Australian X-ray Analytical Association
Newsletter Issue 2 2018

President's Address

Dear AXAA Members and Friends,

On 4th July the National Council visited a number of venues in Brisbane and the Gold Coast, with the view to choosing a venue for AXAA-2020. As mentioned in the most recent Newsletters we considering changes to the conference format, especially regarding the Schools/Workshop component of the programme, and are currently looking at a 3-day event instead of the 5-day event of recent times. We welcome your thoughts on this and other matters, and invite you to contact the National Council with these (see contact details at the end of the Newsletter). We also welcome nominations from the AXAA community for AXAA-2020 Conference Committee members, so if you or someone you know is interested in helping to shape our next conference, please get in touch. We anticipate announcing the venue and dates for AXAA-2020 in our next Newlsetter.

AXAA Student Seminar events will be held in several states over the next few months. These events are an excellent opportunity for students to present their work in a friendly, collegial atmosphere and meet others in the X-ray and neutron scattering community. Prizes will be awarded to the best presentations. Stay tuned for announcements of each of these events.

Nathan Webster
AXAA President

AXAA Student Seminar Events

Dates are being set for this year's AXAA Student Seminars. Open to all students (honours to PhD), with any experience in X-ray or neutron techniques.

Prizes are up for grabs, so please encourage your students to come along and present their research!

Current dates for AXAA Student Seminar Days:

VIC - *"Something to Bragg About"*
October 23rd at CSIRO, Clayton
Contact: Natasha Wright
mailto:Natasha.Wright@csiro.au

WA - *"Bright Scatterers"*
October 25th at Curtin University
Contact: William Rickard
mailto:w.rickard@curtin.edu.au

QLD - *"Braggers"*
November 14th at The University of Queensland
Contact: Nathan Webster
mailto:Nathan.Webster@csiro.au

NSW - *"Scattering Matters"*
Date to be confirmed, at The Univeristy of New South Wales
Contact: Vanessa Peterson
mailto:vanessa.peterson@ansto.gov.au

SA - *"Scatterbrain"*
Date to be confirmed, at The University of South Australia
Contact: Sally Birch
mailto:Sally.Birch@csiro.au

Presenters at the 2016 AXAA Victorian Student Seminar Day.

Powder Diffraction at the Australian Synchrotron and OPAL: A workshop for beginners

25-27 September 2018, The University of Sydney

The powder diffraction teams from the Australian Synchrotron and OPAL in collaboration with Sydney Analytical at the University of Sydney are hosting a 3 day powder diffraction data analysis workshop for beginners aimed at post-graduate students and early career researchers.

This workshop aims to cover all stages of data analysis, beginning at sample preparation, radiation choice, experimental setup and data collection strategies, through to data analysis approaches.

Topics will include; basic crystallography, indexing, search-match, wavelength refinement, geometry corrections and an introduction to advanced analysis techniques. Tutorial sessions will be used to practically reinforce the material presented. Tutorials will be split into 2 parallel sessions: one using TOPAS, one using GSAS II.

Priority will be given to applicants with synchrotron or neutron data or with awarded beamtime. The workshop is free. Accommodation and some meals will be provided. Attendees from institutions that are members of AINSE should contact AINSE directly for travel support.

Lectures and tutorials will be presented by Dr Anita D'Angelo (AS), Dr. Helen Maynard-Casely (ACNS), Dr James Hester (ACNS) and Dr. Matthew Rowles (Curtin).

Applications:

For the application form, please contact: sydney.analytical@sydney.edu.au

The application form and supporting documents (including letter of support from supervisor) should be sent to sydney.analytical@sydney.edu.au by 5:00 pm Monday September 3rd 2018.

EPDIC 2018

The 16th European Powder Diffraction Conference (EPDIC16) was recently held in Edinburgh, UK, and was a great opportunity to attend the richly informative sessions covering the use of diffraction methods to analyse polycrystalline powders. The topics discussed included those on instrumentation, methodology, total scattering and thin film analysis, and the analysis of materials for energy, pharmaceutical and biological applications, plus more. A particular highlight was the EPDIC distinguished powder diffraction award lecture by awardee Bill David, who discussed his career including his work determining the crystal structure of C60. As for the social events, we enjoyed a drinks reception at The Signet Library, which was described as "the finest drawing room in Europe" by King George IV after its completion in 1822. Furthermore, the conference dinner saw delegates sampling Scottish whisky and learning ceilidh dancing. At the conference closing ceremony it was also revealed that the location of EPDIC17 would be the city of Šibenik, Croatia; a beautiful spot to enjoy a European summer and powder diffraction together!

