Society of Crystallographers in Australia and New Zealand

SCANZ

http://www.sca.asn.au

SCANZ Newsletter – April 2011

From the President

(Jose Varghese, CSIRO Division of Materials Sciences and Engineering, Parkville)

The last few years I have been fortunate in re-establishing my relationship with the broader crystallographic community. The early years sharing the driving from Perth to the East across the dusty dirt roads of the Nullarbor in Ted Maslen's old Holden for our early crystallography meetings in the early 70's, seems a life time ago. Having moved over into biology after having traversed a number of disciplines in crystallography from charge density and polarized neutrons to virus crystallography, I had less to do with the SCANZ community.

This exemplifies the dilemma facing crystallography as a discipline in the last decade. The availability of extremely bright diffraction sources, better detectors and accelerating computational power, has led to the rapid determination of atomic resolution structures. Ironically we have been caught by our own success. In particular the spectacular growth of the number of biological macromolecular structures determined by crystallography has led to an entire generation of crystallographers who have developed expertise in molecular biology and protein chemistry and the use automated crystallographic software without necessarily understanding the crystallography discipline behind it. The current debate on the ranking of Crystallography Journals is an example. Acta Cryst. was the journal of choice for my first papers in crystallography with Ted Maslen in the mid 70's. None of my biology papers were published in the Acta Cryst journals. The discipline was becoming more a tool to explore molecular structure and its consequences in Physics, Biology and Chemistry with less emphasis placed on the discipline itself.

In recent years, we at SCANZ played an important role in design and construction of crystallography beamlines and the development of the Australian Synchrotron and the OPAL reactor. One of our current challenges is the continued funding for the Australian Synchrotron in our current economic climate. The advent of the Australian synchrotron and the OPAL reactor, the emergence of XFEL sources and the next generation of Electron Microscopes have enabled new techniques and methodologies being applied in our discipline. There is an opportunity here for us to re-establish crystallography in the context of the new Physics that is emerging, like the exploration of new boundaries of diffraction physics and imaging, the study of the physics of crystallization both in novel materials and in biological systems and obtaining atomic resolution structures from quasi-crystalline material.

I am looking forward to Crystal 27 at Rotarua, New Zealand, and following the very successful Crystal 26 at the Barossa organised by Steve Wilkins, I am sure our New Zealand colleagues will deliver a very enjoyable and scientifically invigorating meeting. We wish Chris Squire and the Organizing Committee a resounding success.
Late next year there will be a combined AsCA/SCANZ meeting in Adelaide that will include the Centennial of Lawrence Bragg's seminal paper marking the birth of crystallography, and all of us will all be working very hard to make it a successful occasion.

Finally I would like us to remember the passing of our colleagues over the last couple of years; including David Cockayne former Director of the Electron Microscopy Unit at the University of Sydney, Lachlan Cranswick formerly of CSIRO Division of Mineral Products, Bryan Wise of Meeco Holdings Pty. Ltd., who was always a strong supporter of SCANZ and Victor Maslen of CSIRO Material Science and Engineering.

Medals Update

At Crystal 26 it was decided to institute two new medals to be awarded by SCANZ. They are:

The **Lawrence Bragg Medal**. For distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging.

The **Sandy Mathieson Medal**. For distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging by a researcher under 40 years of age.

Fittingly, these medals will be first awarded at the joint AsCA'12 / CRYSTAL 28 meeting celebrating the Bragg Centennial.

2010 Australasian Crystallography School (*Brett Collins, Chair, UQld*)

The 2010 Australasian Crystallography School was held at the University of Queensland in Brisbane, Australia. The School was attended by 32 delegates from all around Australia and New Zealand, and included both PhD students just embarking on a career in structural biology, and postdoctoral scientists wanting to learn more advanced methodologies, and get experience with the latest developments in crystallographic structure determination. The School was organised by scientists at the University of Queensland, Monash University and from the University of Cambridge (UK) and we were privileged to have high-profile lecturers from the UK (Prof. Murray Stewart), USA (Pavel Afonine), and all around Australia.

