



e-newsletter

Issue 2, 2014

Australian X-ray Analytical Association

President's Address

Dear AXAA Members and Friends,

The AXAA National Council met recently and one of the discussion items was AXAA-2017, the next instalment of our National Schools, Conference and Exhibition. We are already formulating ideas about possible host cities and conference venues, and will begin to make enquiries and form plans over the coming months. The post AXAA-2014 survey which many of you completed will help shape our next meeting.

Also discussed were our Student Seminar Days which will recommence in 2015. Recently these events have been held in NSW and VIC only, and before AXAA-2017 our goal is to hold them in the other states to engage more students to become part of the AXAA community. Of course, this will require some people on the ground in each state, but with strong support from Council we don't want this to be too onerous a task so please contact us if you would be willing to volunteer.

As AXAA members, we can all do our bit to promote our community and our events so that AXAA continues to remain strong. One strategy Council is looking to employ initially is sponsorship of prizes at related events attended by both current and potential future AXAA Members. Please let Council know of any events you think suitable.

I'd like to draw your attention to a new addition to the Resource Centre of the AXAA website (www.axaa.org), a link to the "IUCr Erice School 2011- The Power of Powder Diffraction". The link contains presentations (slides and audio) from preeminent diffractionists with topics including "Data Collection – Good Practices", "Rietveld Refinement", "Ultrafast Powder Diffraction" and "Taking it to Extremes". This is a truly outstanding resource for anyone who didn't have the opportunity to attend the school in person.

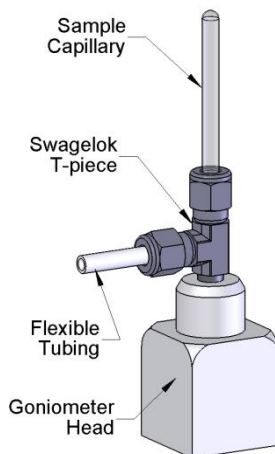
Finally, whilst in Adelaide recently I visited the Royal Institution of Australia, where there is a permanent display honouring the Braggs, complete with a replica Bragg Spectrometer and video describing their life and work. For the mineralogists among us, the minerals display at the South Australian Museum is also very impressive.

Nathan Webster
AXAA President

Matters for Scatterers: The Humble Norby Cell

Despite its simplicity, the Norby cell is an incredibly versatile and indispensable tool for *in situ* powder diffraction and small angle scattering investigations. The same basic design first described by Poul Norby nearly 20 years ago [1], is now routinely used in research laboratories and synchrotron facilities worldwide, and has been crucial to the success of numerous *in situ* experiments. This article celebrates the remarkable contribution of the Norby cell and its derivatives to the field of *in situ* X-ray studies.

The most common implementation of the Norby cell consists of a lightly modified Swagelok T-piece, which allows a glass sample capillary to be mounted and aligned on a standard goniometer head while also enabling the introduction of a cover gas or liquid to the sample. The capillary, which can either be open or closed-ended, is held in place in one tube fitting with a ferrule that provides a gas-tight seal. The opposing tube fitting is often modified to form a blank stub that is compatible with the goniometer head. After alignment, the third (and fourth if a cross-piece is used) tube fitting can then be connected to a flexible tube, through which the cover gas or liquid is supplied. If the capillary is open-ended, this arrangement can be used as a basic flow-through cell. Alternatively, high pressures can be applied to the sample if the capillary is closed. The sample temperature can also be easily controlled by flowing a hot or cold stream of gas over the outside of the capillary, using a hot-air gun or cryostream for example.



Left) Overview of the basic Norby cell design [1]. Above) Photograph of a Norby cell being used during a high temperature oxidation study at the Australian Synchrotron. The cell is being heated by the hot-air blower shown at the bottom of the photo.