IMA2018

XXII MEETING OF THE INTERNATIONAL MINERALOGICAL ASSOCIATION
13-17 AUGUST 2018 | MELBOURNE

The International Mineralogical Association Conference recently took place at the Melbourne Convention Centre. Delegates from Australia and around the world convened to discuss the latest developments in mineralogy, crystallography, and applied mineral sciences, both on Earth and elsewhere in the solar system. Presentation highlights included the discovery of rapid biogeochemical cycling of gold particles all across the world, a series of fascinating cases of meta-stable mineral formation, advances in sustainable metal recovery, including recovery of valuable metals from e-waste, and new insights into the composition of icy bodies such as Titan and Pluto. The exhibition included showcases of Australian mineral and gem collections, which provided some happy perusal during breaks.

The next IMA conference will be in the lovely Lyon region of France, it's only a shame to wait until 2022.

AXAA Website and Contacts

Please visit our website, www.axaa.org, for further information, or follow us on Twitter @axaa_org.

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William Rickard (Curtin University, WA)
Talitha Santini (University of Western Australia, WA)

AXAA Membership

All registered participants of the AXAA-2017 conference are automatically granted AXAA membership for 3 years. Alternatively, new memberships can be obtained free of charge, by making an application to the National Council.

Candidates should provide their CV and a short statement about how they intend to contribute to the organisation. Please send these to the National Council Secretary Mark Styles.

AXAA Resource Centre

There are a range of resources available on the AXAA website, including video recordings of the two Public Lectures at AXAA-2017, tips for Rietveld Analysis, Clay Analysis, XRF tips, and more. We welcome further contributions to our Resource Centre.

Next AXAA Newsletter

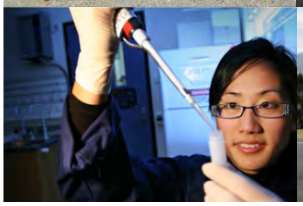
The next issue of the AXAA Newsletter will be distributed in December 2018. Please feel free to send contributions for the newsletter to Jessica Hamilton at *ausxray@gmail.com*. Any comments or feedback about the Newsletter are welcome.

A Day in the Life of an X-ray / Neutron Scientist

We are seeking posts for our 'Day in the Life' series. If you'd like to contribute, or know someone who might be interested, please contact National Council Communications Editor Jessica Hamilton at ausxray@gmail.com.
W:www.axaa.org/a-day-in-the-life.html





Bruker News Australia & New Zealand

Aug-18




Bruker Launches the S6 JAGUAR™ Benchtop WDXRF System for Elemental Analysis in Industry and Academia

Bruker announces the launch of the new S6 JAGUAR™, an exceptionally powerful and versatile benchtop Wavelength Dispersive X-Ray Fluorescence (WDXRF) spectrometer. The S6 JAGUAR extends Bruker's range of XRF instruments by closing the gap between floor standing WDXRF and benchtop EDXRF instruments. It combines excellent analytical performance based on cutting-edge technology with compact size and 'plug & analyze' installations.

The S6 JAGUAR outperforms other compact WDXRF instruments by offering highest sensitivity and 50% reduction in measurement times, due to its compact WDXRF goniometer, closely coupled X-ray optics, and 400 Watt excitation power. Based on the novel, solid-state HighSense XE™ detector with linear range of two million counts per second, the S6 JAGUAR delivers excellent accuracy and precision for quality control in industrial labs for minerals, mining, chemistry, petro-chemistry, and cement. The S6 JAGUAR components are protected by Bruker's SampleCare™ technology, ensuring high instrument uptime and low cost of operation, also when running liquid or powder samples.

The compact WDXRF goniometer combined with the HighSense detector enhance both sensitivity and spectral resolution, providing great flexibility and performance for academic and industrial materials research. With up to four sample masks for different sample sizes, up to four analyzer crystals, and two detectors, the S6 JAGUAR enables fast multi-element analysis for the concentration range from ppm to 100%.

