

e-newsletter

Issue 1, 2012

Australian X-ray Analytical Association

President's Address

Dear AXAA Members and Readers,

Welcome to the first newsletter for 2012!

After a pause year in 2011, 2012 will see the return of our regular AXAA activities - the student seminar days (SSD) and technical meetings. Keep an eye out for the release of the NSW event date in the next newsletter and read on for further information concerning the Victorian SSD.

Before you read on, I take a moment to look at some educational events that were held last year, which saw a significant surge in diffraction education in Australia. 2011 saw the Australasian Crystallography School held in Perth in July, two neutron scattering schools incorporating significant powder diffraction components were held at the Australian Nuclear Science and Technology Organisation (ANSTO), the "Powder Diffraction at Australia's Synchrotron and OPAL Facilities: Experiment Planning to Data Analysis" school was held at the Australian Synchrotron in September, and the "National Workshop On X-ray Powder Diffraction Analytical Methods For Science & Engineering Graduates" was held in Perth, also in September. The latter event will be held again this year in Perth, in August.

The AXAA is also pleased to announce that the International Centre for Diffraction Data (ICDD) has recently established the Robert L. Snyder Student Travel Awards, to attend the Denver X-Ray Conference. The application deadline is 1st May, read further for details.

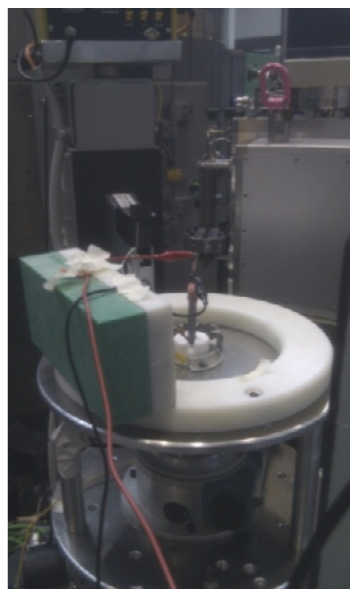
Finally, the National Council met a few weeks ago and voted on our latest round of membership applications. Congratulations to all of our newest members, and if you would like to become a member, please see our "Membership Matters" section in this newsletter.

Vanessa Peterson
National Council President

Matters for Scatterers

The high energy density and compact form of rechargeable lithium ion batteries make them one of the most efficient means of storing energy. However, the performance of a lithium ion battery is only as good as its weakest component. Although anode technology has been significantly developed, the overall performance of lithium ion batteries is being hindered by the shortcomings of current cathode materials.

Many of these shortcomings, such as maximum capacity and cycling stability, are due to irreversible changes of the structure during lithium insertion and extraction. Thus, in order to improve on current cathode materials or design new ones, an understanding of the structural changes that take place during charging and discharging is essential.

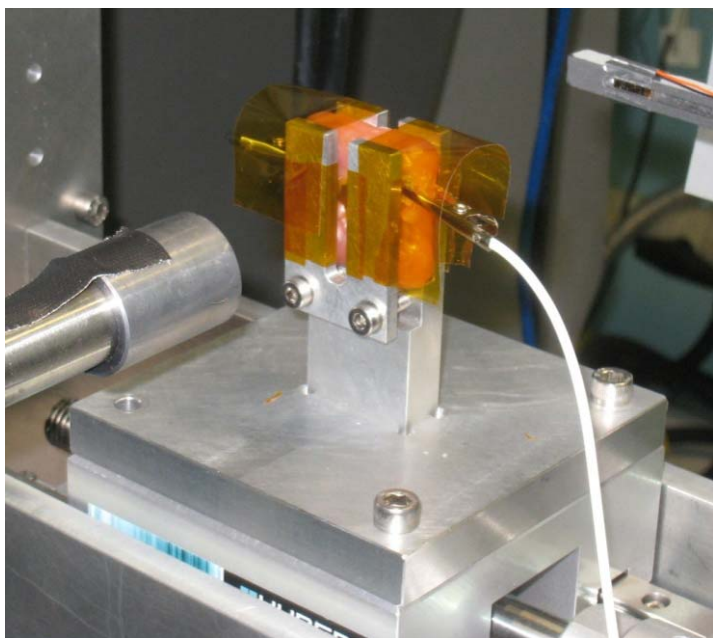


In-situ neutron diffraction cell set up on the WOMBAT diffractometer at ANSTO.

