[Back to SCA Homepage | What's New | Contact Information | SCA Conferences and Events] |

Society of Crystallographers in Australia

SCA

Newsletters

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FROM THE PRESIDENT

People who appreciate the beauty of crystals can be found everywhere. The day after Tim Fisher announced his retirement as leader of the National Party, a journalist recounted in *The Advertiser* how disturbed Tim had been to see how a crystalline formation had been hacked into to provide a path for an electricity cable in a cave somewhere in NSW. Most of us are more concerned every day with the intricacies of the internal structure of crystals, but we know that the external beauty follows from that.

Syd Hall is another who appreciates the beauty of crystals. It may be drawing a long bow to connect Syd with Tim, but they have at least one other thing in common, Syd is retiring also, as Editor of *Acta Crystallographica C*. During his editorship he has been at the forefront of moves to improve the standard of data used in crystal structure analyses reported in the IUCr journals. Hopefully, this will result in raising the level across the board, because there are still too many structures published in chemistry journals that do not reach acceptable standards. The coordinates from these find their way into data bases, where they may be used by the unsuspecting in further research.

The Society, as presently constituted, came into being in 1976 but there were meetings of Australian crystallographers from the early 1960's. Over the intervening time, members have come and gone but it has been brought to my notice that three members who have been involved since those earlier days have resigned this year viz. Colin Kennard, Bryan Gatehouse and J. E. W. L. Smith. Colin has resigned from the University of Queensland, but still keeps a room in the Chemistry Department and can be joined at lunch on Tuesdays. Bryan, who founded crystallography at Monash, says that his interests tend more towards boat-building these days.

I can think of no more concise testimonial to these two than to note that when I asked two former students for some information about them I got immediate responses that would have filled two pages of this *Newsletter*. John Smith was Hans Freeman's first research student. Although not continuing with crystallography, he has kept up an active interest and only a couple of months ago asked me for some

information to pass on to school pupils. He has recently retired from the Callide Power Station in Queensland. I wish them all well.

Right now I am preparing to retire myself, to warmer climes in the northern hemisphere where I will be attending the IUCr Journals Commission Meetings in Manchester and the Congress in Glasgow.

Max Taylor

CRYSTAL XXI

The twenty-first meeting of the Society of Crystallographers in Australia will be held at the Thredbo Alpine Hotel Conference Centre, Thredbo Alpine Village, NSW from February 1-4, 2000.

The important dates are:

- September 1999: Call for abstracts and registration

- November 5th 1999: Deadline for the submission of abstracts and registration and accommodation bookings.

The *1987 Lecture* will be given by Dr Douglas L. Dorset (Electron Microscopy/Diffraction) Principal Research Scientist at the Hauptman-Woodward Medical Research Institute, Buffalo.

Other invited lecturers are: Ian Grey (CSIRO Div. Minerals), Colin Raston (Monash University), Bill David (UK) Peter Colman (BRI) and Stephen Hyde (ANU).

Accommodation

Accommodation at the Thredbo Alpine Hotel will be $90 per person/day for single, and $45 per person/day for twin or double rooms. Apartment accommodation is also available at $35 pp/day with a mixture of twin and single rooms.

A wide range of accommodation is available in Thredbo, but we would encourage use of the that which we have arranged at these very favourable group rates since the more people using this accommodation will lower the cost of our use of the conference rooms. We will ask those requesting apartment accommodation to nominate possible room mates in the event that they are allocated a twin room and will endeavour (where possible) to meet such preferences. Further information can be obtained from the conference at website: http:// rsc.anu.edu.au /~welberry/crystal21/.

Alison Edwards

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

The Australian Synchrotron Research Program at the Advanced Photon Source, Chicago.

Introduction

In a previous article Drs Garry Foran and James Hester described how the Australian National Beamline Facility (ANBF) evolved into the Australian Synchrotron Research Program (ASRP). The authors gave a detailed account of the original facility at the Photon Factory, which has yielded so much excellent science and continues to go from strength to strength.