SPECTRA.ELEMENTS™, the new S6 JAGUAR software, provides quick setup of applications, enhanced evaluation, and comprehensive reporting. The standardless quantification software SMART-QUANT WD™ delivers accurate results, even for unknown samples, based on powerful fundamental parameter algorithms.

Bruker's multilingual TouchControl™ interface and EasyLoader™ sample handling ensure intuitive, fail-safe operation. In addition to its broad application range, the S6 JAGUAR is suited for minerals and cement with the ready-to-analyze solutions GEO-QUANT Basic™ and CEMENT-QUANT™. Pre-calibrated application packages and minimum installation requirements, using standard electrical outlets, and not requiring compressed air, make the S6 JAGUAR a 'plug & analyze' tool. The AXSCOM™ automation interface enables integration of the S6 JAGUAR into automated industrial laboratories.

Dr. Kai Behrens, the Bruker XRF Product Line Manager, commented: "The speed and analytical flexibility of the S6 JAGUAR are unique in its class. Analytical precision and accuracy based on 400W excitation power in its small benchtop form factor make the S6 JAGUAR an excellent WDXRF analyzer for industrial research and QC, as well as for academic and government research laboratories."

For more information about the S6 JAGUAR, please visit **www.bruker.com/s6jaguar**

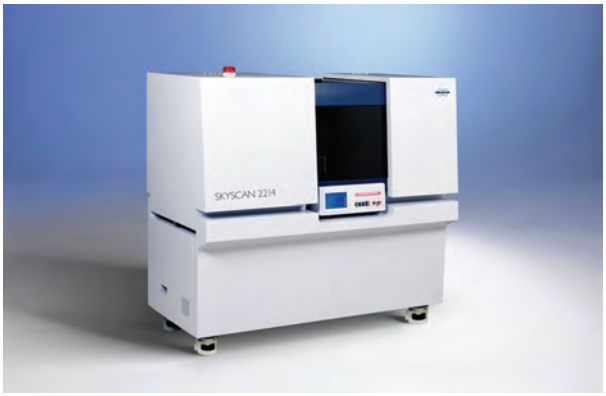
Bruker Introduces New SKYSCAN 2214 Ultra-High Resolution Nano-CT

Bruker announces the launch of the SKYSCAN™ 2214, a multiscale X-ray nano-CT (computed tomography) system with a unique X-ray source and detector geometry that generates sharper images with outstanding precision. The SKYSCAN 2214 offers unprecedented, ultra-high resolution for larger fields of view in larger objects, which makes nano-CT practical and truly useful for industrial and academic research.

The SKYSCAN 2214 features an innovative, modular design which accommodates up to four detectors, allowing customers to select the most appropriate detector for their samples and applications. This flexibility offers the scanning of a wide variety of samples types and sizes in one instrument, reducing the need for multiple, different CT systems. The four detectors are field-upgradeable for cost-effective expansion of the SKYSCAN 2214, in order to accommodate changing analytical requirements.

The SKYSCAN 2214 pushes the boundaries for measuring larger objects at ultra-high resolution. Its uniquely large field of view allows for the analysis of objects up to 300 mm in size. For objects up to 12 mm in size, it provides better than 500 nanometer true 3D resolution. The achievable voxel size is 60 nanometer. Its unique detector design encompasses a 6 Megapixel (Mp) flat-panel, and three optimized 8/11 Mp cooled CCD cameras. The SKYSCAN 2214 produces up to 8K x 8K pixels in every slice, which is 16 times larger than any other nano-CT system available on the market.

While delivering cutting-edge, research-grade results, the SKYSCAN 2214 comes equipped with user-friendly, comprehensive software for excellent data collection and high-end analysis capabilities. Spiral scanning enables distortion-free data acquisition and artefact-free reconstruction. The world's fastest 3D reconstruction software speeds up imaging an object's internal microstructure 10-100 times compared to traditional CT reconstruction algorithms. The SKYSCAN 2214 requires almost no



maintenance, thus enhancing system uptime and reducing cost of ownership.