The easy control over gas/liquid environment, vacuum, pressure and temperature, as well as its compatibility with the Debye-Scherrer transmission geometry employed at most synchrotron facilities, makes the Norby cell ideal for a wide range of *in situ* applications. These include the study hydrothermal reactions (e.g. [2]), gas-solid reactions (e.g. [3]), phase transitions (e.g. [4]), gas loading of porous materials and hydration/dehydration experiments, to name a few.

Since its first appearance, the Norby cell has been augmented to include additional features, such as integrated heaters [5,6], *in situ* fluid injection [7] and more robust fluid handling capabilities [8]. Although these more sophisticated cells are undeniably useful for achieving certain environmental conditions, the humble Norby cell remains an excellent solution for many *in situ* X-ray experiments and is certainly worthy of recognition.

Mark Styles
Newsletter Editor

- [1] Norby P., *Mater. Sci. Forum*, 1996;228-231:147.
[2] Francis R.J. and O'Hare D., *J. Chem. Soc. Dalton Trans.* 1998:3133.
[3] Krogh Andersen E. *et al.*, *J. Solid State Chem.*, 1998;141:235.
[4] Blanchard D. *et al.*, *J. Alloys Compd.*, 2005;404-406:743.
[5] Palancher H. *et al.*, *J. Appl. Crystallogr.*, 2005;38:370.
[6] Chupas P.J. *et al.*, *J. Appl. Crystallogr.*, 2008;41:822.
[7] Norby P. *et al.*, *J. Appl. Crystallogr.*, 1998;31:481.
[8] Jensen T.R. *et al.*, *J. Appl. Crystallogr.*, 2010;43:1456.

Crystals in the City 2014

Do you know where your atoms are? If not, then crystallography is here to rescue you!

In the International Year of Crystallography, Helen Maynard-Casely from ANSTO and Neeraj Sharma from UNSW have joined forces to develop an exhibition of life-sized crystal structures. We hope that these models entertain, educate and inspire the general public. We also hope that our fellow scientists and engineers (including AXAA members) enjoy these exhibitions and are proud to be affiliated with crystallography. So, go on check out the models and tell your friends, family and colleagues about crysta-what? Crystallography.

Don't forget to engage with social media, take photos with the models and have some fun with it too!

The 'Crystals in the City' project, launching in August is here to celebrate the [UN International Year of Crystallography](#) 2014. We'll be showcasing a number of GIANT crystal structures in cities across Australia and explaining how we know where each and every one of their atoms are.



From a material that keeps your phone functioning, to the shiny gem on your finger, to medicines that treat millions every year – our giant structures will explain how and why the science of crystallography has made all of our lives better.

We currently have five of the giant crystal structures rolling out across Australia, with the first of them to be unveiled in Sydney in August, as part of National Science Week. These are:

A very useful material – Perovskite

Centennial Parklands, Sydney – Friday 1st August - Monday 1st September 2014
UNSW Australia from Monday 1st September onwards

From batteries to the centre of our Earth this structure is all around us – and yet many of us have never heard of it.

A bit of glam – Diamond

Royal Botanical Gardens, Sydney – Friday 1st August - Monday 1st September 2014

Carbon is the versatile element that builds us all and the environment around us. We'll be explaining why this element is everywhere.

A building block of nuclear medicine – Molybdenum

From Friday 8th August at the Australian Museum

Forming one of the most basic crystal structures, but helping diagnose millions of patients every year, molybdenum is a vital metal.

A variation on a theme - SrFeO₃ to SrFeO₂

Questacon Q-Lab until December 2014
Australian Synchrotron from 2015 onwards

We don't really know how networked square planar iron in SrFeO₂ should behave, so the discovery of this structure gives us our first chance to find out.

And there's more in the pipeline (neuraminidase and glucose), and they will be moving about – look out for them popping up somewhere near you. Photos of the structures and smaller 3D printed structural models will be showcased at the Verge Gallery, Sydney University and at Southern Cross University shortly.

