The Australian Synchrotron in the International Year of Crystallography

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The Australian Synchrotron has been providing world quality X-ray diffraction instrumentation and expertise to the scientific community via the Powder Diffraction and two Macromolecular Crystallography beamlines since 2007. These capabilities reach across the scientific landscape from studies of advanced materials for applications such as electronics displays and new energy technologies, to development of new pharmaceuticals, studies of disease and other fundamental biological processes.

The Australian Synchrotron in Melbourne (Figure 1) is one of Australia's premier research facilities and, at over $250 million, represents one of the biggest single investments in scientific excellence in the nation's history. Operated by the Australian Nuclear Science and Technology Organisation, the Australian Synchrotron produces intense beams of X-ray and infrared light at experimental end-stations, providing unique experimental capabilities. Since commencing user operations in 2007 the Australian Synchrotron has become an integral part of the Australian and New Zealand research scene. The facility has now supported over 2500 experiments and more than 20,000 user visits resulting in scientific research that has already had significant and lasting impact.

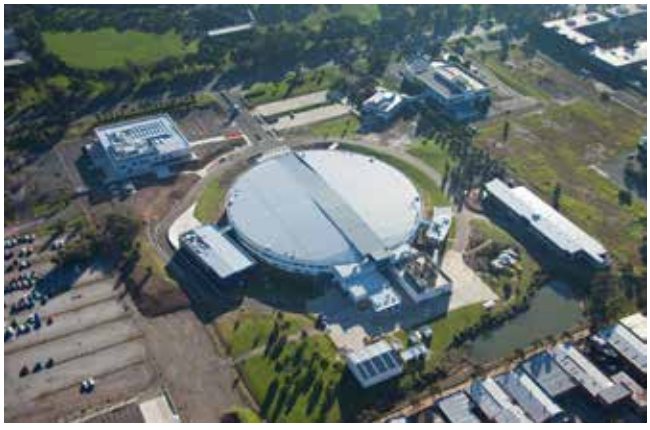

Figure 1: The Australian Synchrotron and National Centre for Synchrotron Science (top left).

Research performed at the Australian Synchrotron has seen world-leading results in: medical and life sciences, including key insights into diseases such as malaria and diabetes; advanced materials and engineering, including drug delivery systems and new types of electronics; and earth and environmental sciences including reduced CO_2 emissions in cement manufacture and hydrogen storage materials. Many of these results are underpinned by the use of crystallography and it is fair to say that the technique is a workhorse for synchrotron facilities around the world. In this UN-declared international year of crystallography, it is a good time to showcase some of the outstanding science produced at the Australian Synchrotron and which was made possible by the work of "Australia's" W. L. and W. H. Bragg just over 100 years ago.

"...the use of crystallography.... is a workhorse for synchrotron facilities around the world"

The history of crystallography in Australia is a rich one, many aspects of which are well documented. John Jenkin's biography, for instance, of the Bragg's, William Henry and William Lawrence, provides a wonderful tour of the scientific, the personal and the societal environment surrounding the "Most Extraordinary Collaboration in Science". What may be less well appreciated are the extent and the connectedness of the crystallographic links in the Australian research story, particularly from the 1950's onwards. Any attempt in a brief note such as this to definitively represent the pioneers and achievements of crystallography through that period to the current day is doomed to failure. Instead, allow this random sampling to demonstrate the impact crystallography has had and the connections it has spawned on the national research scene.

In the 1950's A. D. Wadsley set up an X-ray lab in Melbourne with a series of high resolution Guinier cameras, bits of which are still in use at CSIRO (thanks to

Ian Grey for this piece of social history). He was also a pioneer in the use of electron microscopy in tandem with diffraction to solve structures in the very early era of electron diffraction. Some of the initial attempts in this space were pursued, at Wadsley's suggestion, by John Cowley and Alex Moodie also from CSIRO who were of course seminal researchers in that field. Wadsley was asked to submit a case for the Nobel prize but unfortunately died before it could be considered, but does have the honour of having the high pressure mineral, Wadsleyite named for him.

In the 1960's Ted Maslen, who had worked at Oxford with Dorothy Hodgkin on molecular structures, came back to the University of Western Australia and set up a crystallography lab. Among many others he supervised Hugo Rietveld, and it is the Rietveld method that is so critical to refinement of crystal structures from powder diffraction data. Maslen was a driving force in getting diffraction up and running at the 10 MW HIFAR reactor at Lucas Heights, Sydney, establishing a long tradition of, what is now, the Australian Nuclear Science and Technology Organisation's involvement in crystallographic methods.

"A synchrotron light source provides an increase in brightness of the X-ray light by more than a factor of a million compared to laboratory sources."

