Issue 3, 2013

Australian X-ray Analytical Association

President's Address

Dear AXAA Members and Friends.

The 2014 National Workshops, Conference, and Exhibition is almost here! In just over two months we will converge on the Pan Pacific Hotel in Perth for an action-packed five days of learning, research dissemination, discussions and networking. The Conference Program Committee has been busy putting together an exciting program, and Sarah our conference secretary has put together an excellent social program too! Earlybird registration closes this Friday 13th December, so don't waste any time making the most of these reduced rates. In addition, the poster abstract submission deadline had been extended, please read on for further details.

Since our last Newsletter we have had student seminar events in both NSW and Victoria. Both were very well attended and showcased the work of some of our very talented student members. Read further on for reports on both. Thanks to PANalytical for supporting the NSW event, and to Bruker and the Australian Synchrotron for supporting the VIC event.

Finally, the 2014 Conference marks the time when a new AXAA Council for the period 2014-2017 is to be elected. Details of the nomination procedure can be found later in the Newsletter.

For now that's all from me, see you in Perth!

Vanessa Peterson National Council President

AXAA 2014 Workshops, Conference and Exhibition

EARLY BIRD REGISTRATIONS CLOSE FRI 13TH DEC 2013 POSTER ABSTRACT SUBMISSION DEADLINE EXTENDED TO 10TH JAN 2014



Plenary speakers

Professor David Bish (Indiana University, USA)
Dr Pamela Whitfield (Oak Ridge National Laboratory, USA)
Mr John Fowler (Intertek, WA)
Professor Bill David (ISIS, UK)
Dr Robert von Dreele (Argonne National Laboratory, USA)

Please register and submit your poster abstracts through: www.axaaconference.info

Please visit the website for details of invited speakers, a preliminary conference program including details of the preconference workshops, and details of the exciting opportunity to submit a paper for publishing in *Powder Diffraction*Journal.

A very special thank you to our Platinum Sponsors:



Student Seminar Days

NSW, 19th September 2013

Aurivillius-sillen, prussian blue analogues, tungsten bronzes and the humble perovskite, these were some of the notable structures adopted by the materials presented in this year's NSW Student Seminar Day. I had the pleasure to host the event at the School of Chemistry, University of New South Wales on September 19th. Approximately 25 people attended to hear the young researchers present their work. The attendees were not disappointed, the breadth and depth of research on show was a testament to the diverse range of fields that AXAA covers. The presenters, from three universities, were all excellent public speakers and they will most certainly go on sharing their science with the world. The presenters were Emily Reynolds, Tom Whittle, Stephen Ogilvie and Samuel Liu from the University of Sydney, Neamul Khansur and Patrick Tung from the University of New South Wales, and Simon Hager from the University of Western Sydney.

The audience and presenters engaged in lively discussion following the talks with beer, wine and pizza as facilitators. The food and drinks were proudly sponsored by PANalytical and we thank them for sponsoring this meeting and putting up the prize money for the best presentations. Everyone that attended really appreciates the support you give the students, Universities and AXAA.

On the night, the prizes went to:

First Place: Samuel Liu (University of Sydney)

Second Place: Patrick Tung (UNSW)

Third Place: Tom Whittle (University of Sydney)







(Top left) First place winner Samuel Liu with Scott Gilroy from PANalytical; (top right) second place winner Patrick Tung; (left) enjoying pizza and drinks afterwards.

Congratulations to the winners. Every year we say the judges had a tough time, but this year really took the cake.

Neeraj Sharma & Vanessa Peterson

VIC, 9th October 2013

The 2013 AXAA VIC Student Seminar Day was held at the National Centre for Synchrotron Science and was very well attended with an audience of about 30 AXAA members and guests. Seven student presentations were given in PhD and honours categories – each having a strict 15 min time limit with five mins for audience questions. The students were from three Victorian Universities (Monash, Deakin and Melbourne), with Monash students being the clear majority at this year's event with a ratio of 5:2.

First item on the agenda was a very interesting presentation given by Dr. Helen Brand (Beamline Scientist, Australian Synchrotron) titled "Studying Hydrated Sulphates using Scattering Techniques". Next up were the students who were all eligible for either a full bursary to attend AXAA 2014 or a cash prize in one of two student categories. The stakes were high and the student presentations were all excellent which made the job of the three judges very difficult.

The winner in the PhD category was Anita D'Angelo from Monash University – her presentation titled "Cerium Based Oxides as Oxygen Selective Absorbents" proved hard to beat. Anita was awarded a full AXAA-2014 bursary, and we look forward to her welcoming her into the AXAA community and her future AXAA-2014 conference presentation. A close second "cash prize" in the PhD category was awarded to Jingchao Song from Monash University – his presentation titled "Interpretation of Growth Dynamics of Binary and Ternary Topological Insulators using In Situ Synchrotron X-ray Diffraction" was also very well received by the judges.