Organisations currently providing funding to this project include UNSW Australia, the Australian Nuclear Science and Technology Organisation, the Australian Synchrotron, the Society of Australian and New Zealand Crystallographers (SCANZ), the University of Queensland, Walter and Eliza Hall Institute, DCS Technical with the Royal Australian Chemical Institute (RACI), and the Australian Institute of Nuclear Science and Engineering (AINSE). Affiliated organisations include the Centennial Parklands, the Royal Botanical Gardens, Questacon, Powerhouse Museum, the Australian Academy of Sciences, the University of Sydney, and Southern Cross University. Various people from a range

of institutes have contributed to this project and we would like to thank everyone for their efforts!

Read more at www.crystalsinthecity.com.au and keep up to date @Crystal_in_city

Also, don't forget about the Crystallography365 - <http://crystallography365.wordpress.com>

Crystallography: an Australian science

Why should Australians be one of the proudest crystallographic nations? Well, Australia was at one time home to the Nobel Prize-winning father and son - William Henry Bragg (father) and William Lawrence Bragg (son) - who developed the fundamental equation, $n\lambda = 2d\sin\theta$, that is the cornerstone of crystallography. Every piece of crystallographic equipment relies on this equation and it is used to determine every crystal structure. Bragg's equation has led to countless advances in science and technology with immeasurable benefits for society, and is one of the most important equations ever derived, alongside Einstein's $E=mc^2$.

To this day, Australia packs a significant punch in the world-wide crystallographic community and will continue to do so in the future. Australians should be proud of our historical role in this field and the work Australian scientists have done, and continue to do, using this technique.

Neeraj Sharma
University of New South Wales

Denver X-ray Conference DXC 2014 – Wrap-Up

28 July – 1 August 2014
Big Sky Resort, Montana USA

This year, the Denver X-ray Conference was held nowhere near Denver but in the mountainous ski resort area of Big Sky in Montana. The main base and conference centre is at an elevation of 2,289 m (7,510 ft) above sea level (about the height of Australia's highest peak Mt Kosciuszko) but with Lone Mountain, 3,403 m (11,166 ft) forming the backdrop to the centre. If the views were not sufficient to take your breath away, then the altitude certainly did.



The first two days of the meeting consisted entirely of workshops with themes ranging from Rietveld analysis, latest developments in 2-D detectors, modulated structures, trace element analysis by XRF and micro XRF. It was my privilege to be invited to participate in a full day Quantitative Phase Analysis (QPA) using

diffraction techniques workshop, along with Arnt Kern (Bruker AXS, chair), Mark Raven (CSIRO Land & Water) and Pam Whitfield (ORNL). This workshop provided the basis for QPA along with details of the many pitfalls awaiting unsuspecting analysts.

The conference proper included sessions on New Developments in XRD & XRF Instrumentation, Texture Measurement with X-rays, Electrons & Neutrons, General and Micro XRF, Applied Materials Analysis as well as a session on Small Angle X-ray Scattering for Nanomaterials Characterisation. Australians were well represented in both the audience and the scientific program.



Dr X-ray Ted meets, for the first time, Ms. Sue de Voigt (teD.Phil).

A conference is nothing without the opportunity to catch up with old (and new) friends. The place to be on Tuesday night was in at the Oktoberfest in July sponsored by Bruker where bratwurst, sauerkraut and an endless supply of beer was on offer. Dr. X-ray Ted made the

acquaintance of a new employee at the POWGEN instrument at ORNL, Ms Sue de Voigt (teD.Phil)*. It is understood that they were discussing their campaign to encourage all facilities (i) to employ their own mascot and (ii) bring them to significant conferences to engage in a teddy bear's picnic, er, pub-crawl.

The highlight at the end of the week (on the weekend of course, I wouldn't dream of skipping sessions) was a visit to Yellowstone National Park (~1.5 hours drive from Big Sky). Yellowstone is one of the world's great national parks and is home to one of the largest calderas with over 10,000 thermal features and more than 300 geysers, has wonderful scenery and a wide range of wildlife (bison blocked the road on more than one occasion).



The Grand Prismatic at Yellowstone National Park (photo courtesy of Arnt Kern).