The expansion of the ASRP into the Advanced Radiation Source (APS) in Chicago now gives Australian researchers access to third generation synchrotron radiation (SR). Highly collimated and intense light from the APS will open up such areas as time-dependent studies of crystalline and amorphous condensed matter systems, as well as allowing us to use traditional X-ray scattering techniques on micron-sized sample regions. In addition, the X-ray energies generated by APS insertion devices and bending magnets extend the SR energy ranges normally available at second generation sources to well above 100keV (less than 0.124Å in wavelength). This will open the way to scattering studies of high-Z materials for which X-ray absorption at more "conventional" energies is a serious problem.

The Australian involvement in a number of Collaborative Access Teams (CATs) at APS is first and foremost a science-driven enterprise, designed to complement our existing facility at the ANBF in Japan. This is reflected in the choice of beamline sectors to which the ASRP contributes funding and manpower. Our support of these sectors has guaranteed us substantial beam time, a sizable influence on the scientific directions taken by these facilities and a point of ingress for Australian scientists into the larger APS community.

Collaborative Access Teams at the APS

Each CAT "owns" at least one sector on the APS storage ring. Each sector contains two primary radiation sources; a bending magnet and an insertion device (usually an undulator). An undulator beamline will typically accommodate experiments where highly intense and well-collimated beams with small spatial dimensions (1mm down to 1μ m) are required. Bending magnet beam lines, on the other hand, are more suited to applications where larger beam footprints are required (as is often the case for imaging) or in applications such as multiple-wavelength anomalous diffraction (MAD) where a smooth energy spectrum profile is advantageous.

The instrumentation and beamline facilities available at the APS are far too numerous to document here in detail, although a brief outline of each of the sectors directly involving the ASRP will be given. We would like to encourage interested researchers to visit the following web sites for more information:

- www.ansto.gov.au/natfac/asrp.html - for an overview of the ASRP, how to apply for beamtime, e-mail contacts and links to relevant web sites.

- www.aps.anl.gov - for an overview of the Advance Photon Source in Chicago and links to all its CATs.

- cars1.uchicago.edu/chemmat/chemhome.html - for an overview and details of the ChemMatCARS CAT (sector 15).

- cars1.uchicago.edu/biocars/biocars_home_page.html – for an overview and details of the BioCARS CAT (sector 14).

- www.aps.anl.gov/sricat/ - for an overview and details of the SRI-CAT (sectors 1 – 4).

ChemMatCARS (Sector 15)

This sector is devoted to the study of chemistry and materials science. The insertion device beamline (15-ID)

is currently under construction and well on the way to completion, with a bending magnet beamline (15-BM) planned within the next few years.

This facility is run by the University of Chicago and includes a number of other universities and institutes in its consortium. Initially, this CAT will service four distinct areas:

- Single crystal crystallography
- High energy resolutions XAFS
- Static and time-dependent reflectometry on liquid and solid surfaces
- Static and time-dependent small and wide angle X-ray scattering (SAXS /WAXS) on liquids and 'soft' solids such as polymers and fibers.

Dr David Cookson is the ASRP scientist stationed at this sector. He previously worked with Dr Garry Foran at the ANBF in Japan for five years before relocating to Chicago.

BioCARS (Sector 14)

Also run by the University of Chicago, this CAT is devoted to protein and virus crystallography. It has been fully constructed and is now accepting Australian users. It has three separate beam lines:

1) Insertion beamline 14-ID-B, is designed for both high-resolution monochromatic crystallography (including MAD), and for time resolved studies using pink beam (ie white beam with higher energies removed) in Laue configuration.

2) Bending magnet beamline 14-BM-C, designed for monochromatic protein and virus crystallography. This is the "work horse" beamline optimized for more "routine" protein diffraction experiments.

3) Bending magnet beamline 14-BM-D, designed for MAD, monochromatic and Laue experiments.Dr Harry Tong is the ASRP scientist stationed at this sector. Harry joined the ASRP one year ago, having had a number of years of protein crystallography experience working in Australia, Canada and the Netherlands.