(Left) Second place winner in the PhD student category Jingchao Song with Chris Kelaart from Bruker; (right) enjoying refreshments at afternoon tea.

In the honours category there were also two prizes awarded, the first given to Jessica Hamilton (also from Monash University). Jessica's presentation titled "Trace Metal Mobility During Mineral Carbonation" was excellent; in fact I found it remarkable that a presentation of this very high standard was being given by an honours student. Jessica was awarded a full bursary to attend AXAA-2014, and we also look forward to welcoming her into the AXAA community and her AXAA-2014 (cont'd)

conference presentation. The "cash" second prize in the honours category was awarded to Connor Turvey, again from Monash University for his presentation on "Using Portable X-ray Diffractometers for Field Based Carbon Accounting at Woodsreef Chrysotile Mine, NSW, Australia".

Our congratulations to all the student presenters and many thanks to our three judges, Justin Kimpton (Australian Synchrotron), David Hay (CSIRO) and Rod Clapp (Diffraction Technology) who were given a very difficult task. Thank you to Bruker for their generosity, funding the PhD student cash prize and finally our special thanks to several Australian Synchrotron staff who allowed us to use their facilities free of charge to hold this important VIC AXAA event.

Natasha Wright and Nathan Webster

Young Tall Poppies

The prestigious annual Young Tall Poppy Science Awards, run by the Australian Institute of Policy and Science, aim to recognise the achievements of Australia's outstanding young scientific researchers and communicators. Award winners ('Tall Poppies') participate in education and community outreach programs in which they become role models to inspire school students and the broader community about the possibilities of science.

AXAA President Dr. Vanessa Peterson (Bragg Institute, ANSTO) and AXAA Member Dr. Neeraj Sharma (School of Chemistry, UNSW) were among nine 2013 NSW Award Winners. They were presented with their awards at a ceremony held at the Powerhouse Museum on 31st October, which was attended by more than 50 leading representatives of the science, technology, engineering and education sectors from universities, business and industry groups.



Vanessa (front centre) and Neeraj (second from right) with the other NSW Young Tall Poppies winners. (acknowledgement: Daniel O'Doherty)

In addition to Vanessa's research, which centres on how materials work at the atomic scale and uses this information to improve important technologies and discover new materials (she currently leads a group researching materials in "energy technologies" like batteries that power laptop computers and phones), Vanessa participates in a range of outreach activities such as National Science Week events "Science Fact or Fiction" and "Snag a Scientist".

Neeraj's research aims to create new materials and devices that can better utilise the energy we generate and store. He uses X-ray and neutron techniques to "see" how atoms are distributed in energy-related devices and how these change when the device is used. Neeraj regularly presents his work to the public, including annual guest lectures entitled 'The Nuclear Debate' at the International Grammar School, Sydney, and in early 2013 presented the Occasional Address at Sydney Technical High School Speech Day to an audience of over 900 students, parents and teachers.

Congratulations Vanessa and Neeraj!

AXAA National Council, 2014-2017

In accordance with the requirements of the AXAA-Inc constitution, the current National Council will vacate their positions at the next AGM, to be held during the AXAA-2014 conference.

We seek nominations for the 2014-2017 National Council, comprising six members, with three being nominated by the retiring Council and three being nominated by the AXAA members. The retiring AXAA National Council announces our three Council nominees who have accepted their nominations:

Nathan Webster (nominated for President) Vanessa Peterson (nominated for Vice-President) Natasha Wright (nominated for Secretary)

We request that AXAA members forward their nominations for any National Council position, including General Council, President, Vice-President, Secretary, Treasurer and Newsletter Editor positions, to the AXAA Secretary Natasha Wright (natasha.wright@csiro.au).

Closing Date for Nominations: 10th January 2014

Upcoming events

1. Internet XRD Courses (Basic and Advanced Levels): 2014

The I-XRD (Basic and Advanced Levels) Courses have been designed for people who are new practitioners or more experienced XRD analysts.

Features of the course include -

- o Start at any time, subject to the availability of places.
- Self-paced instruction to accommodate the needs of busy people.
- Study materials transmitted as e-mail attachments in the form of 10 modules, with an assignment being set for each module.
- Feedback on the assignments provides excellent mentoring.
- May be used as a vehicle for in-house XRD training.