The development of inorganic crystallography was soon followed by proteins. Early developments of structural biology work through Hans Freeman at the University of Sydney and Ted Baker in New Zealand (who was also a past chair of the Scientific Advisory Committee of the Australian Synchrotron) included the solutions of plastocyanin and actinidain respectively in the 1970's. The structural biology field has generated many notable alumni since then (many of whom such as Peter Colman and Mitchell Guss have played important roles in the development and direction of the Australian Synchrotron serving respectively on the board of the operating company and as the chair of the Scientific Advisory Committee – more of these connections can be followed in other better-informed summaries such as Jenny Martin's [1], herself a previous member of the Scientific Advisory Committee), and the growth of both inorganic and protein work continues at a rapid pace.

A huge increase in that pace came about with the advent of synchrotron light sources as user facilities. A process which began in the 1980's but has accelerated in the 1990's and, for Australian researchers, in 2007 when the Australian Synchrotron commenced operations. A synchrotron light source provides an increase in the brightness of the X-ray light by more than a factor of a million compared to laboratory sources. To take advantage of the signal-to-noise advantage and the tunability of the X-ray energy, synchrotron beamlines develop a sophisticated arsenal of sample handling and treatment options. At the Australian Synchrotron for instance, the crystallography beamlines offer automatic sample changing, cryogenic puck mounting systems, UV laser for radiation damage induced phasing, xenon pressure chamber for isomorphous replacement phasing, tunability for single or multiple anomalous diffraction methods, micro-collimation, in tray screening and the list goes on. At the powder diffraction beamline high and low temperature stages, high pressure environments, gas flow environments and other *in situ* capabilities are commonly in use. All these are coupled with high data rate acquisition, analysis storage and remote access. It is little wonder then that outputs from the facility have been rising steadily since 2007, with now more than 1600 publications, many of which rely on crystallography.

But it is not just the raw numbers that are impressive. Access to the world-class facilities at the Australian Synchrotron creates an opportunity for research that can't be done any other way. As a result some of the best in research from Australia, New Zealand and beyond has been facilitated by access to the Australian Synchrotron. For instance, researchers have reported findings relating to understanding how insulin binds to its primary receptor [2] – a result that could have profound implications for the design of more robust forms of synthetic insulin. Other results provide insight into the operations and triggers of the immune system [3]. In this the International Year of Crystallography, results such as these published in leading journals such as *Nature, Cell* and *Science*, are signposts in excellence for the innovation and translational research that often follows to the benefit of the economy and the health of society.

Powder Diffraction at the Australian Synchrotron

The *Powder Diffraction* (PD) beamline at the Australian synchrotron [4] provides the research community with a cutting edge crystallographic tool. The high

flux of X-rays delivered to the beamline from a bending magnet source, combined with the high-resolution, and a position-sensitive Mythen II microstrip detector [5] enables the collection of an entire diffraction pattern simultaneously. This allows processes to be tracked *in situ*, with real-time crystallographic information collected continuously, avoiding artefacts and loss of information on sampling. The wide range of available sample environments, and the ability to design and construct bespoke environments, provides the crystallographic community of Australia with a unique capability to study the structure and function of crystalline materials. The popularity and success of the beamline is evident in the publication record which has continued to increase year-on-year; publishing more than 330 peer-reviewed journal publications since 2008.

In the near future the *in situ* capabilities of the *Powder Diffraction* beamline will be extended further with robotic sample changers and remote access schemes designed to optimise high throughput. In addition, a higher energy, *Advanced Diffraction and Scattering* (ADS) beamline based upon a superconducting wiggler X-ray source is planned as part of the next suite of beamlines to be built at the Australian Synchrotron. The ADS beamline will have access to higher energy X-rays with a greater flux for more sample penetration, and will be focussed horizontally to minimise divergence. This will open up a new exciting sector of science with opportunities for techniques such as rapid texture analysis and 2D materials mapping scanning diffraction tomography, energy dispersive diffraction studies and high resolution 3D strain scanning of large volume materials from areas as diverse as high pressure mantle geology to studies of lead-free piezoelectrics.

Powder Diffraction Case studies

(i) Nucleation and crystallisation of minerals: Jarosite

Jarosite minerals are widespread in a number of industrial and environmental settings; for example, jarosite is deliberately produced to remove iron from hydrometallurgical circuits in zinc production facilities, [6] however in metal bioleaching systems the formation of jarosite inhibits the desired reaction [7]. Jarosites are also a major component of acidic soils, and present in significant amounts in acid mine drainage environments [8]. Researchers are developing sustainable solutions to jarosite stockpiles created as by-products of mineral and industrial processes. On Mars, jarosite may represent the key to unlocking the geological history and environmental context of water on the red planet. [9,10] Understanding jarosite formation, mineralogy and stability is essential for streamlining industrial processes that involve jarosites, and understanding the geological evolution of the environments in which they abound.