The most powerful tools available for the study of structural changes in cathode materials are neutron and synchrotron X-ray diffraction. We have performed (cont.)

multiple *ex-situ* investigations on the cathode material $\text{Li}_{0.18}\text{Sr}_{0.66}\text{Ti}_{0.5}\text{Nb}_{0.5}\text{O}_3$ following insertion of lithium via chemical and electrochemical means. While synchrotron X-ray diffraction has allowed us to investigate phase changes at various stages of lithium insertion, neutron diffraction has been invaluable in locating lithium in the structure. The combination of both techniques has allowed inferences to be made on lithium diffusion pathways and the factors which limit the amount of lithium inserted within the structure. However, *ex-situ* analysis does not allow for the direct correlation of structure and properties due to possible changes that occur during extraction of the cathode material from the cell.

In order to directly study the effect of structural changes on electrochemical properties, custom *in-situ* cells were developed both for neutron and synchrotron X-ray diffraction. Approximately 800 data sets were collected using the neutron *in-situ* cell over two days covering several charge/discharge cycles to different voltages. In addition, 900 data sets were collected over three days using our custom synchrotron X-ray *in-situ* cell. The synchrotron cell was particularly challenging to design due to the absorption losses of the X-ray beam passing through some of the battery materials. Sequential Rietveld refinements of models to these data sets provide a comprehensive understanding of the structural changes which take place during cycling, making this study one of a few which fully characterises a cathode material *in-situ*.



In-situ synchrotron diffraction set-up on the powder diffraction beamline at the Australian Synchrotron.

William Brant
PhD Candidate
The University of Sydney

2012 AXAA Student Seminar Days

After a hiatus in 2011 due to the 2011 AXAA Conference, 2012 will see a return of the AXAA Student Seminar Days. These events give Honours, Masters and PhD students using X-ray, neutron, light and electron scattering in their research the chance to meet each other and present their work to other students, researchers and members of industry. The Victorian event is planned for Sept/Oct 2011; stay tuned for further details, and details about events in other states.

Vanessa Peterson Elected as Director-at-Large of the ICDD

Our National Council President, Vanessa Peterson, was recently elected onto the Board of Directors of the ICDD, and assumed office on 22 March 2012. Details can be found at: <http://www.icdd.com/profile/whatsnew/2012bod.htm>

Robert L. Snyder Student Travel Awards

The ICDD has recently established the Robert L. Snyder Student Travel Awards, which honour his life and work. The awards offer travel support (\$1000) which assists undergraduate and graduate students attending the Annual Denver X-ray Conference, to be held from 6-10 August 2012 in Colorado Springs. Further details and the application form can be found at <http://www.icdd.com/resources/awards/snyder.htm>

The application form can also be found at the end of this newsletter.

Editor's note: Professor Brian O'Connor (Curtin University) submitted a tribute to Professor Snyder which appeared in the 4th edition of the 2011 AXAA newsletter.

AXAA Website

A makeover is planned for the AXAA Website to bring the information on there up to date. This is in its initial stages; further details will be provided in future editions of the Newsletter.

Membership Matters

AXAA-Inc membership is for the 3-year period starting from the 2011 AXAA National Conference (existing membership will be re-approved in 2014). Membership is free. Candidates should provide a brief CV and a short statement of intention about what they intend to do in the organisation. Please send these to National Council Secretary Natasha Wright. The council votes on membership applications at least once every 6 months.