Internet XRD Course (Basic) - Series 2, 1914

The basic-level course has been designed to give new XRD practitioners a grounding in the use of powder XRD for materials analysis, with particular reference to sample preparation and XRD mounting; XRD data measurement; phase identification and phase composition determination by line ratio analysis. It provides an excellent foundation for the Internet XRD (Advanced) course (see below).

Course fee: \$2,795 including GST

Internet XRD Course (Advanced) - Series 1, 2014

The advanced-level course has been designed to give established XRD practitioners a grounding in advanced methods for powder XRD materials characterisation. Participants will already have some familiarity with very basic crystallography and diffraction principles; sample preparation and mounting; XRD data measurement; phase identification; and quantitative phase composition analysis by line ratio methods.

The principal foci of the advanced course are –

- Crystallography for XRD data analysis, including space group concepts.
- Managing bias in the XRD pattern due to the instrument and the sample, including microabsorption and preferred orientation effects.
- o Pattern simulation using CIF crystal structure files.
- Rietveld characterisation of materials, including phase composition analysis.
- o Indexing a powder diffraction pattern, with space group determination
- o Structure solution when a CIF file is not available.
- Crystallite size and strain analysis.

Course fee: \$2,795 including GST

I-XRD Courses Director: Dr Brian O'Connor

Further information and enrolment:

brian oconnor@iprimus.com.au (Tel 08 9291 7067)

2. Internet XRF Course: Series 7, 2014

The course provides XRF analysts, particularly those new to the field, with on-site instruction on the practical principles of wavelength dispersive XRF. Features of the course include -

- Start at any time
- Self-paced instruction to accommodate the needs of busy people
- Study materials transmitted as e-mail attachments in the form of 11 modules; with an assignment being set for each module.
- Feedback on the assignments provides excellent mentoring.

The course has a substantial number of international participants, as well as Australians, and is being used by companies as a vehicle for in-house XRF training.

Course Director: Dr Brian O'Connor

Course fee: \$2,795 including GST

Further information and enrolment:

brian oconnor@iprimus.com.au (Tel 08 9291 7067)

AXAA Contacts http://\

http://www.axaa.org/

NATIONAL COUNCIL PRESIDENT Vanessa Peterson, ANSTO

Telephone: (02) 9717 9401

e-mail: vanessa.peterson@ansto.gov.au

NATIONAL COUNCIL SECRETARY

Natasha Wright, CSIRO Telephone: (03) 9545 2041

e-mail: natasha.wright@csiro.au

-g...g

NATIONAL COUNCIL TREASURER

Gordon Thorogood, ANSTO

Telephone: (02) 9717 3183

e-mail: gordon.thorogood@ansto.gov.au

NEWSLETTER EDITOR

Nathan Webster, CSIRO

Telephone: (03) 9545 8635

e-mail: nathan.webster@csiro.au

Diffraction Technology

Instruments and accessories for X-ray analysis

Introducing the NEW Nova SxD Now you can upgrade your XRD with a fast X-ray Detector



The addition of a fast Nova SxD detector allows you to scan 30x faster with the same counting statistics. It can give you a real boost in throughput without the expense of a new instrument.

The fast Nova SxD shown fitted to a GBC EMMA

The Nova SxD can be added to any XRD where stepping motor pulses are available. It is stand-alone and there is minimal intrusion into the normal functioning of the XRD. Scanning is done with the XRD operating software, data collection is done on a separate PC and a file is saved.

The Nova SxD comes as a complete system with detector, power supply and software. The only installation required is to take out the stepping motor pulses from the XRD controller.

Documentation is included, and Diffraction Technology can offer the installation service.

Diffraction Technology e-mail diffraction@bigpond.com phone 03 9787 3801 Web www.diffraction.com.au





New in 2014....

Taking analysis from the laboratory into the mine!

- Grade Control
- Process control
- Easy installation
- Best performance!

Visit our stand at the AXAA conference for details



PANalytical launches Epsilon 1 - Small and powerful EDXRF

Focus on easy analysis

PANalytical further extends its benchtop portfolio with Epsilon 1, a low-cost, fully integrated energy dispersive XRF analyzer consisting of a spectrometer, built-in computer, touch screen and analysis software. The well designed optical path, a wide range of excitation capabilities and a highly sensitive SDD detector make it a star performer in the category of low-cost benchtop instrument. When higher performance and sample throughput is required, other benchtop XRF analyzers like Epsilon 3 and Epsilon 3 XL that operate at higher power and are equipped with a

sample changer are available.