"...*in situ* X-ray diffraction experiments, continuously collecting scattering data and observing jarosite formation in real time"

In a collaboration between the Australian Synchrotron, the Bragg Institute (ANSTO) and the CSIRO group that grew out of Arthur Wadsley's original X-ray lab, we carried-out *in situ* X-ray diffraction experiments, continuously collecting scattering data and observing jarosite formation in real time (see Figure 2). Without the signal-to-noise capabilities of the Mythen II detector it would not be possible to observe the initial stages of jarosite formation, pushing to the limit the amount of crystalline material which can be detected. In addition, thanks to the high resolution available, a new structural type of jarosite was discovered [11], with significant implications for the study of frustrated antiferromagnetic materials. Kinetic analysis of the *in situ* diffraction data showed that jarosite forms in a single nucleation event. This is a key finding for industrial jarosite applications: if this step can be promoted or suppressed, then jarosite formation can be controlled [12].

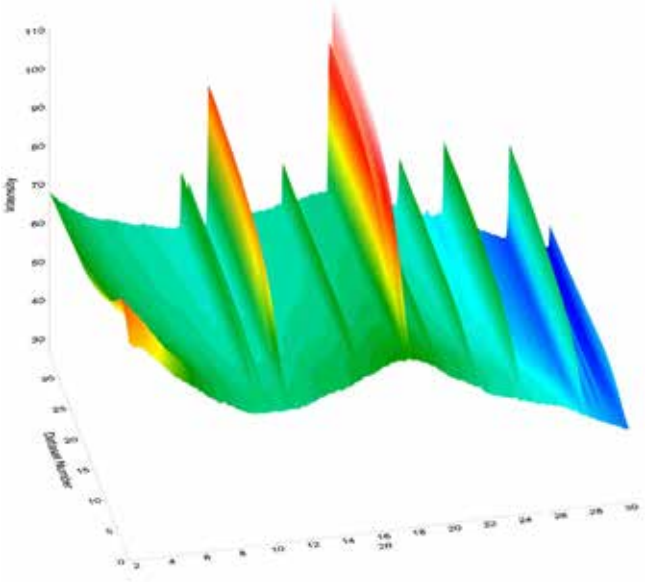

Figure 2: 3D diffraction pattern showing the formation of jarosite from solution versus time.

(ii) Lithium- and sodium-ion batteries

Lithium- and sodium-ion batteries are used worldwide to power portable electronic devices. The technology has many benefits and considerable research is underway to further improve performance, with many researchers focusing on optimising the electrodes. *In situ* X-ray powder diffraction provides an opportunity to examine the reactions at the active electrodes and gain a greater understanding of the mechanisms involved during the charge and discharge cycles. Researchers at the PD beamline typically use a modified coin cell [13-15]. Holes through the centre of the cell casing, sealed from the atmosphere with Kapton film, allow the synchrotron X-rays to scatter from the internal components of the cell during electrochemical discharge (see Figure 3).

Figure 3: An example of a the contents of a battery cell used for *in situ* cycling

(iii) Hydrogen storage materials

Hydrogen is an attractive alternative to petrochemicals as source of clean energy. A key area for further exploitation of hydrogen fuel cell technology is the need for safe and highly-efficient hydrogen storage materials. A great deal of research into compounds with high hydrogen content and excellent performance is carried out at the beamline. Researchers are interested in the amount of hydrogen which can be stored in a material as well as the stability of the compounds created and the ability of the materials to release hydrogen as desired. Using X-ray powder diffraction at the Australian Synchrotron (see Figure 4), researchers investigate the structure of the new compounds formed on hydrogen uptake [16] and have demonstrated high gravimetric hydrogen densities and favourable dehydrogenation targets in a number of metal hydride systems [17,18].

Macromolecular Single Crystal Diffraction at the Australian Synchrotron

Macromolecular crystallography has a wide range of applications to chemical, technological, geological, biological, medical and pharmaceutical sciences. The Australian Synchrotron currently hosts two Macromolecular Crystallography (MX) beamlines: the high-throughput MX1 beamline and the micro-focus MX2 beamline.

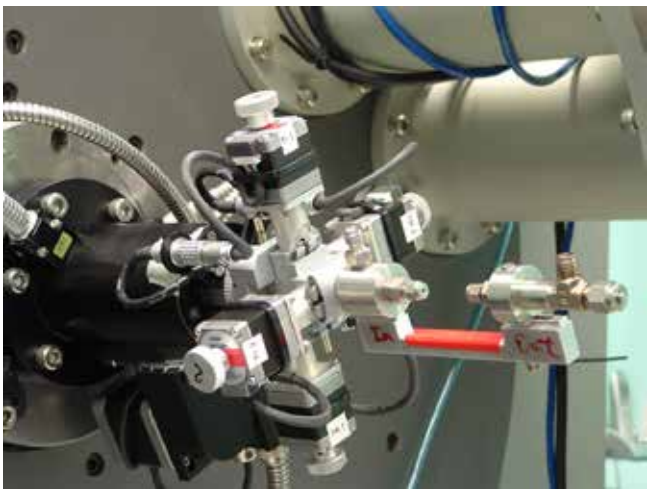

Figure 4: Gas flow through cell at the Powder Diffraction beamline for determination of the structures of hydrogen storage materials.