The goal of the course was to provide students with a broad theoretical understanding of X-ray crystallography, in particular as applied to macromolecules, and significant hands-on experience with modern software packages for data processing, structure determination and structure refinement. In addition students were given a demonstration of remote access data collection at the Australian Synchrotron, as an introduction to the automation and robotics that are now changing the way that we collect crystallographic diffraction data. Over seven days the students covered topics from protein crystallisation, basic diffraction theory, data processing, molecular replacement and experimental techniques for phasing, structure refinement, model building and structure validation. Generally subjects were divided into theory lectures, followed by hands on tutorials using computing facilities at the University of Queensland, with each student given access to their own desktop system.

We have had very positive feedback from the students following the course. This is the second of the Australasian Crystallography Schools that have been held and there are already plans to host the third one this year in Perth, to be organised by Prof. Alice Vrielink, Prof. Charles Bond (UWA) and colleagues.

We are very grateful for the enthusiastic support we received from sponsors and funding agencies, ARC Molecular and Materials Structure Network, University of Queensland, SCANZ, The Australian Synchrotron, Rigaku/Meeco, Bruker and Oxford Instruments.

Programs, lecture notes and photos from the School are available at:

http://www.imb.uq.edu.au/index.html?page=123027

Vale David John Hugh Cockayne, FRS (*Peter S Turner*)

David Cockayne, friend and colleague of so many Australian microscopists, died peacefully at his home in Oxford on December 22, 2010, following a long battle with cancer. It has been a joy and privilege for me to know David as dear friend and inspiring colleague since we were graduate students together in John Cowley's Diffraction Group at Melbourne University Physics School in 1964. All of us who have known and worked with David are in mourning while we cherish memories of our times with a remarkable person and brilliant scientist. In particular, I recall many stimulating and productive visits to EMU at Sydney University for research collaborations.

David's research career started with his MSc project to test the Cowley-Moodie Multislice theory using convergent beam electron diffraction with Alex Moodie and Peter Goodman, and continued with DPhil and post-doctoral studies in Oxford. Then back to Australia for that remarkable quarter-century as Director of EMU at Sydney University, before returning to Oxford in 2000.

David's retirement from Oxford Materials in September 2009 was marked with a splendid 1-day conference, attended by over 100 scientists from many countries. Many of us present went with a heavy heart, knowing of David's illness. But it was a joyful day of loving tributes – a memorable occasion. Poignantly, the special issue of *Phil Mag* in which the papers presented are published appeared in December 2010. The first paper is a very fine biographical tribute by Sir Peter Hirsch, which brings back many memories of David's rigorous but inclusive approach to research, teaching and leadership of the microscopy community in Australia and internationally.
(http://www.informaworld.com/smpp/section?content=a924771017&fulltext=713240928 - references).

Our deepest sympathies go to Jean Cockayne and Sophie, Tamsin and James and all of David's family.

Vale Lachlan Cranswick

Lachlan Cranswick went missing from his home in Deep River, Canada around the 18th January 2010, and his body was found in Welsh Bay on the 15th June 2010. While only 41, Lachlan was a remarkable contributor to a number of areas of crystallography. The following tribute was written by Armel Le Bail and Ian Swainson while he was still missing.

It is already one month now that Lachlan Cranswick has been listed as a missing person by the police of Deep River, Ontario, Canada, and we have, unfortunately, to consider the possibility that he may never come back. As a friend of us, we have to tell you two or three things about him.

Lachlan M.D. Cranswick was astonishingly hyperactive in the fields of the methods and computer programs for crystallography, both powder and single crystal, organizing all kinds of events such as satellite workshops during international congresses and independent events; round robins about the Rietveld method, SDPD, search-match; Internet stuff like Newsgroups (sci.techniques. xtallography), mailing lists (Rietveld, SDPD); editor of many IUCr Newsletters (Crystallography Computing, Powder diffraction and Teaching Commissions); etc. The CCP14 (from 1998 to 2003) - http://www.ccp14.ac.uk/ - gave him an opportunity to extend his activities of cataloging the most efficient computer programs. He was not himself a developer but was constantly arguing with them in order to obtain algorithm improvements, texts to publish in newsletters explaining more about their software, etc. Thousands of his emails are out there that concern these topics.