2015 DXC Conference

The 2015 DXC will be held 3-7 August at the Westin Westminster, Westminster, Colorado, USA. 2015 will be a joint conference with the 16th International Conference on Total Reflection X-ray Fluorescence Analysis and Related Methods (TXRF 2015). Watch the website for details of the program and abstract submission deadlines <http://www.dxcicdd.com/index.htm>

Ian Madsen
CSIRO Mineral Resources Flagship
* Sue de Voigt = pseudo-Voigt
(shamefully, I didn't get it immediately either)

PANalytical Award for Young Scientists

PANalytical is one of the world's leading suppliers of analytical X-ray instrumentation and software. The company embarked on an initiative to reward young scientists that have demonstrated innovative thought to their research when using an X-ray analytical technique with a € 5,000 prize. There are no restrictions on the manufacturer of the X-ray equipment that was used.



Ms. Ana Cuesta, affiliated to the Department of Inorganic Chemistry, University of Málaga (Spain) was elected as winner of the PANalytical Award 2013 for her splendid investigation of yeelimite, the most important phase in calcium sulfoaluminate cements. She is currently working on her PhD thesis and plans to invest the prize money in furthering her education. More details about Ms. Cuesta's prizewinning article are described on www.panalytical.com/award.

The winner of the first PANalytical Award in 2012, Dr. Thomas Bennett, appreciated the international recognition of his work in X-ray diffraction, provided by the award. *"Shortly after the award, I was elected to a highly competitive research fellowship at Trinity Hall, University of Cambridge. I was able to use the PANalytical award as evidence of my international standing, which can prove crucial in setting young academics apart from one another."*

The PANalytical Award has now been launched for the third year in a row. The winner of the award would have published a paper that appeared in print during the period from 1 January 2013 until 1 December 2014 and that demonstrates groundbreaking thinking in a topical field. The prize will be decided by a selection committee that includes established research scientists unaffiliated to PANalytical.

Applying for the award is easy via www.panalytical.com/award, with a closing date of 1 December 2014. Correspondence or questions about the award can be addressed to award@panalytical.com.

AXAA Membership

All registered participants of the AXAA-2014 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, a nomination letter from an existing AXAA member, and a short sentence about how they intend to contribute to the organisation. Please send these to the National Council Secretary Natasha Wright (see AXAA contacts) if you would like to apply.

AXAA Website and Contacts

AXAA has a new-look website! Please come and have a look at: www.axaa.org

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Please email contributions for Issue 3 of the 2014 AXAA Newsletter to Mark Styles by Friday the 28th of November. Any comments or feedback about the Newsletter are welcome.

Upcoming Events

MEDSI 2014



The Australian Synchrotron is hosting the 2014 Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI) conference at the Hilton on the Park, Melbourne Victoria, from the 20th to the 24th of October.

MEDSI 2014 will showcase international leading-edge developments in design and research on high end accelerator engineering and technology. The conference features an exciting program, highlighting innovations in UHV Vacuum Technology, Magnet Design and Technology, Accelerator and Beamline Design, Insertion Devices and Endstation Design.

Poster abstracts are still being accepted until the 29th of August. To register, visit: <http://www.meds2014.org/>

Australian Synchrotron Users Meeting 2014 – Incorporating New User Symposium 2014

19-21 November
National Centre for Synchrotron Science, Melbourne

The Australian Synchrotron User Meeting 2014 showcases the best research undertaken at the Australian Synchrotron, and provides updates on the latest technique and applications developments, both here and at our sister light sources overseas.

For the first time, New User Symposium 2014 will be held immediately prior to the User Meeting on 19 November. This one day symposium is aimed at novice users wishing to learn more about how synchrotron, accelerator and neutron based techniques can benefit their research.

User Meeting 2014 and New User Symposium 2014 will be held at the Australian Synchrotron's National Centre for Synchrotron Science (NCSS).

Registration and abstract submission open in late August.

