dr Narsimha Reddy

INSTRUMENTS

Kenneth has been making good use of our **Mass Spectrometer**, **XRD**, **TGA-DSC** and **SEM-EDS** to characterise his samples.



Hyun Min
School of Science



RESEARCH

Hyun Min is a Master of Research student with the School of Science. Hyun has been creating spin crossover coordination cages by experimenting with a combination of different ligands and metals. Spin crossover materials are a type of molecular switch, which can reversibly change between two bistable states. By incorporating this magnetic property into coordination cages (which are large molecules containing internal voids) it can be used for a variety of multifunctional applications.

IMPACT

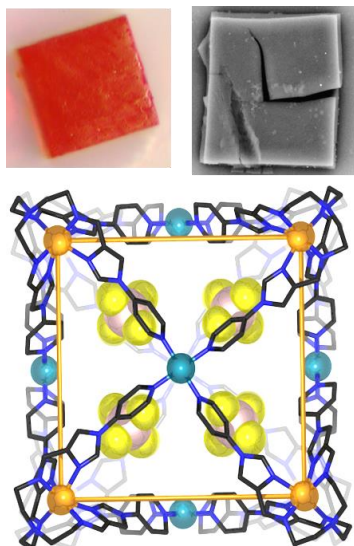
Materials which have the ability to “switch” can be used in a plethora of potential applications. These compounds can be used in nanotechnology for data storage and processing materials. Furthermore, these complexes can be used in medicine, where a molecule can be designed for drug delivery to specific areas for encapsulation and release.

SUPERVISORS

Dr Feng Li

INSTRUMENTS

Hyun has been using our **Mass Spectrometer**, **XRD**, **SEM-EDS**, **XRM** and **TGA-DSC** to characterise his coordination cages.



RESEARCHER FOCUS:

Dr Maggie Davidson

BACKGROUND

Dr Maggie Davidson is a senior lecturer and Occupational Hygienist in Environmental Health and Management at the WSU School of Science.

RESEARCH

Dr Davidson's research involves characterising the components of occupational aerosols (e.g. dust) in order to identify particles that may harm a person's lungs. She is also working with industry to find ways to eliminate or minimise exposures to protect worker health.

Presently, Dr Davidson is studying the constituents of fine hemp-based dusts with particles less than $<18\text{ }\mu\text{m}$, that can enter the respiratory region of the lung. It is important to characterise hazards, develop control strategies and establish exposure limits to protect workers in the emerging Australia hemp industry. Due to its illegal status, there is much we do not know about dust diseases associated with inhalation of cannabis containing dusts, and they are being found to be a complex mixture of organic and inorganic components, including the ubiquitous crystalline silica.

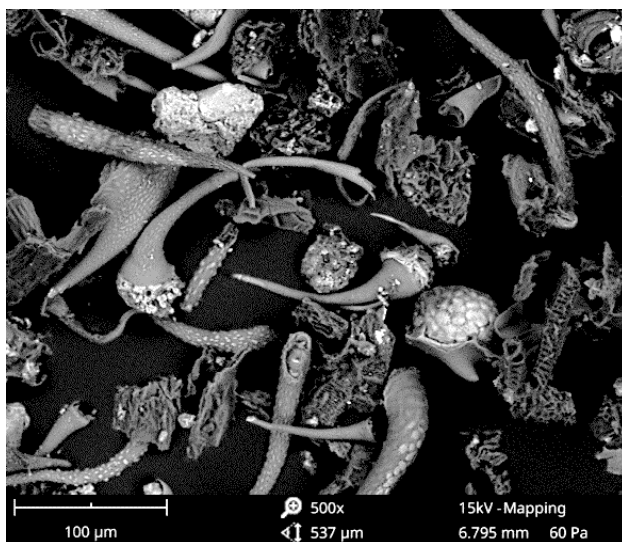
The health risk associated with cannabis dusts is complicated because they contain components that may have immunological (cannabis pollen, microorganisms, danders), toxic (pesticides, metals), infectious (microorganisms), irritant (soil, crystalline, plant material), and even carcinogenic effects (crystalline silica). This is a joint project between School of Science, the AMCF and NGS laboratory, and the Australian Industrial Hemp Alliance. Additionally, Maggie has also been analysing artificial stone dusts at the AMCF to identify if it contains components other than the crystalline silica which may pose a hazard to workers. This is part of an icare Dust Diseases Project called "Beyond Respirable Crystalline Silica: What makes artificial stone so toxic?".

IMPACT

Dr Davidson's work will help inform construction and hemp industries about the dangers present in occupational aerosols and will help avoid preventable deaths related to these workplace environments.

USE OF AMCF INSTRUMENTS

Dr Davidson has been using a number of instruments at the AMCF including our Phenom XL and Jeol 6510 Scanning Electron Microscopes with Energy Dispersive Spectroscopy (SEM-EDS), as well as our X-ray Diffractometer (XRD).



An SEM image of some particles that make up HEMP dust.