SRI-CAT (Sectors 1 to 4)

The Synchrotron Radiation Instrumentation CAT is run by the APS itself under the Experimental Facilities Division (XFD). This CAT was formed with dual missions: to perform basic research in synchrotron-based optics and techniques, and to develop and operate strategic instrumentation that takes full advantage of the capabilities of the APS. As was originally envisioned, new CATs building their own facilities at the APS have used much of the technology arising from SRI-CAT research, especially in the area of high-heat load optics.

About 80 XFD staff members are directly involved with beam-line operations. Three of the four sectors run by the CAT are currently operational with the fourth scheduled to take first light next year. A summary of the sectors and their associated beam lines follows:

Sector 1: Time resolved studies, high-energy X-ray studies and high heat load studies.

This sector has presently one undulator line and one bending magnet line. It has flexible beam lines, which would be suitable for Australian users wishing to use third-generation radiation in an ad hoc setup.

- 1-ID (undulator line): Energy range from 5-130 keV. Scattering from disordered materials, X-ray

diffraction, high-energy microprobe studies (40-60 keV).

- 1-BM (bending magnet): Time resolved spectroscopy, energy dispersive XANES, dispersive diffraction.

Sector 2: X-ray microprobe (including micro-tomography, fluorescence and diffraction), high-resolution soft X-ray spectroscopy and deep X-ray lithography.

This sector has one bending magnet line, and four branched undulator lines, two taking radiation from a soft X-ray undulator and two using a hard X-ray undulator.

- 2-ID-B (soft X-ray undulator): high-resolution micro imaging (tomography, fluorescence, diffraction etc), coherent scattering and interferometry.

- 2-ID-C (soft X-ray undulator): high-resolution soft X-ray spectroscopy. Spectromicroscopy and diffraction of surfaces and near surface regions. Magnetic studies.

- 2-ID-D and 2-ID-E (hard X-ray undulator): high resolution micro-fluorescence imaging , micro-diffraction and coherence based techniques.

- 2-BM (bending magnet): micro-tomography, diffraction, fluorescence microprobe, high-resolution fluorescence spectroscopy, deep X-ray lithography for prototyping micromachined parts.

Sector 3: Inelastic X-ray and nuclear resonant scattering studies.

3-ID (undulator): High energy-resolution X-ray scattering in the 6-30 keV range.

Sector 4: Polarization/magnetic studies.

This sector is being built and will become operational next year. The sector will comprise a soft and hard X-ray undulator line both delivering circularly polarized light and both being able to operate in parallel. Present magnetic/polarization studies are pursued mainly in sectors 1 and 2.

Dr Anton Stampfl is the ASRP scientist stationed at these sectors. Prior to this position, Anton worked in Germany at the Fritz Haber Institut and Freie Universität in Berlin and at La Trobe University in Melbourne.

David Cookson, Harry Tong,

Anton Stampfl, Richard Garrett

Call for applications for the "E.N.(Ted) Maslen 1987 Studentships and Scholarships"

CRYSTAL XXI

Thredbo, NSW, February 1-4, 2000

The Council of the Society of Crystallographers in Australia is calling for applications from postgraduate students of crystallography for the "E.N.(Ted) Maslen 1987 Studentships and Scholarships" to fund attendance at the twenty-first meeting of the Society of Crystallographers in Australia to be held at Thredbo

Village, New South Wales from February 1-4, 2000.

Details of the conference are available on the internet at: http://rsc.anu.edu/~welberry/crystal21/.

SCA student members from both Australia and New Zealand are invited to apply for the Scholarships, which will make a substantial contribution to the travelling costs. Selections will be based upon merit, geographic distribution and previous and/or future opportunities of the candidates. As the SCA Council regards these awards as an important means of introducing young crystallographers to the national and international scientific community, students awarded Scholarships will be expected to make a presentation of their work at the meeting.

The method of application is straightforward, but a strict deadline will apply.