USER MEETING 2014

20-21 NOVEMBER

<http://um2014.synchrotron.org.au>

Enquiries: um2014@synchrotron.org.au

NEW USER SYMPOSIUM 2014

Synchrotron, accelerator and neutron techniques
19 NOVEMBER

<http://nus2014.synchrotron.org.au>

Enquiries: nus2014@synchrotron.org.au

X-ray Materials Analysis Internet Courses – Wavelength Dispersive XRF and Powder XRD

Mode of Instruction for XRF and XRD Courses

These internet-delivered courses provide XRF and XRD analysts, particularly those new to x-ray analysis, with on-site and/or at-home instruction on the underlying principles and principal analytical methods. Features of the two courses -

- 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 a set of modules; with an assignment being set for each module.
- Feedback on the assignments provides excellent mentoring.

The courses have a substantial cohort of international participants, as well as Australians, and are being used by companies as vehicles for in-house XRF and XRD training.

Courses Director: Dr Brian O'Connor

Internet XRF Course: Series 7, 2014

The Internet XRF Course comprises modules on - XRF Overview; X-ray Excitation of the Specimen; X-ray Dispersion and Detection; XRF Data Measurement; Data Analysis Basics; Methods of Quantitative Analysis; Absorption-Enhancement Corrections; Specimen Preparation; Major Component Analysis Using Fusion Buttons; Trace Element Analysis Using Powders; and Analysis of Sub-Milligram Environmental Samples.

Course fee: \$2,795 including GST

Internet XRD Course: Series 2, 2014

The internet XRD Course comprises modules on - XRD Overview; Essential XRD Fundamentals; XRD Measurement Strategies (I); XRD Measurement Strategies (II); Search/Match Identification Analysis (I); Search/Match Identification Analysis (II); Case Studies in Search/Match identification Analysis; Phase Composition Analysis Using Line Intensities; and Introduction to Advanced Methods (indexing, Rietveld phase analysis, structure solution, etc.)

Course fee: \$2,795 including GST

Further Information and Enrolment Procedure:

brian_oconnor@iprimus.com.au (Tel 08 9291 7067)

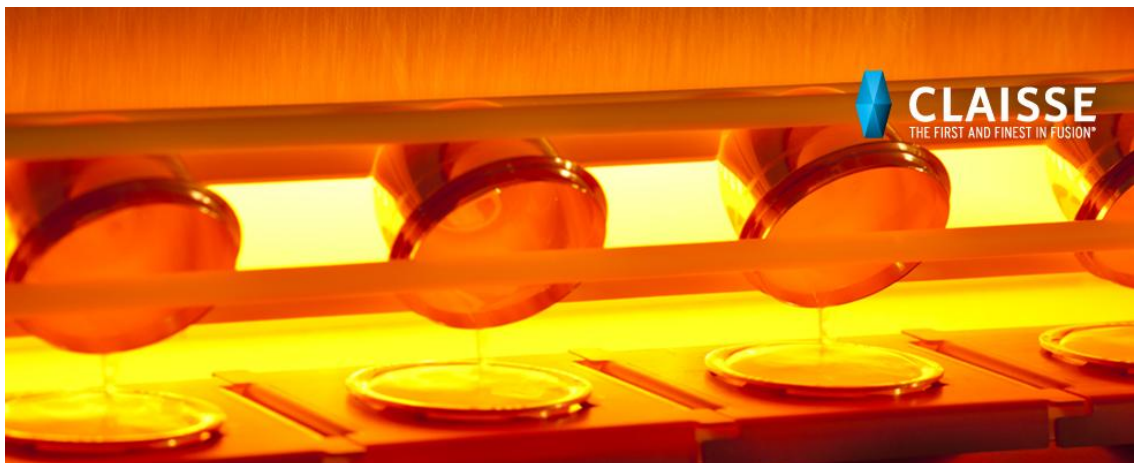
NEWS RELEASE

Acquisition of La Corporation Scientifique Claisse Inc.