The bending-magnet MX1 beamline delivers hard X-rays in the energy range from 6 to 18 keV, and is used for standard macromolecular crystallography and most chemical crystallography measurements. The beamline is equipped with a *Stanford Automated Mounting system* (SAM)-type robot [19], and a Quantum 210r CCD (charge coupled device) detector *(Area Detector Systems Corporation)* mounted to allow variable sample to detector distances between 76 and 800 mm. A motor actuated CryoJet 5 *(Oxford Instruments)* maintains a sample temperature of 100 K during measurement to prevent radiation damage. A sensitive silicon-drift fluorescence detector (Vortex 90EX, *Hitachi*) is installed so as to actuate to a position a few millimetres from the sample to enable excitation scans of metal absorption edges during Multiple wavelength Anomalous Diffraction (MAD) experiments.

"Macromolecular crystallography has a wide range of applications to chemical, technological, geological, biological, medical and pharmaceutical sciences"

The micro-focus MX2 beamline is the prime macromolecular crystallography beamline at the Australian Synchrotron. Powered by a small-gap in-vacuum undulator, it is designed for challenging projects such as small crystals, weakly diffracting crystals and crystals with large cell dimensions. Wavelength selection at the beamline is achieved using a cryo-cooled double-crystal monochromator (DCM) which is currently equipped with a Si-111 crystal set. The DCM is designed to select

energies in the range 6 keV to 20 keV, while maintaining a fixed exit beam geometry. The sample positioning and detection systems are essentially the same as the MX1 beamline. Further equipment for crystal alignment with respect to the X-ray beam is achieved with a high-resolution sample video microscope and its video stream is embedded in the *Blu-Ice* control system [20].

Both MX beamlines feature automated indexing and data processing, with a suite of programs being triggered by the collection of a diffraction image. Statistical descriptors of the data are harvested from the processed data and displayed by a web client at the beamlines in close to real-time, allowing data collection to be assessed on-the-fly. The system is useful in helping strategic experimental decisions to be made by users of the beamline. An automated structure determination software pipeline system (called Auto-Rickshaw) [21,22] has been installed on MASSIVE (a high-performance computing cluster) [23]. The system is triggered from the beamline computers when the auto-processed X-ray data indicates an anomalous signal. Apart from the automatic system, Auto-Rickshaw can be triggered for structure solutions using various phasing methods over a web-based user interface by selecting appropriate parameters and the processed datasets.

The macromolecular crystallography beamlines are supported by a PC2 certified biochemistry laboratory with fume hoods, pH meters, centrifuges, balances and other common laboratory equipment. A range of heavy atom and halide salts is available for derivatisation of protein crystals. A pressure chamber (Hampton Research) is located in the sample preparation laboratory and can be used to produce Xenon derivatives of macromolecular crystals [24,25] for mapping solvent channels or location of molecular oxygen within protein crystals, or for experimental phasing [26,27]. A UV laser has been installed on MX1 beamline for radiation-damage-induced phasing of disulphide containing proteins [28] or selenomet protein crystals [29], and for generating additional phase information [30].

MX1 and MX2 began hosting experiments in 2007 and 2008 respectively and have run a fully subscribed user-program to the present day. In 2013 the mode of access to the macromolecular crystallography beamlines changed from three proposal rounds per year, to an annual *Collaborative Access Program* (CAP). Under the CAP system, users from different universities and research groups send crystals, students and staff on each experimental visit to collect over an intensive 24 hour period. Depositions of protein structures determined using Australian Synchrotron data in the worldwide Protein Databank (PDB) have been steadily increasing year-on-year and recently exceeded 750; while peer-reviewed publications from the two beamlines currently exceed 600 (Figure 5).