Upcoming Events and Conferences

National XRD Course
X-ray Powder Diffraction Analytical Methods,
Curtin University, Perth
Saturday 25 Aug – Tuesday 28 Aug, 2012

Venue: Department of Imaging and Applied Physics, Curtin University, Bentley (Perth), Western Australia. [Client-specific version of the course can be presented at the customer's site].

Duration of Curtin Course: 4 days

Dates: 25-28 August, 2012

Course Presenters: Professor Brian O'Connor and Dr Robert Hart

Enquiries and further information:
B.O'Connor@curtin.edu.au

Cost: \$2,585 including GST

Availability of places strictly limited

Overview: The course has been designed to give participants a theoretical and practical grounding in the principal characterisation methods which make use of X-ray powder diffractometry data. Approximately 60% of the course involves hands-on instruction. Participants personally collect diffractometry data sets and then process these, both manually and with PC computers, in exercises on various analytical methods, including Rietveld analysis.

Public domain software will be used, including *WINPLOTR* and *Rietica*. The course also includes overviews and demonstrations of the commercial software packages *X'Pert HighScore Plus* and *Diffracplus Topas*. While the course is relevant to the analysis of all classes of crystalline materials, attention will be devoted mainly to materials relevant to the mining and mineral processing sector.

Date	Event	Location	Further Information
30 June-4 July 2012	AINSE Winter School	AINSE, ANSTO	http://www.ainse.edu.au/events2/winter_schools
9 July 2012	2012 Synchrotron and Neutron New Users Symposium	Australian Synchrotron	http://www.synchrotron.org.au/index.php/news/events/australian-events
28-31 Oct 2012	13th European Powder Diffraction Conference EPDIC 13	Grenoble	http://epdic13.grenoble.cnrs.fr/
2-5 Dec 2012	AsCA 12/Crystal 28: Celebrating 100 years of Crystallography	Adelaide Convention Centre	www.sapmea.asn.au/crystal2012
6 Dec 2012	Bragg Symposium: Celebrating 100 Years of Crystallography	University of Adelaide	www.sapmea.asn.au/crystal2012
22-25 April 2013	Accuracy in Powder Diffraction IV	NIST	http://www.nist.gov/mml/apdiv_conference_2013.cfm

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Denver X-ray Conference

Robert L. Snyder

Student Travel Award Application

In pursuing its dynamic commitment to the education of the scientific community, the International Centre for Diffraction Data is offering a limited number of travel awards to help students attend the **2012 Denver X-ray Conference**, being held in Denver, Colorado, 6–10 August 2012. Grants are awarded in the amount of \$500 for students living within the USA, and \$1,000 for students living outside of the USA. Denver X-ray Conference also offers a reduced student registration fee and student housing. (see www.dxcicdd.com for full details).

Students are required to participate in the technical program by submitting an abstract for oral or poster presentation. To apply for assistance, submit this completed form, a copy of your abstract and a supporting letter from your research advisor. The deadline for applications is May 1, 2012.

First Name	_____	Last Name	_____
Dept.	_____	Univ.	_____
Street	_____	Box/Apt. #	_____
City	_____	St/Prov.	_____ Zip/Postal Code
Country	_____	Telephone	_____
Fax	_____	E-mail	_____

Are you a:

Undergraduate Student Post doc Associate Graduate Student

Other (explain) _____

Name of Professor or Research Advisor:

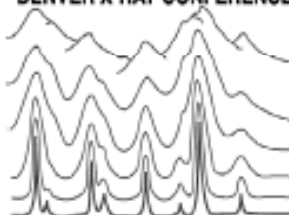
Signature of Professor or Research Advisor/Date

Signature of Applicant/Date

Submit Application To:

Robert L. Snyder Student Travel Award
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273
E-mail: DXCtravelgrants@icdd.com
Fax: (610) 325-9823

DENVER X-RAY CONFERENCE™



Don't forget!

- Complete each section of this form
- Attach a copy of your abstract to this application
- Attach a letter of support from your Professor or Research Advisor
- Contact ICDD to confirm receipt of application

Diffraction Technology



Do you want a simple low-cost, no-frills X-ray Powder Diffractometer for routine materials characterisation?