Method of Application

Postgraduate students applying for a "1987 Scholarship" should forward to the Secretary, Dr Brendan Kennedy, School of Chemistry, University of Sydney, NSW 2006 the following:

- An abstract of the presentation sent, or to be sent, to the Organising Committee.

- A covering letter from the applicant' supervisors with a brief reference and verifying that the applicant is a *bona fide* student at the time of the meeting.

- An indication of what other funding may be available from the applicant's own institution.

- An indication as to whether the applicant has previously received funding from the SCA.

It is expected that he deadline for applications will be December, 1999, the exact date to announced in the next *Newsletter*.

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

Department of Applied Physics,

Curtin University of Technology.

The present laboratory had its origins in the X-ray analysis facility established in 1967 by John de Laeter, the founding Head of Physics at the Western Australian Institute of Technology (renamed Curtin University of Technology in 1987). The facility was mainly used in the initial years to provide X-ray powder diffraction and fluorescence spectrometry support for mineral science, meteorite and cultural heritage projects. Geoff Kerrigan and Ian Bailey shared laboratory direction during this period.

Brian O'Connor was appointed to lead the laboratory in 1971 having gained a PhD in crystallography at the University of Western Australia (UWA) with the late Ted Maslen, and then having worked as a post-doctoral fellow with Terry Willis at Harwell and Dorothy Hodgkin at Oxford, and again with Ted Maslen on electron density studies. Brian had not even seen a powder diffractometer on arrival at Curtin.

Some 15 years ago, Brian and Mark Raven (then a student) committed to the development of Rietveld modelling for microstructural characterisation whereas the technique had been largely used up to that time as a crystal structure refinement tool. While atom position definition is now of interest to the Curtin team, their

principal focus with Rietveld analysis continues to be the development of procedures for absolute phase abundance measurements, texture, strain, crystallite size, etc.

The laboratory is currently equipped with a Bragg-Brentano Siemens D500 diffractometer for pattern acquisition, and a multi-purpose D5000 instrument for pole-figure, residual stress and grazing incidence diffraction. Extensive use is also made of neutrons (MRPD and HRPD powder instruments at Lucas Heights, mainly for high temperature data acquisition), and synchrotron radiation (BIGDIFF at the Photon Factory, Tsukuba, Japan) to supplement laboratory-based X-ray diffraction measurements. The laboratory also has a Siemens X-ray fluorescence/emission (XRF) spectrometer which is invaluable for applying attenuation corrections to diffraction data according to Compton scatter intensities.

Crystallographic expertise is largely provided by Deyu Li, Arie van Riessen, Craig Buckley and Brian O'Connor. Li joined Brian at Curtin in 1987 from the Shanghai Institute of Ceramics where he had acquired the Rietveld disease after gaining a PhD under the distinguished Russian crystallographer Valentin Simonov.

The laboratory has produced various crystallographers-cum-materials scientists in recent years including Bruno Latella (now at ANSTO), Bee K Gan (UTS), John Carter (Australian Fused Materials), Husin Sitepu (NIST, USA) and Mark Raven (CSIRO). We were delighted when Bee and Bruno married during their time as PhD students. Recently the group has become a popular choice for Indonesian postgraduates, notably Pheman Suherman, Dwi Asmi, Suminar Pratapa, Athanasius Bayuseno and Simon Sembiring. The large Curtin Rietveld gang (approximately 15 at any one time) is fortunate to have Hugo Rietveld as a mentor through Hugo's regular visits to Perth to see family.

The laboratory is now one of the principal facilities of the Curtin Materials Research Group which specialises in industry-directed research. The most substantial research achievements in recent years have involved (1) bauxite processing by the Bayer method, (2) processing of alumina-matrix advanced ceramics, and (3) metal corrosion. Craig Buckley's recent arrival has expanded the diffraction research armoury to include small-angle neutron scattering measurements and computational modelling of electron density distributions.

Brian O'Connor

Society of Crystallographers in Australia

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