Dr. Frank Burgaezy, President of the Bruker AXS division, commented: "The SKYSCAN 2214 is a game-changer for ultra-high resolution nano-CT in the material sciences. Its superior high resolution for larger objects offers new opportunities for developers of composite materials, as well as for geology, where precision is key to determine porosity and grain size. In metrology, the precision of the SKYSCAN 2214 enables exact internal dimension measurements at the submicron scale. Ultra-high resolution is also critical for the development of lithium batteries and other energy storage devices."

Dr. Wulf-Ingo Jung, President of the Bruker BioSpin Preclinical Imaging division, added: "The SKYSCAN 2214 enables new capabilities in preclinical imaging as well. Its large field of view combined with true high-resolution allows a wide range of samples to be imaged ex vivo, offering artefact-free analysis of soft tissues, e.g. in lung imaging or tumour vascularization. This top-of-the-line, new nano-CT system is also the ultimate tool in the growing fields of zoology and entomology, where very small objects can be studied with extreme precision."

For more information, visit
https://www.bruker.com/skyscan2214

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Malvern Panalytical
a spectris company

MINERALOGICAL ANALYSIS OF HARD-ROCK LITHIUM ORES

Figure 1. Hard-rock lithium ore

Summary

Knowing the qualitative and quantitative mineral composition of lithium ore means additional information for mine planning and downstream processing. Using a benchtop diffractometer in a laboratory or an automated environment helps to achieve optimal efficiency and lowest energy costs during mining and beneficiation.

Introduction

Mining companies have promised to add 20 lithium production sites to the 16 currently operating due to a sudden increase in demand for electric vehicles, which are competing with laptops and smartphones for lithium ion batteries (Bloomberg Businessweek September 2017).

Lithium is mined from two types of deposits: lithium-rich brines (lithium salts) or hard-rock granite pegmatite deposits. This case study focuses on the latter one. Lithium-containing minerals that occur in granite pegmatites are spodumene, apatite, lepidolite, tourmaline and amblygonite of which spodumene is the most common lithium-bearing mineral. Lithium hard-rock recovery can be broken down into a few key steps: (i) crushing of the ore, (ii) concentration by froth flotation, (iii) thermal treatment in a rotary calcining kiln to convert α-spodumene into the β-modification. This allows the lithium present in the ore to be extracted during the further processing steps.

The determination of the mineralogical composition with X-ray diffraction (XRD) is essential for optimizing operational efficiency of the mining and beneficiation process of hard-rock lithium ores. The Minerals edition of Aeris is the first benchtop X-ray diffractometer designed for process control and geometallurgical characterization in the mining industry. This case study shows a typical example of the fast and precise analysis of mineralogical ore compositions with the Aeris Minerals edition.

Experimental

The presented data were collected on an **Aeris Minerals** edition industrial benchtop diffractometer operated at 600 W using copper radiation and the highly acclaimed PIXcel^{1D} strip detector which allows rapid, high-quality analysis of rocks, ores and minerals. The measurement time for each sample was 10 minutes. Data evaluation including phase identification and quantification using the Rietveld full-pattern method was done using the HighScore Plus suite (version 4.6) [1].

Results and discussion

Fourteen samples from both raw ore of a hard-rock lithium deposit as well as processed material were analyzed.
The obtained results show that the samples are characterized by a complex mineralogy. Main minerals are spodumene $LiAl(SiO_3)_2$, quartz SiO_2, albite $NaAlSi_3O_8$, anorthite $CaAl_2Si_2O_8$; minor amounts of lepidolite $K(Li,Al)_3(Al,Si,Rb)_4O_{10}(F,OH)_2$, orthoclase $KAlSi_3O_8$ and traces of tourmaline (elbaite) $Na(Li_{1.5}Al_{1.5})Al_6Si_6O_{18}(BO_3)_3(OH)_4$ and beryl $Be_3Al_2(SiO_3)_6$ are also present in the samples.

Figure 2 shows an example of a full-pattern Rietveld quantification of a hard-rock lithium ore analyzed in this case study. The obtained quantitative phase compositions of all analyzed samples are plotted in ***Figure 3*** and summarized in ***Table 1***.