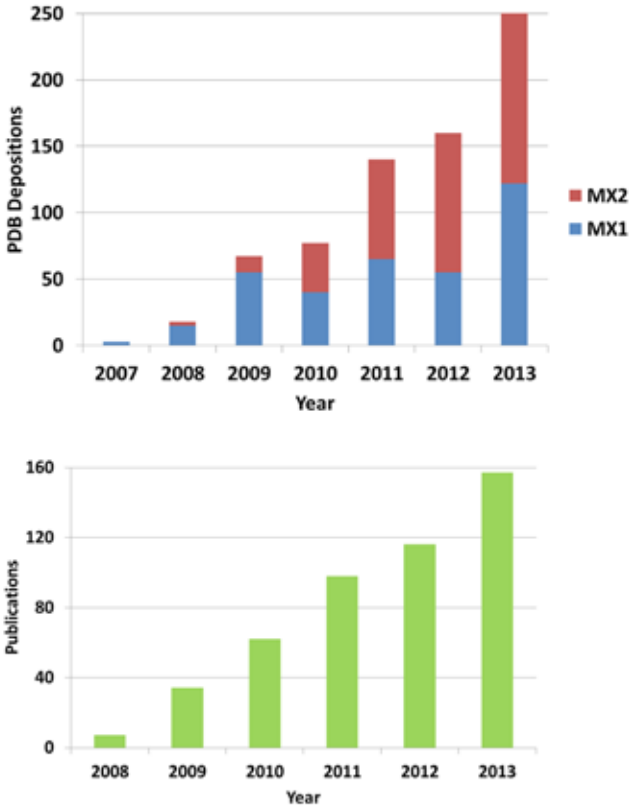

Figure 5: Protein structures determined using Australian Synchrotron MX beamlines and deposited in the PDB and peer-reviewed publications.

More broadly, the impact of the Australian Synchrotron on the field of protein crystallography can be seen by comparing all structures deposited in the World Wide Protein Data Bank by researchers from Australia and New Zealand - that comparison shows that in 2013, more than 60% of all structures from the region are derived from the Australian Synchrotron.

Macromolecular Crystallography Case Studies

The Australian structural biology community regularly produces internationally-significant research outcomes using data from the MX1 and MX2 beamlines. Recent highlights include insights into the regulation of blood clotting [31], diabetes [2], understanding the body's immune response [3,32] and the immune defence mechanisms of plants [33], as well as discoveries that could

lead to more-effective treatments for some cancers [34], leukaemia [35] and neurodegenerative diseases [36]. In addition, the chemical crystallography community generates a range of outcomes in relation to new catalysts [37], organic light-emitting materials [38], and metal organic frameworks [39,40].

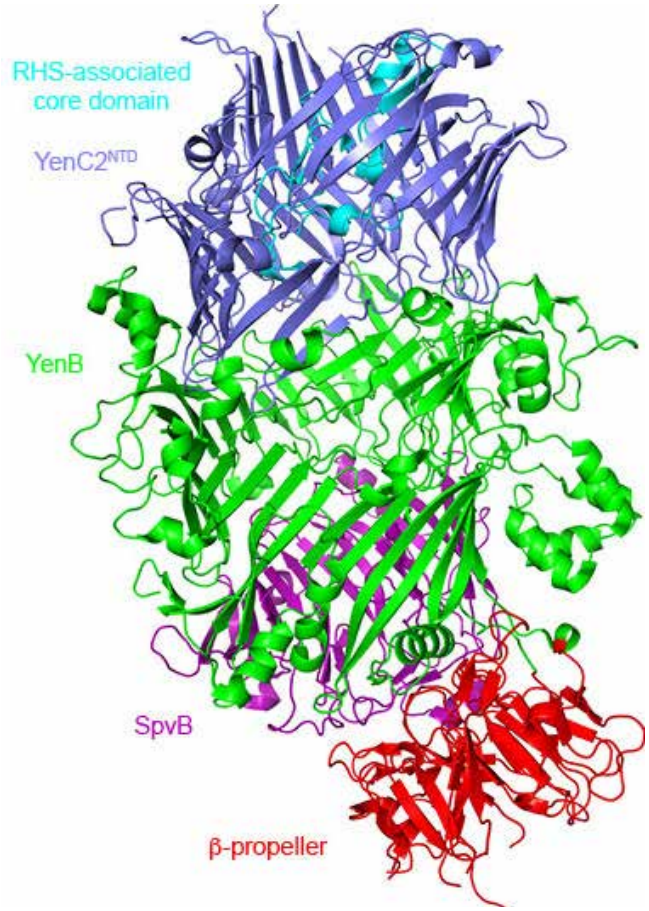

Figure 6: Crystal structure of the YenB/YenC2NTR complex (Busby et al., Nature 2013). The β-propeller domain of YenB is shown in red, the conserved SpvB sequence in purple, and the rest of YenB in green. YenC2NTR is coloured blue and the conserved RHS-associated core domain is coloured cyan

(i) Structures of Protein Complexes

The ABC toxin complexes, composed of three core subunits (A, B and C), are best characterised from insect pathogens such as *Yersinia entomophaga* (the related *Yersinia pestis* is associated with the cause of the black plague). The toxins produced by such bacteria are of interest owing to their potent insecticidal activity and potential role in human disease. The three-dimensional structure of the complex formed between the B and C proteins determined to 2.5 Å (Figure 6) was published in the journal Nature, and helped to elucidate the role of the B protein in the mechanism of toxicity [41], and helped to elucidate the role of the B protein in the mechanism of toxicity. The high-resolution native dataset was collected at the MX2 beamline while X-ray data for phasing were collected at the MX1 beamline. The experimental phasing was performed with the use Auto-Rickshaw and via combination of four selenium single-wavelength anomalous diffraction (SAD) datasets and a tantalum bromide derivative.