He was concerned about the difficulties to do science in developing countries and distributed his NEXUS CD Rom where Internet access was not possible or difficult (Cuba, etc). That regularly updated CD contains a huge list of open software and documentation about crystallography, and more. He was also interested in so many things that it is difficult to summarize: philosophy, history, literature, poetry, etc. Flavors of his life from Australia to Canada passing by the United Kingdom are still available at his personal homepage in Melbourne: http://lachlan.bluehaze.com.au/, a mixture of humorous and serious things. Moreover, quality of life was important to him: he preferred finally Chalk River in a wonderful nature, Canada to another job opportunity at Berkeley. He was involved in many social and sporting activities: he was the vice-president of the Deep River Curling and Squash Club, an avid dinghy sailor on the Ottawa River in the summer, and enjoyed walking and cross-country skiing in the winter.

Two citations from him reveal his professional concerns. The first citation is from a paper about the future of crystallography: "Research institutes and departments that are not willing to reinvest in expert staff, as well as invest in the time and effort it takes to develop scientific leadership in supporting fields such as crystallography, may suffer a precipitous decline in their abilities to perform leading-edge research." (Z. Kristallogr. 217, 2002, 293-4). The second citation is from an Acta Crystallographica paper (A64, 2008, 65-87): "Unless a sufficient body of people continues to dismantle and re-build programs, the knowledge encoded in the old programs will become as inaccessible as the knowledge of how to build the Great Pyramid at Giza." Lachlan co-authored or authored at least 53 papers listed in the Web of Science, one of them entitled "Superconductivity in LaFe(1-x)CoxAsO" (Phys. Rev. B78, 2008, 104505) appears to be destined to attract a large number of citations (already 60 by 2009). He had written chapters in the most recent books about powder diffraction. His career was just beginning, he was

aged only 41.

Lachlan has worked for the NRC's Canadian Neutron Beam Centre for seven years. "His collaborators from universities across Canada praise his effectiveness in supporting their research," said Daniel Banks, a spokesman for the centre. "He was a driving force in developing our scientific tools to the leading edge." Indeed, he was a driving force not only for the NRC but for the world!

Those of us who know him well miss him as a good friend. But the entire community of crystallographers will also miss him professionally, probably finding much less information on the Web about the tools they may use in order to solve their problems. Forgive us the joke, but we prefer to believe that he was captured by aliens wanting to improve the level of crystallography on their planet, rather than to imagine something worse.

A timeline of Lachlan's passing can be found on his website (http://lachlan.bluehaze.com.au/update.html). There was a special session in his honour at the American Conference on Neutron Scattering in Ottawa in 2010 and there is one on computational crystallography coming up in the 2011 American Crystallographic Association meeting which is being held in New Orleans. A more formal obituary has now appeared in *J. Appl. Cryst.* (2010, **43**, 1134; http://scripts.iucr.org/cgi-bin/paper?S0021889810035971), and highlights of his funeral service can be found on Youtube (search for "Lachlan Cranswick").

A new mineral (cranswickite), discovered by R.C. Peterson, was also named in honour of Lachlan. The abstract of the manuscript announcing its discovery is as follows:
Cranswickite is a new mineral of composition $MgSO_4$•4(H_2O) from Calingasta, Argentina (IMA2010-016). Cranswickite is monoclinic, space group Cc, a = 11.9183(3)Å, b= 5.1709(1)Å, c = 12.1888(3)Å, β = 117.537(2)°, V= 666.1 Å^3, Z =4. The mineral occurs as a soft white vein filling in a metasedimentary rock (d_{calc} =1.918 Å^3). The atomic structure has been determined by direct methods and refined by Rietveld refinement of powder diffraction data. The atomic structure consists of chains of corner-sharing magnesium-containing octahedra and sulfate tetrahedra. All the water molecules directly coordinate magnesium in the structure. The five strongest lines in the powder X-ray diffraction data are [d_{obs} in Å (I)(hkl)]: 5.259 (100) (200), 3.927 (46) (1 1 -2), 3.168 (45) (1 1 -3), 4.603 (29) (1 1 -1), 2.570 (23) (3 1 1). Infra-red and Raman spectra are very similar to the spectra measured from starkeyite. Cranswickite is closely related to starkeyite $MgSO_4$•4(H_2O) that has an atomic structure where two sulfate tetrahedra and two magnesium octahedra share corners to form a four-membered ring and not a chain as in cranswickite.