The results show that after flotation, the concentrate (sample # 11) consists of 89.6% α-spodumene and minor amounts of feldspar, quartz and traces of tourmaline (elbaite). Main minerals in the tailing (sample 12) after flotation are quartz, feldspar and lepidolite with a remaining 0.9% of α-spodumene.
After the calcination of the α-spodumene concentrate the resulting product (sample 13) mainly consists of β-spodumene (92.2%) with a trace amount (0.6%) of remaining α-spodumene. The main mineral in the residue of this process (sample 14) is analcime $NaAlSi_2O_6 \cdot H_2O$ with some remnant of β-spodumene.

This study shows that X-ray diffraction (XRD) analysis using a benchtop instrument is an excellent tool for a reliable process control of lithium hard-rock recovery, enabling the ore grade analyses and monitoring of the relevant mineral concentrations during processing to ensure the most efficient use of energy and reagents.

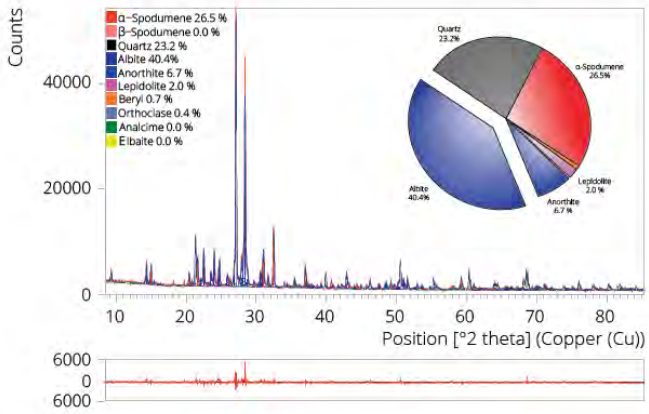

Figure 2. Quantitative Rietveld analysis of a complex lithium ore

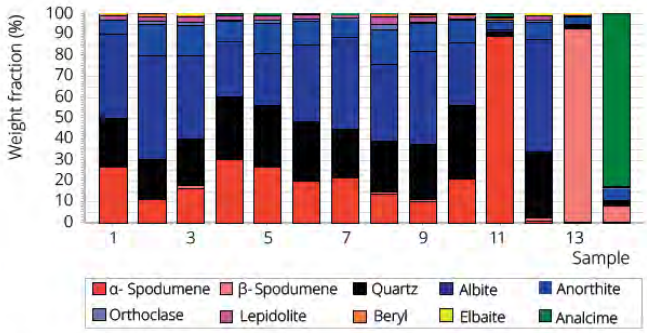

Figure 3. Mineralogical composition of 14 raw and processed lithium samples

Table 1. Mineralogical composition of raw and processed lithium samples

Sample type	#	Spd-α	Spd-β	Qtz	Ab	An	Or	Lpd	Brl	Elb	Anl
Ore	1	26.5	-	23.2	40.4	6.7	0.4	2.0	0.7	-	-
Ore	2	11.3	0.7	18.1	49.6	15.2	1.6	1.9	1.5	-	-
Ore	3	16.6	1.3	22.3	39.8	14.7	1.6	2.6	1.1	0.1	-
Ore	4	30.5	0.3	29.7	26.2	9.9	0.7	1.7	0.2	0.1	0.8
Ore	5	26.7	0.8	28.9	24.5	14.9	1.6	2.0	0.5	-	0.2
Ore	6	20.1	0.4	27.8	37.2	11.4	0.7	2.0	0.5	-	-
Ore	7	21.2	0.9	22.6	44.3	8.6	0.3	1.7	0.0	0.2	0.1
Ore	8	13.8	0.9	24.1	36.9	16.6	2.4	3.5	1.7	-	-
Ore	9	10.1	1.0	26.5	44.2	13.7	0.5	2.4	0.9	-	0.5
Ore	10	20.9	0.6	34.4	30.4	10.6	0.5	1.9	0.2	-	0.5
Concentrate	11	89.6	0.4	1.3	1.4	3.7	0.6	0.8	0.3	0.6	1.5
Tailing	12	0.9	1.3	31.9	53.5	8.6	0.8	2.2	0.6	0.2	-
Calcined	13	0.6	92.2	1.9	0.4	3.3	0.4	0.4	0.6	0.1	-
Residue	14	0.4	7.6	2.4	-	6.3	0.1	-	0.4	-	82.8

1. [1] T. Degen et al., HighScore Suite (2014) Powder. Diffr. **29** (S2) S13-S18.