The Epsilon 1 range complements PANalytical's energy dispersive X-ray fluorescence series with four application-specific benchtop solutions. These are cost-effective, factory pre-calibrated packages for a range of key analytical processes. Dedicated solutions are available for:

- mining
- determining sulfur in fuels
- determining additives in
- lubricating oils
- research and education



Epsilon 1 for the mining industry: Accurate and safe quantification of rocks and ores

X-ray fluorescence spectrometry is widely used in the mining industry during exploration, mine resource planning and mineral beneficiation. Epsilon 1 easily and precisely determines elemental concentrations of rocks, soils and a wide range of

ore types. The instrument is calibrated with Omnian, PANalytical's market-leading standardless analysis package, used on our more advanced instruments. As an out-of-the-box solution, Omnian can be used to analyze a wide variety of sample compositions from sodium to americium across the periodic table.

With its small footprint and very simple installation requirements, the Epsilon 1 can be placed very close to where the analysis is needed, for example in the quarry or mine-site office.

Epsilon 1 for determining sulfur in fuels: Guarantee your fuel production quality

Levels of sulfur in fuels are heavily regulated because of the environmental impact and their influence on engine lifetime. This is reflected in several test methods and standards, like ASTM D4294, ISO 20847, ISO 8754 and IP 496 where energy dispersive X-ray fluorescence (EDXRF) is the specified analytical technique.

On top of the generic EDXRF benefits, such as low operating costs, Epsilon 1 offers out-of-the box norm-compliant analysis. ASTM D4294 is currently the most stringent test method for the determination of sulfur in fuels and Epsilon 1 easily complies with it.

Epsilon 1 for determining additives in lubricating oils: Compliant analysis

Producers of lubricating oils must also comply with increasingly stringent environmental requirements, like ASTM D6481. Measurement precision is a key requirement of this test method. Epsilon 1 is the ideal analytical solution for the determination of phosphorus, sulfur, calcium and zinc in unused lubricating oils. Total cost of ownership is typically less as compared to techniques such as AAS, ICP and wet-chemical methods which additionally require a dedicated skilled operator.

Epsilon 1 for research and education: Flexible elemental analysis

If you want to liven up your university classes or enhance your serious cutting-edge research, the Epsilon 1 provides an easy-to-operate and X-ray safe soliution. It provides pre-programmed 'out-of-the-box' XRF analysis from simple element identification and quantification to more sophisticated analysis like fingerprinting, standardless and layer analysis.

For further information, visit http://www.panalytical.com/Epsilon-1-range.htm or contact your local PANalytical representative.



A success story continues: X'Pert PRO becomes X'Pert³

PANalytical recently introduced the next generation of multipurpose X-ray diffractometers, the X'Pert³ family. X'Pert³ continues the long successful history of X'Pert systems. Users can now enjoy improved performance and reliability in powder diffraction (X'Pert³ Powder) and thin film metrology (X'Pert³ MRD and X'Pert³ MRD XL) by innovations proven on our latest Empyrean platform. This state-of-the-art XRD technology ensures that the X'Pert³ family is ready for the future.

The X'Pert³ family now uses the patented corrosion-resistant incident smart beam path (CRISP) technology. CRISP prevents X-ray-induced corrosion on any of the incident beam path components, from the X-ray tube, tube housing to incident beam optics, thus maximizing the uptime of your equipment. Toxic wastes, such as lead oxides and beryllium oxides are prevented. In combination with the lead-free tube tower and PANalytical's eco-friendly tube disposal policy this guarantees 'green' operation.

Another feature providing maximum uptime is the introduction of pneumatic shutters and beam attenuators. We have learned from the Empyrean that these type of actuators are the most reliable choice for these frequently operated system components. Smooth operation throughout the system's lifetime is thus quaranteed.

Also adopted from our latest Empyrean system is the 2nd generation PreFIX technology. Reconfiguring your XRD system and optics positioning are now easier and more accurate than ever. Naturally this 2nd generation PreFIX is compatible with the 1st generation, making any transition to a newer system very economical – your existing optics can just be reused. Additionally you can of course benefit from our latest and any future developments on optics, sample stages and solid-state detectors.

The X'Pert³'s new control electronics are now more powerful and networkenabled, offering improved service possibilities by remote monitoring of the complete instrument in the future.

Last but not least these new-generation systems comply with the latest safety standards.

All these innovations make the X'Pert³ systems supreme solutions for many applications of today and tomorrow.

X'Pert³ Powder



The cost-effective multipurpose system for:

- Crystallographic phase analysis (identification and quantification)
- Microdiffraction
- Small-angle scattering (SAXS)
- Pair distribution function (PDF)
- Stress analysis
- Thin film analysis
- Non-ambient XRD





X'Pert³ MRD (XL)

The standard in high-resolution analysis for:

- Thin films
- Reflectivity
- Rocking curve
- Reciprocal space mapping
- Texture analysis
- Stress analysis
- Wafer mapping