Dr Leigh Shepard

BACKGROUND

Dr Leigh Sheppard is a senior lecturer and Director of Academic Program (Advanced Engineering and the WSU-UNSW Collaborative Program) in the School of Engineering, Design and Built Environment.

Dr Sheppard's background is in advanced material processing. His primary research interests relate to the development of novel materials for sustainable hydrogen production via solar-driven photo-electrochemical water-splitting. Leigh has also contributed to the development of metallic coatings for orthopaedic applications, ultra-high strength nanocomposites, photocatalytic oxides, and graphene growth.

RESEARCH

Dr Sheppard's research is centred about understanding the relationships that exist between the way in which materials are processed, and the unique set of properties they possess as a result.

In recent years this has involved the use of reactive magnetron sputtering to make thin film deposits on objects. Using this instrumentation, materials with a controlled elemental composition can be deposited at thicknesses ranging from 5 nm to several 1000 nm. Simultaneous control of thickness and composition enables the fabrication of layered nanocomposites with properties that vary according to their depth from the surface.

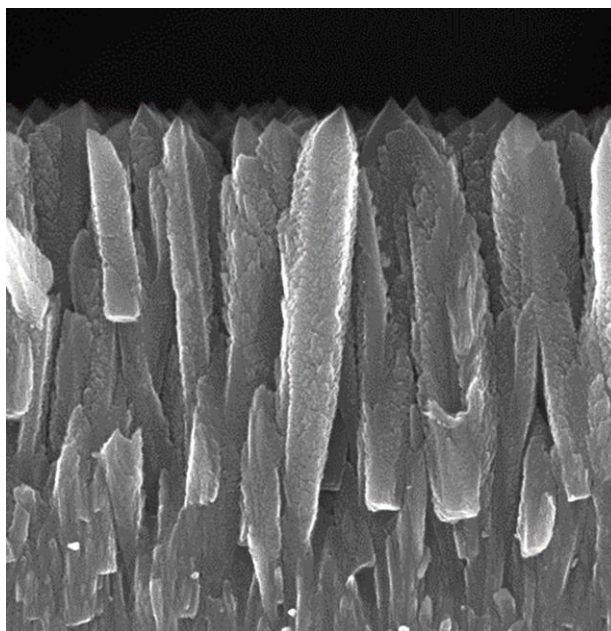
Understanding the crystal morphology of these films adds an additional dimension and is the basis behind the SEM image shown on this page. Leigh's expertise in material processing synergises closely with the characterisation expertise of the AMCF staff and they frequently collaborate on projects concerning advanced materials design and development.

IMPACT

Achieving a carbon-free route to hydrogen fuel will play a critical role in addressing climate change whilst securing the energy needs for growing standards of living. Towards this ultimate goal, Leigh's research is fundamental in nature and seeks to solve critical material challenges, such as achieving high chemical stability from an efficient solar material which must operate for years in sea water under full (or concentrated) sunlight.

USE OF AMCF INSTRUMENTS

Dr Leigh Sheppard has been using a number of instruments at the AMCF including our Zeiss Field Emission Gun - Scanning Electron Microscope (FEGSEM), Phenom XL and Jeol 6510 Scanning Electron Microscopes with Energy Dispersive Spectroscopy (SEM-EDS), as well as grazing incidence measurements on our X-ray Diffractometer (XRD).