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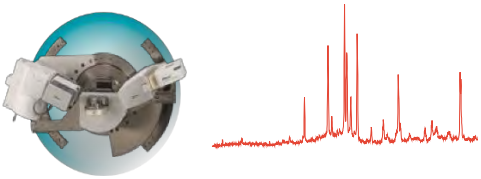
INTELLIGENT MULTICORE OPTICS THAT ELIMINATES PAINFUL MANUAL INTERVENTION

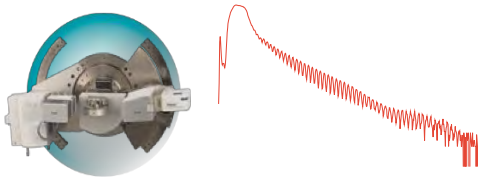
Introducing Empyrean, Malvern Panalytical's third generation X-ray diffractometer that is equipped with intelligent iCore and dCore multi optics. It is the first fully automated multipurpose diffractometer that allows the largest variety of measurements without any manual intervention.

- Smart technology and software enables seamlessly transition between advanced XRD techniques
- Run heterogeneous sample types and different applications in one uninterrupted batch
- Great for central labs
- Intuitive for beginners
- Reduce user training time by 30%
- Reduce the possibility of mistakes in data collection
- Simplify the creation of Standard Operating Procedures in regulated environments

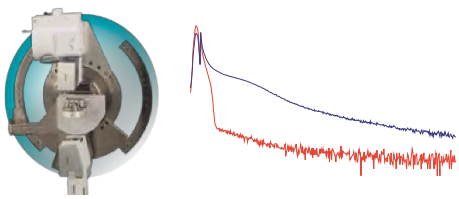
Phase identification/quantification



X-ray reflectivity



Small-angle X-ray scattering



Empyrean III, the market's intelligent diffractometer
Grand launch at our Sydney XRD Symposium. Stay tuned!

www.malvernpanalytical.com/Empyrean

Press Release

TESCAN Acquire Manufacturer of 3D and 4D X-ray Imaging Systems

TESCAN ORSAY HOLDING a.s. (TESCAN), a leading global developer and supplier of electron, ion and light microscopy systems, recently acquired XRE NV, a Belgian-based designer, and manufacturer of dynamic 3D and 4D X-ray imaging systems.

The XRE team was part of the founding team of Ghent University Centre for X-ray tomography. Since forming XRE, they have been continuing to push the bounds of what is possible with the technology, resulting in systems that bring synchrotron-like performance to your laboratory. The extensive publication list produced by the XRE team members and users of their systems is a testament to their quality and capabilities.

With a collaborative, developmental and interactive philosophy, they have specialised in producing systems tailored to the exacting requirements of their clients. Using a flexible and open architecture, they tailor system using different X-ray sources, detectors and sample stages. This platform allows users to upgrade their systems as new technologies/components become available and to upgrade as finances become available. This in turn results in an upgradable and future-proof tool for your lab.

At the heart of the XRE X-ray tomography system is the intelligent software that is fully integrated with the hardware. It has been designed to help users go beyond what other system offer, to collect time-resolved 3D datasets, or 4D datasets. Although this may seem relatively straight forward, the XRE software deals with the complex problem that includes enormous datasets, temporal artefacts and continuous rapid data collection to generate high quality, accurate data. Best of all, the software allows users to easily manage, interpret and maneuver data including deconstruct and reconstruct to give you a non-destructive insight into the inner workings of your sample or material.

XRE systems have also been optimised for in situ experiments. This allows you to directly observe the dynamic behaviour of your sample under changing experimental conditions. This property can vastly accelerate the time required to develop a product as it more accurately simulates the actual operating conditions a component is subjected to.

They currently have 3 platforms:

1. **CoreTOM** – Designed for the earth sciences, CoreTOM is a multi-resolution 3D X-ray microscope optimized for high resolution, large field of view imaging of full cores down to microplugs.
2. **DynaTOM** - a unique and first of its kind dedicated system for fast dynamic *in situ* imaging and 4D studies
3. **UniTOM** – a flexible high resolution platform designed for maximum image quality and resolution that can also cater for multiple X-ray sources and detectors

TESCAN's XRE product range is now available through AXT who have a wealth of experience in X-ray related technologies including XRD, XRF, microanalysis, XRM and non-destructive testing. For more details please visit www.axt.com.au.