This is what the MMA and now the eMMA is designed for.



It is lightweight, bench-top mounted, and can be moved or transported without losing alignment. The unique Harmonic Gearbox goniometer and the tube-shield are attached to the cabinets, so the whole instrument moves as one.

It has a radius of 250mm, so there is adequate resolution for separating closely spaced mineral peaks.

It can be fitted with a 10-sample loader, which is unobtrusive so can be left in place permanently if desired.

AND – it can be driven from your Laptop via the Ethernet port either directly or via a network by software which is integrated with ICDD ® databases for rapid qualitative identification.

For more information: www.diffraction.com.au
Or contact Rod Clapp at diffraction@bigpond.com

Cutting-edge technology. Ultimate commitment.

Experience our innovative X-ray solutions for mining



Axios^{MAX}-Minerals: offers a dedicated XRF solution to the industry and includes a complete set of traceable standards.

Axios FAST: is the fastest simultaneous XRF spectrometer on the market.

CubiX³ Minerals: most accurate and fastest diffractometer for production and process control, the perfect solution for grade control of drill cores and ores.

Epsilon 3 range: range of cost-effective benchtop energy dispersive X-ray fluorescence systems, ideal for accurate grade control and exploration materials.

In-line real-time process control
Sodern CNA cross-belt analyzers from PANalytical provide real-time elemental analysis.

Epsilon 5: polarized EDXRF spectrometer is an essential tool for geological applications; this spectrometer excels in the analysis of heavy metal trace elements in addition to major and minor light elements.

For more information please contact:

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The Analytical X-ray Company



Bruker Expands its Small Angle X-ray Scattering (SAXS) Product Portfolio for High-Throughput Nanostructure Analysis



Bruker have recently announced the strategic expansion of its X-ray diffraction and scattering product portfolio into high-throughput nanoparticle analysis, based on Bruker's recent acquisition of Kratky Small Angle X-ray Scattering (SAXS) technology developed previously by Hecus X-ray Systems GmbH in Graz, Austria.

A further performance breakthrough has now been achieved in SAXS measurement speed and sample throughput by the integration of the **ImS™** microfocus X-ray source and Bruker's **VANTEC-1™** detector into the Kratky **MICRO™** series of SAXS cameras. A gain factor of 2x-3x over the best conventional instruments opens up new fields of applications where either measurement speed or primary beam flux density are essential to collect data from weakly scattering materials or solutions. The new **MICROCalix™** system even enables researchers in chemistry and drug discovery to simultaneously execute SAXS and calorimetric investigations, while the new **MICROPix™** system is ideal for high-throughput analysis of protein size, shape and size distributions in 10 minutes, while requiring less than 10 microliter quantities of diluted sample.

Professor Peter Laggner, Director of Nanostructure Solutions at Bruker AXS, commented: "With this strategic expansion Bruker can now provide SAXS tools for both major nanoscience and nano-analysis segments: the physical and materials research market with the established Bruker high-end **NANOSTAR™**, and the biomedical and pharmaceutical market with the compact new **MICROPix** and **MICROCalix** systems."

Dr. Lutz Brügemann, Director of R&D and Marketing at Bruker AXS, stated: "The cutting-edge X-ray source and detector technologies developed by Bruker are key in enabling this major technological step. Merging our performance-leading X-ray components into an innovative scientific and analytical SAXS tool opens new market opportunities in molecular biology and drug discovery which so far were accessible only when using large-scale research facilities with synchrotron sources."



For further information, please contact Bruker on (03) 9474-7000 or email sales@bruker.net.au

NEXT GENERATION OF BRUKER HAND-HELD XRF ANALYSERS



Inspection and Testing Equipment specialist, Russell Fraser Sales Pty Ltd is proud to unveil the next generation of Bruker Hand-Held XRF analysers, coming soon. This follows the success of the S1 Turbo analyser with Bruker's X-Flash Silicon Drift Detector (SDD). The all new S1 Titan XRF analysers (for heavy elements and light elements) will also incorporate X-Flash SDD technology, but with additional features for improved speed and accuracy.