Spectris plc ('Spectris' or the 'Company') (LSE: SXS), the productivity-enhancing instrumentation and controls company, today announces that it has acquired the business and assets of the Canadian company La Corporation Scientifique Claisse Inc. ('Claisse'), a global market leader in sample preparation for atomic spectroscopy (including X-ray) analysis, for an undisclosed sum. Revenues for the year ending March 2014 were CAD 13 million.

Claisse designs, manufactures and sells consumables and instruments used to prepare consistent and comparable samples for spectroscopic analysis in mining, pharmaceutical, academic research and industrial applications. Claisse will become part of the Materials Analysis segment and will be integrated into PANalytical, combining two leaders in fusion and X-ray fluorescence (XRF) analysis.

Eoghan O'Lionaird, Spectris Business Group Director, said: "Claisse is a strong strategic addition to Spectris' Materials Analysis segment as it deepens our presence within the sample preparation market. Claisse is renowned for its innovation and fusion technology leadership, and we are confident that the market will benefit from PANalytical's support of Claisse's continued product and application development plans. We believe there is a strong cultural fit with PANalytical, and that the combined capabilities will create significant value for our XRF customers, as well as increasing PANalytical's resilient revenues."

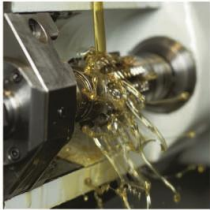




PANalytical

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- Superb energy resolution
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- Operation with all common characteristic X-ray emission lines

The LYNXEYE XE is the first energy dispersive one-dimensional detector for ultra fast X-ray diffraction measurements. It enables high-speed data acquisition up to 450 times faster than conventional point detector systems with a superb energy resolution making $K\beta$ filters and secondary monochromators redundant. Operating with all common characteristic X-ray emission lines (Cr, Co, Cu, Mo, and Ag radiation) it enables outstanding angular resolution (FWHM) and perfect line profile shapes.

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Scancia offers custom-tailored fluxes for your application. We can vary the Li:B ratio, the granulometry and non-wetting agent or oxidizer content.

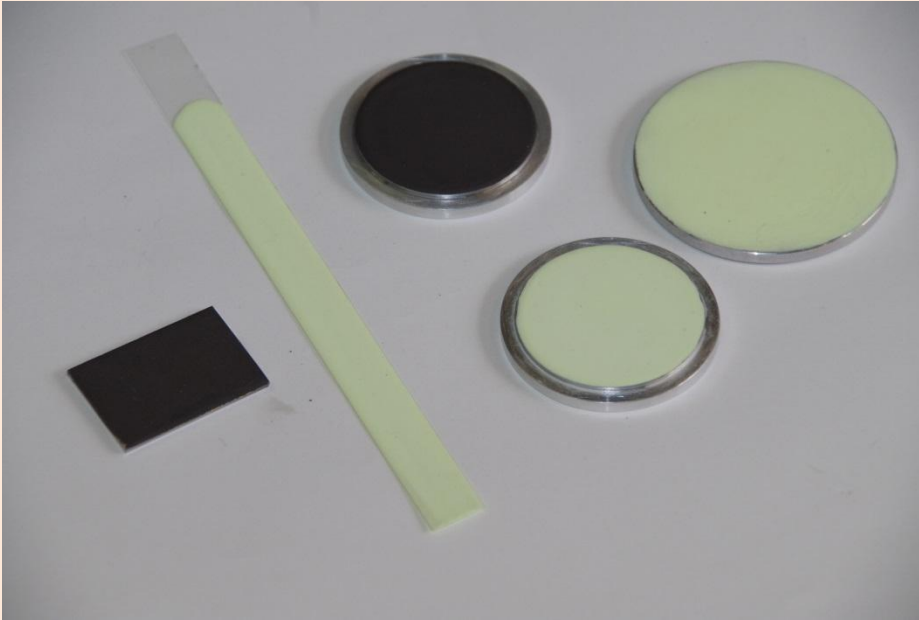
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Contact Rod Clapp.

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