Press Release

Cutting Edge Small Molecule XRD System Installed at the University of Melbourne

Sydney, Australia, July 12, 2018 - Crystallographers at the University of Melbourne received a boost following the installation of a state-of-the-art small molecule X-ray diffraction (XRD) machine. The XtaLAB Synergy-S from Rigaku Oxford Diffraction (ROD) is a class-leading instrument that marries cutting edge technologies that will enable their researchers to generate world-class data. The system was installed by AXT Pty. Ltd. ROD's distributor in Australia and New Zealand.

The XtaLAB Synergy-S incorporates the latest PhotonJet high flux dual wavelength (Molybdenum/Copper) X-ray source that will allow their researchers to better resolve smaller crystals with poor crystallinity. Equally important is the HyPix 6000HE detector that utilises the latest Hybrid Photon Counting technology with no dead time or background noise. In combination with the Kappa goniometer and user influenced software, the Synergy-S becomes an enviable system.

The Synergy-S becomes the flagship instrument in the X-ray Diffraction Facility at the University of Melbourne. It adds to the small molecule capabilities partnering a Rigaku SuperNova system installed in 2010 and was the logical replacement for an older Rigaku system.

The University of Melbourne team with ROD Applications Specialist. (L to R) Dyanne Cruickshank from ROD, with Martin Van Koeverden, Robert Gable and Brendan Abrahams from The University of Melbourne.

Dr Robert Gable, Manager of the X-Ray Diffraction Facility said of their purchase, "Selecting the Synergy-S system was largely based on experience. The CrysalisPro software used on other Rigaku systems we have used had proven extremely effective at characterising materials and generating publication quality data from twinned or poor quality materials we work with. Combined with the high intensity dual wavelength X-ray source, our ability to characterise materials is greatly enhanced. Furthermore, using the same software has simplified our training and enables users to seamlessly move between instruments when required."

The system will serve researchers of all levels from undergraduate through to postdoctoral and academic staff. As more researchers are inducted, the utilisation of the Synergy-S will increase with a sizeable user-base already identified. Dr Gable envisages that it will be used by a range of different research teams for a host of different compounds including organic biomolecules, minerals, coordination polymers, metal complexes used for catalysis or cancer treatment and polyoxometallates.

Speaking more about the additional capabilities afforded by the new system, Dr. Gable mentioned that, "the Synergy-S will allow us to collect data on smaller crystals that do not give usable diffraction data on the SuperNova. It will also significantly decrease the analysis time for complex samples."

The system was purchased following a successful LIEF grant bid submitted by the University of Melbourne and other university and research institutes. The University of Melbourne is grateful to the Australian Research Council for their contribution towards the purchase.

The Rigaku Oxford Diffraction product range are part of AXT's extensive range of analytical X-ray instruments, including XRD, XRF, XRM, CT, EDS and WDS sourced from suppliers from around the globe. For more details, please visit www.axt.com.au.