(ii) Towards a vaccine for Celiac Disease

Crystal structures solved using Australian Synchrotron X-rays have revealed the molecular face of celiac disease, paving the way for potential treatments and diagnostics. Research published in *Nature Structural and Molecular Biology* described the interaction between T-cells of the immune system and the peptide (gliadin) that is present in gluten, and was found to be a trigger for celiac disease [42]. The study examined how different T-cells bound to gliadin, with the aim of developing a therapeutic that could turn off the immune response. This study was carried out by an international team of researchers from the ARC Centre of Advanced Molecular Imaging based at Monash University, Leiden University (The Netherlands), and the US biotech company (*ImmusanT*) that is involved in developing a peptide-based vaccine for celiac disease (Nexvax2®). The study showed that the majority (~95%) of coeliac sufferers carry one of two genes for a protein linked to susceptibility for the disease (HLA–DG2). In 2012, the research team found a similar trigger for the other 5% who have the other susceptibility gene (HLA–DQ8) [43].

"...the Australian Synchrotron is a participant in the new Australian Research Council Centre of Excellence for Advanced Molecular Imaging..."

Conclusion and the Future

In a nice bookend to the role that physics has played in crystallography over more than 100 years it is fascinating to note that Australians again have a lead role in the next stage in understanding the structure and function of proteins. The use of X-ray Free Electron Lasers to determine structure from nano-crystals and, perhaps, even single molecules is an exciting development. It is also one where Australian physicists, such as Henry Chap-

man [44-49], John Spence [45-49] and (former Australian Synchrotron director) Keith Nugent [50,51] have made key discoveries. The Australian Synchrotron is also playing a role in developing new methodologies that will link existing synchrotron-based approaches with XFEL capability. In this endeavour the Australian Synchrotron is a participant in the new *Australian Research Council Centre of Excellence for Advanced Molecular Imaging* [52], which integrates physics, chemistry and biology (which is one of the great strengths of synchrotron facilities) to unravel the complex molecular interactions that define immunity.

Crystallography in Australia has been underpinned by a rich history of innovators in the field striving to use and develop cutting edge scientific tools to answer real-world questions. The infrastructure developed, and upgrades planned, at the Australian Synchrotron will allow future pioneers to continue to be at the forefront of scientific discovery.