Bruker's 2nd generation S1 Titan XRF analysers now feature a rear in-built viewing screen and weigh-in at only 1.43kg, (battery included) making them the lightest hand-held units on the market. The S1 Titan offers improved analytical performance with a 20-50% lower Limit of Detection (LOD) for metallic trace elements. All metal calibrations have been upgraded for higher accuracy and improved versatility based on new calibration platform used in other Bruker XRF (laboratory) analysers. The light element of Magnesium can now also be captured at a 50% lower LOD than that achieved previously.

The S1 Titan is simple to use, featuring one touch start-up and with no ongoing sample standardization required. A 25% increase in battery life will extend in-field use and the improved ruggedness and weather-proofing (IP54 rated) of the S1 Titan ensures operator confidence in any environment.

For Positive Material Identification and Quality Assurance inspection, the Bruker S1 Titan instruments will enable fast and reliable data capture which can be transferred via USB flash drive for reporting purposes. Company branding can also be applied to reports through Bruker's optional S1 Data Tool reporting package. Other instruments will follow for specific applications such as Mining and RoHS applications.



For all of your Bruker Hand-Held XRF requirements, contact Russell Fraser Sales Pty Ltd:

Tel: +612 9545 4433 Fax: +612 9545 4218

Email: rfs@rfsales.com.au Web: www.rfsales.com.au

What's New from AXT Pty Ltd

Rigaku have a new website and visitors can also download the highly respected Rigaku Journal here: www.rigaku.com/download/rigakujournal This journal contains the best of the scientific research and applications in XRF and XRD that Rigaku undertake in its applications, research and development facilities.



AXT have also updated their website. The first stage is up and you can see the new look here: www.axt.com.au

New Rigaku Miniflex 300/600 Benchtop XRD.

Now the 5th Generation of the highly successful Miniflex has been released, more power more flexibility more results!



See the video here:

<http://video.comparenetworks.com/services/player/bcpid102811046001?bckey=AQ~~,AAAAAH9G3tk~,9fesXRDi9S5ysqhJqdOgCv18zyTclOz1&bclid=0&bctid=1414480664001>

The new MiniFlex 300 and 600 features :

- MiniFlex 600 600W power for faster and more reliable results
- MiniFlex 300 300W features built in chiller no external utilities required
- Range of detectors available from Scintillation Counter to D/Tex Ultra solid state Si strip detector
- Range of attachments available including auto samplers and holders for air sensitive samples

Full Range of Benchtop XRF available

From the entry level Nex QC to the benchtop SuperMini WDXRF Rigaku have got all the applications covered!

Nex QC Low Cost Benchtop EDXRF



- The Nex QC is a small easily transportable (16kg) EDXRF which can measure Na-U.
- Various packages are available e.g. for the wood Treatment industry and S analysis in fuels.
- 50kV for wide element range, can analyse solids, liquids, pastes, slurries, thin films
- Built in microprocessor control, smartphone style touch screen and Ethernet connection for easy export of results

Nex CG Cartesian EDXRF High Sensitivity Benchtop EDXRF

- 50kV for wide elemental range Na-U in solids, liquids, pastes, slurries, thin films
- 3D Cartesian Geometry with secondary excitation for best peak to background ratio's and low minimum quantifiable levels
- Fundamental Parameters approach for either standardless calibrations or reducing number of standards required
- Variety of autosampling options available



SuperMini Sequential Benchtop WDXRF

- 50kV 200W Able to measure F-U in solids, liquids, pastes, slurries, thin films
- Full vacuum operation for exceptional performance esp light elements with high precision
- 12 position sample changer with spinner standard
- Less than ½ the price of a full system
- Perfect as back up system, or for operations that have a requirement for timely precise results but have a modest throughput