DECTRIS
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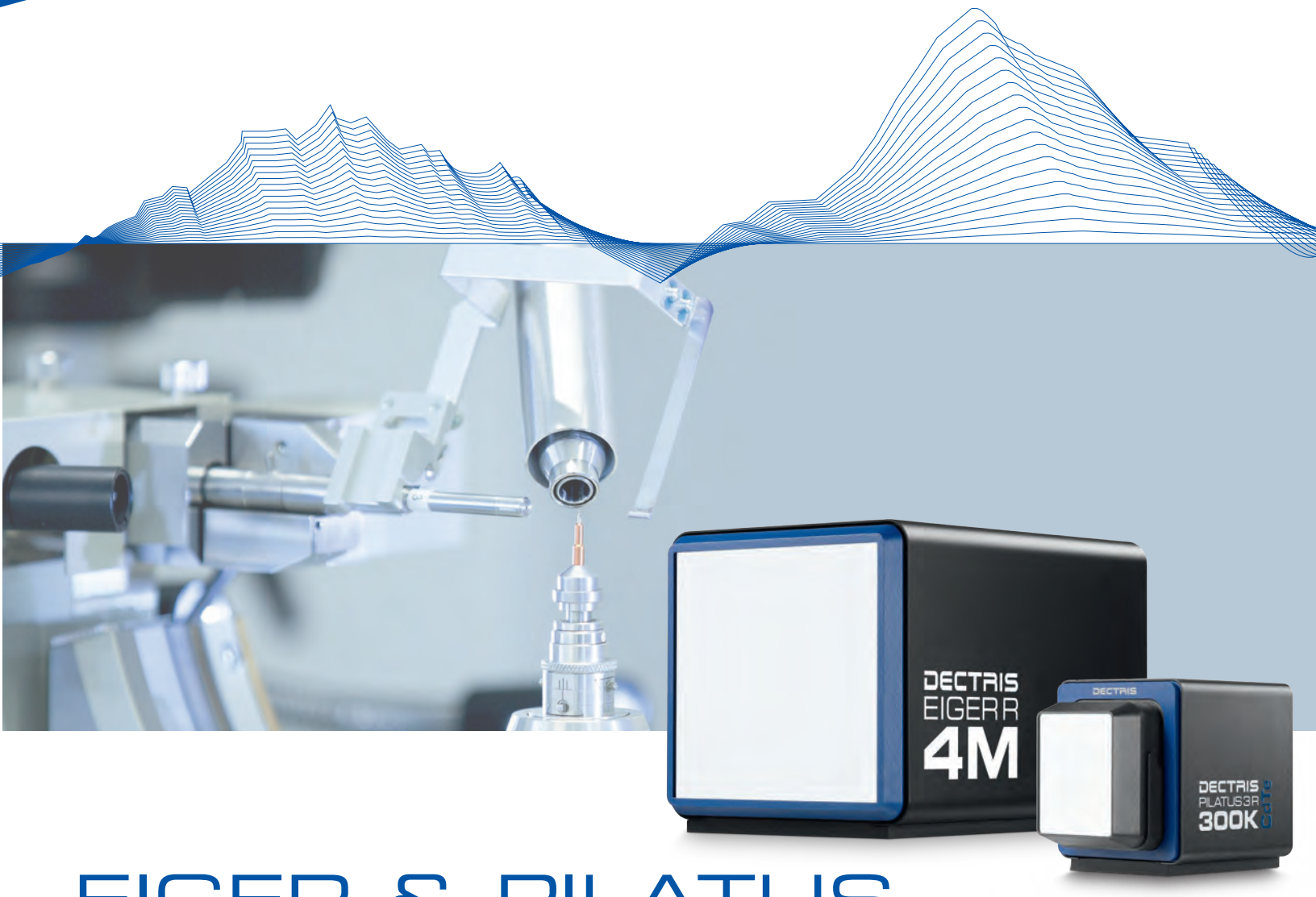

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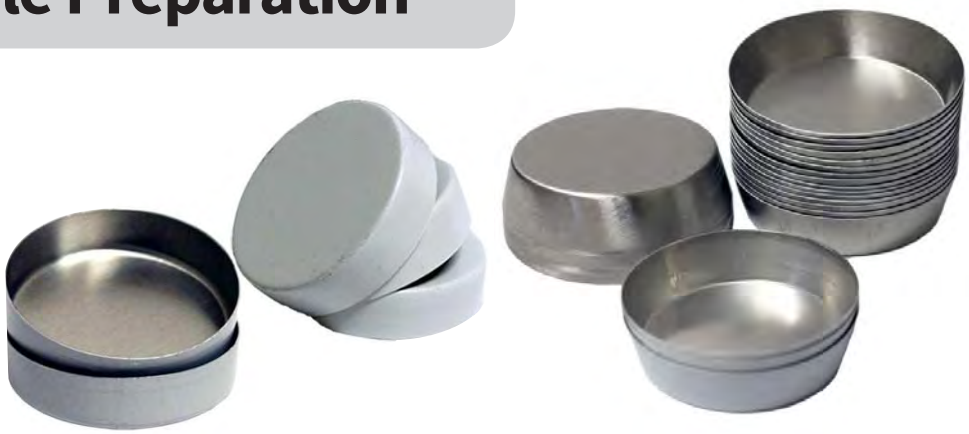

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