References

1. http://www.iucr.org/news/newsletter/volume-14/number-1/crystallography-in-australia-and-new-zealand
2. J.G. Menting, J. Whittaker, M.B. Margetts, L.J. Whittaker, G.K.-W. Kong, et al., Nature **493**, 241 (2013).
3. R. Berry, N. Ng, P. M. Saunders, J. P. Vivian, J. Lin, et al., Nature Immunology, **14** 699 (2013).
4. K. S. Wallwork, B. J. Kennedy & D. Wang, AIP Conference Proceedings **879**, 879 (2007).
5. B. Schmitt, Ch. Bronnimann, E.F. Eikenberry, F. Gozzo, C. Hormann, R. Horisberger and B. Patterson, Nuclear Instruments and Methods in Physics Research A, **501**, 267 (2003).
6. J. E. Dutrizac, and J.L. Jambor, Reviews in Mineralogy and Geochemistry, Mineralogical Society of America, **40**, 405 (2000).
7. E. J. P. Jones, T.-L. Nadeau, M. A. Voytek, and E. R. Landa, J. Geophys. Res. **111**, G01012 (2006).
8. L. C. Basciano, and R. C. Peterson, American Mineralogist **92**, 1464 (2007).
9. G. Klingelhöfer, R. V. Morris, B. Bernhardt, C. Shröder, D. S. Rodinov, P.A. de Souza, A. Yen, R. Gellert, E. N. Evlanov, B. Zubkov, et al., Science, **306**, 1740 (2004).
10. J. J. Papike, J. M. Karner, and C. K. Shearer, Geochimica et Cosmochimica Acta **70**, 1309 (2006).
11. N. V. Y. Scarlett, I. E. Grey, and H. E. A. Brand, American Mineralogist **95**, 1590 (2010).
12. H.E.A. Brand, N.V.Y. Scarlett, I.E. Grey, N. Kirby and R. Knott, J. Synchrotron Radiation **20**, 626 (2013).
13. W.R. Brant, S. Schmid, G. Du, Q. Gu and N. Sharma, J. Power Sources **244**, 109 (2013).
14. W. M. Dose, N. Sharma and S. W. Donne, J. Power Sources **258**, 155 (2014).
15. W. K. Pang, V. K. Peterson, N. Sharma, C. Zhang and Z. Guo, J. Phys. Chem. C **118**, 3976 (2014).
16. K. Nogita, S. D. McDonald, A. Duguid, M. Tsubota and Q. F. Gu, J. Alloys and Compounds, **580**, S140 (2013).
17. Q. Gu, L. Gao, Y. Guo, Y. Tan, Z. Tang, K. S. Wallwork, F. Zhang and X. Yu, Energy & Environmental Science **5**, 7590 (2012).
18. Z. Tang, Y. Tan, H. Wu, Q. Gu, W. Zhou, C. M. Jensen, X. Yu, Acta Materialia **61**, 4787 (2013).
19. A. E. Cohen, P. J. Ellis, M. D. Miller, A. M. Deacon and R. P. Phizackerley, J. Applied Crystallogr. **35**, 720 (2002).
20. T. M. McPhillips, S. E. McPhillips, H. J. Chiu, A. E. Cohen, A. M. Deacon, P. J. Ellis, et al., J. Synchrotron Radiation **9**, 410 (2002).
21. S. Panjikar, V. Parthasarathy, V. S. Lamzin, M. S. Weiss and P. A. Tucker, Acta Crystallogr. D **61**, 449 (2005).
22. S. Panjikar, V. Parthasarathy, V. S. Lamzin, M. S. Weiss and P. A. Tucker, Acta Crystallogr. D **65**,1089 (2009).
23. W. J. Goscinski, P. McIntosh, U. C. Felzmann, A. Maksimenko, C. J. Hall, et al., Frontiers in Neuroinformatics **8**, March 27 (2014).
24. M. S. Soltis, M. H. B. Stowell, M. Wiener, G. Phillips, D. Rees, J. Appl. Crystallogr. **30**, 190 (1997).
25. S. Panjikar and P. Tucker, J. Appl. Crystallogr. **35**, 261 (2002).
26. T. S. Peat, S. Balotra, M. Wilding, N. G. French, L. J. Briggs, S. Panjikar, N. Cowieson, J. Newman and C. Scott, Mol. Microbiol. **88**, 1149 (2013).
27. V. Richter, C. S. Palmer, L. D. Osellame, A. P. Singh, K. Elgass, D. A. Stroud, H. Sesaki, M. Kvansakul and M. T. Ryan, J. Cell Biology **204**, 477 (2014).
28. M. H. Nanao and R. B. Ravelli, Structure **14**, 791 (2006).
29. S. Panjikar, H. Mayerhofer, P. A. Tucker, J. Mueller-Dieckmann, and D. de Sanctis, Acta Crystallogr. D **67**, 32 (2011).
30. D. De Sanctis, P. A. Tucker and S. Panjikar, J. Synchrotron Radiation **18**, 374 (2011).
31. R. H. P. Law, T. Caradoc-Davies, N. Cowieson, A. J. Horvath, A. J. Quek, et al., Cell Reports **1**, 185 (2012).
32. A. J. Corbett, S. B. G. Eckle, R. W. Birkinshaw, L. Liu, O. Patel, et al., Nature, **509**, 361 (2014).
33. S. J. Williams, K. H. Sohn, L. Wan, M. Bernoux, P. F. Sarris, C. Segonzac, T. Ve, Y. Ma, S. B. Saucet, D. J. Ericsson, et al., Science, **344**, 299 (2014).
34. J. Moeker, T. S. Peat, L. F. Bornaghi, D. Vullo, C. T Supuran, S.-A. Poulsen, J. Medicinal Chemistry, **57**, 3522 (2014).
35. S. E. Broughton, T. R. Hercus, M. P. Hardy, B. J. McClure, T. L. Nero, M. Dottore, et al., Cell Reports **8**, 410 (2014).
36. L.A. Miles, G.A.N. Crespi, L. Doughty, M.W. Parker, Scientific Reports, **3**, 1302 (2013).
37. K. Q. Vuong, C. M. Wong, M. Bhadbhade and B. A. Messerle, Dalton Transactions, **43**, 7540 (2014).
38. W. J. Gee and S. R. Batten, Crystal Growth & Design **13**, 2335 (2013).
39. C. S. Hawes, Y. Nolvachai, C. Kulsing, G. P. Knowles, A. L. Chaffee, P. J. Marriott, S. R. Batten and D. R. Turner, Chemical Communications, **50**, 3735 (2014).
40. Y. Wu, V. K. Peterson, E. Luks, T. A. Darwish, C. J. Kepert, Angew. Chem. Int. Edit. **126**, 5275 (2014).
41. J. N. Busby, S. Panjikar, M. J. Landsberg, M. R. H. Hurst, J. S. Lott, Nature **501**, 547 (2013).
42. J. Petersen, V. Montserrat, J. R. Mujico, K. L. Loh, D. X. Beringer, et al., Nature Structural & Molecular Biology **21**, 480 (2014).
43. S.E. Broughton, J. Petersen, A. Theodossis, S.W. Scally, K.L.