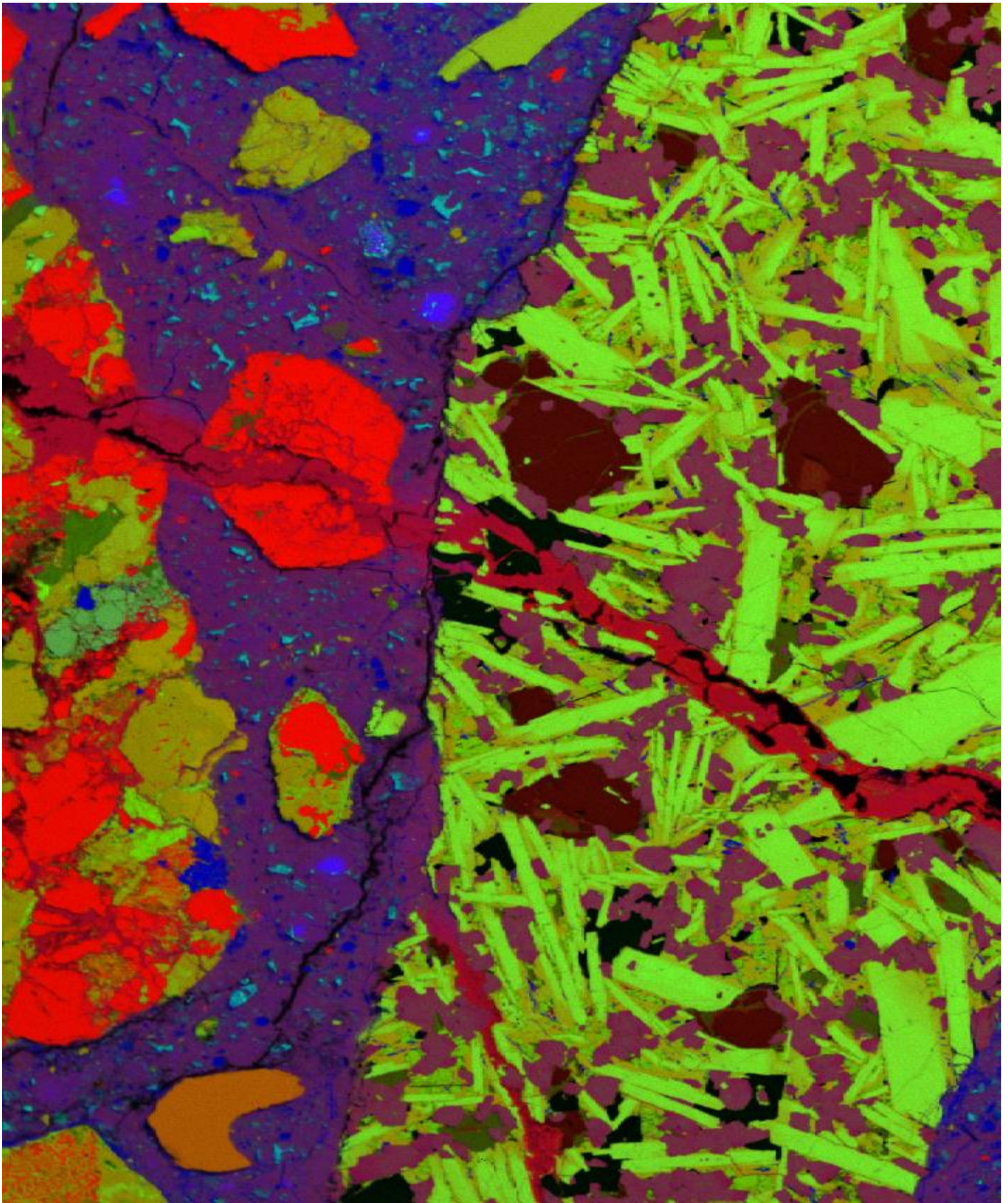


A FEG-SEM image showing crystallite growth formed during thin film deposition.

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2. Johanna Wong-Bajracharya, Vasanth R. Singan, Remo Monti, Krista L. Plett, Vivian Ng, Igor V. Grigoriev, Francis M. Martin, Ian C. Anderson, and Jonathan M. Plett, (2022), "The ectomycorrhizal fungus *Pisolithus microcarpus* encodes a microRNA involved in cross-kingdom gene silencing during symbiosis", *Proceedings of the National Academy of Sciences*, 119(3), e2103527119.
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8. Kash A. Bhullar, Michael M. Horgan, Ashley Le, David Fania, Richard Wuhrer, Valentin Razmovski- Naumovski, Kelvin Chan, Patrice Castignolles, Marianne Gaborieau, (2022), "Assessing the quantification of acetylation in konjac glucomannan via ATR-FTIR and solid-state NMR spectroscopy", *Carbohydrate Polymers*, 291, 119659.
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10. Mihee Shin, Min Zhang, Annika vom Scheidt, Matthew H. Pelletier, William R. Walsh, Penny J. Martens, Jamie J. Kruzic, Björn Busse, Bernd Gludovatz, (2022), "Impact of test environment on the fracture resistance of cortical bone", *Journal of the Mechanical Behavior of Biomedical Materials*, 129, 105155.
11. Santha Herath, Dharmappa Hagare, Zuhaib Siddiqui & Basant Maheshwari, (2022), "Microplastics in urban stormwater—developing a methodology for its monitoring", *Environmental Monitoring and Assessment*, 194(3), 1-15.
12. Jung-Eun Lee, John Connolly, Wen Yang, Guillaume Freychet, Taifeng Wang, Steven A. Herrera, Satoshi Murata, Phani Saketh Dasika, Devis Montroni, Anna Pohl, Chenhui Zhu, Mikhail Zhernenkov, Richard Wuhrer, Leigh Sheppard, Michiko Nemoto, Atsushi Arakaki, Pablo Zavattieri, & David Kisailus, (2022), "Fibrous anisotropy and mineral gradients Within the radula stylus of chiton: Controlled stiffness and damage tolerance in a flexible biological composite", *Journal of Composite Materials*, doi:10.1177/00219983221121867.
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14. Bhawantha M. Jayawardena, Resmi Menon, Mark R. Jones & Christopher E. Jones, (2022), Spectral Phasor Analysis of Nile Red Identifies Membrane Microenvironment Changes in the Presence of Amyloid Peptides. *Cell Biochemistry and Biophysics*, doi.org/10.1007/s12013-022-01105-0.
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16. Bhawantha M. Jayawardena, Lorraine Peacey, Roland Gamsjaeger & Christopher E. Jones, (2022), "Essential Role of Histidine for Rapid Copper (II)-Mediated Disassembly of Neurokinin B Amyloid", *Biomolecules*, 12(11), 1585.
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