Powder Diffraction Workshop

The Australian Synchrotron will be hosting the first (of what will hopefully be an annual) joint AS-PD / OPAL-PD workshop entitled "Powder Diffraction at Australia's Synchrotron and OPAL Facilities: Experiment Planning to Data Analysis" on 6th-9th September 2011.

The workshop targets early career researchers who have used, or plan to use the powder diffraction facilities at OPAL or the AS. We aim to provide information covering applying for instrument time and planning the experiment through to data analysis. Over the 4 days participants will hear lectures from experts in the field and also be given several opportunities to gain hands-on experience with data analysis software.

AsCA'12 / CRYSTAL 28

The next AsCA meeting, the Bragg Centennial meeting, will be held jointly with CRYSTAL 28 at the Adelaide Convention Centre on November 2-6, 2012.

Bragg Centennial Symposium (*Steve Wilkins, CSIRO*)

On 11 November 1912 at the age of 22 and while still a PhD student at Cambridge, William Lawrence Bragg presented a lecture to the Cambridge Philosophical Society on the interpretation of the X-ray diffraction data for Zincblende (ZnS) that had been recorded by Max von Laue and colleagues in Gottingen earlier that year. Based on the theory he developed of coherent reflection of X-rays from planes of atoms and an understanding of the nature of the X-ray spectrum involved, Lawrence was able to correctly determine the structure of Zincblende cf von Laue and colleagues who had proposed a simple cubic structure from their data. Thus was begun the field of modern crystallography and the start of a revolution in our ability to determine the structure of matter.

Lawrence Bragg was born in Adelaide in 1890, the son of William Henry Bragg, Professor of Mathematical and Experimental Physics at the University of Adelaide. His schooling was at St Peter's School in Adelaide. In 1915, Lawrence and his father were awarded the Nobel Prize for Physics (jointly with von Laue) for their development of X-ray crystallography. Lawrence remains the youngest Nobel Prize winner in Physics and the only Australian born scientist to achieve this honour. It is therefore very fitting that we hold a special centennial symposium to mark his pioneering of X-ray crystallography and that we hold it in Adelaide. A number of eminent speakers are planned to talk on the role of Lawrence Bragg and the way in which his discovery have led to major developments in structural science. The Symposium will immediately follow on from the planned AsCA/SCANZ meeting, also in Adelaide, and Australian Institute of Physics Congress in Sydney, commencing on 9 December.

Proposed dates and venue for the Lawrence Bragg Centennial Symposium are:

6-7 December 2012, Adelaide Convention Centre

Upcoming Meetings

April 27-30, 2011	CRYSTAL 27 meeting Rotorua, NZ http://www.crystal27.org.nz/
July 18-22, 2011	2011 Australasian Crystallography School UWA, Perth
August 22-30, 2011	XXII Congress and General Assembly of the IUCr Madrid http://www.iucr2011madrid.es/
September 6-9, 2011	Powder Diffraction at Australia's Synchrotron and OPAL Facilities: Experiment Planning to Data Analysis Australian Synchrotron, Melbourne
November 2-6, 2012	Joint AsCA'12 / CRYSTAL 28 meeting Adelaide
November 6-7, 2012	Bragg Centennial Symposium Adelaide

THE UNIVERSITY OF WESTERN AUSTRALIA

Achieving International Excellence

2011 Australasian Crystallography School

(macromolecular and small molecule crystallography)

University of Western Australia

Date:

July 18 – 22, 2011

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