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Dr Helen Brand has been a beamline scientist on the Powder Diffraction beamline at the Australian Synchrotron since December 2011, following a postdoctoral fellowship jointly funded by CSIRO Process Engineering and ANSTO. She is a Planetary Geologist by training and was awarded a PhD from University College London for investigations of highly-hydrated sulphate minerals with relevance to geological processes within the Galilean satellites of Jupiter. Her research interests focus on determining the thermoelastic properties and the crystal chemistry of a range of minerals which are of interest in a variety of environmental, planetary geology and industrial settings.

Dr Santosh Panjikar earned his PhD in Protein Crystallography from Friedrich-Schiller University (Jena, Germany) in 2001. He held a postdoctoral, Senior Technical Officer and Staff Scientist appointments at the EMBL Hamburg Outstation, Germany with Dr Paul A. Tucker between 2001 and 2011. Currently he is working as a Beamline Scientist at the Australian Synchrotron. He is an Adjunct Research Fellow at the Department of Biological Science and Biochemistry, Monash University, Australia and a member of the IUCr commission on crystallographic computing. His research interests focus on structural biology, method developments in structural biology, synchrotron instrumentation and software development in macromolecular crystallography.

Loh, A. Thompson, et al., Immunity **37**, 611 (2012).

44. H. N. Chapman, A. Barty, M. J. Bogan, S. Boutet, et al., Nature Physics, **2**, 839 (2006).
45. H. N. Chapman, P. Fromme, A. Barty, T. A. White, R. A. Kirian, et al., Nature, **470**, 73 (2011).
46. M. M. Seibert, T. Ekeberg, F. R. N. C. Maia, M. Svenda, et al., Nature, **470**, 78 (2011).
47. S. Boutet, L. Lomb, G. J. Williams, T. R. M. Barends, A. Aquila, et al., Science, **337**, 362 (2012).
48. L. Redecke, K. Nass, D. P. DePonte, T. A. White, D. Rehders, A. Barty, et al., Science, **339**, 227 (2013).
49. J C H Spence, U Weierstall and H N Chapman, Rep. Prog. Phys., **75**, 102601 (2012).
50. H. M. Quiney, A. G. Peele, Z. Cai, D. Paterson and K. A. Nugent, Nature Physics, **2**, 101 (2006).
51. B. Abbey, K. A. Nugent, G. J. Williams, J. N. Clark, A. G. Peele, M. A. Pfeifer, M. de Jonge & I. McNulty, Nature Physics, **4**, 394 (2008).
52. http://www.imagingcoe.org/

Conferences 2013-14

20-24 October 2014
MEDSI 2014 - Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation Monday, Melbourne.
www.medsi2014.org

26-29 October 2014
Australasian Radiation Protection Society Conference , Hobart
www.arpsconference.com.au

26–31 October 2014
XRM2014 — 12th International Conference on X-ray Microscopy Melbourne, Vic
www.xrm2014.com

3-6 November 2014
The Periphery of Disks Monday, Sydney
www.atnf.csiro.au/research/conferences/2014/ThePeripheryOfDisks/

2-5 December 2014
OSA Optics and Photonics Congress on Light, Energy and the Environment (LEE) ANU, Canberra
www.osa.org/energyOPC

7-11 December 2014
21st Australian Institute of Physics Congress. ANU, Canberra, ACT
www.aip2014.org.au

3-6 February 2015
Annual Condensed Matter and Materials Meeting ("Wagga 2015")
Wagga Wagga campus of the Charles Sturt University, NSW
pems.unsw.adfa.edu.au/cmm/2015/

8-12 February 2015
AMN7 Advanced materials & Nanotechnology. Nelson, New Zealand
www.amn-7.com

18-23 July 2015
2nd Asia-Oceania Conference on Neutron Scattering Saturday, Manly, NSW
www.aocns-2015.com/

5-9 October 2014
7th Vacuum and Surface Sciences Conference of Asia and Australia (VASSCAA-7) Hsinchu, Taiwan
vasscaa-7.tcfst.org.tw/index_4.html

19 November 2014
User Symposium: Synchrotron, Accelerator and Neutron techniques 2014
Australian Synchrotron, Clayton, Vic
www.synchrotron.org.au/news/events/australian-events/

20-21 November 2014
Australian Synchrotron User Meeting 2014
Australian Synchrotron, Clayton, Vic
www.synchrotron.org.au/news/events/australian-events/event/

9-12 February 2015
The Most Massive Galaxies and their Precursors
Sydney, NSW
www.aao.gov.au/conference/massive-galaxies-2015

20 February 2015
Physics Teachers Conference
Monash University, Clayton, Vic.
www.sciencevictoria.com.au/confVCE.html