



## CXS Annual Workshop 2007

Organising Committee Meeting  
Wednesday 16th May, 2007

### POST\_MORTEM

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#### 1. Budget

See budget on pages 3 to 4.

- 145 participants/registrants
- Extra-money could be used as seed funding for the 2008 workshop.

#### 2. Report

See report on pages 5 to 9.

Janos Hajdu suggested a couple of speakers on X-ray laser topics. Farenc Krause (MPQ, Munich), Henry Chapman, (LLNL, DESY), Roger Falcone (ALS, slicing sources); Richard W. Lee (UCB, LLNL), Anton Barty (LLNL))

Consider (x-ray) lasers as a theme?

#### 3. 2008 meeting

- We will need to discuss at the next Executive Committee meeting who will be in the 2008 Organising Committee.

It is important to have both physicists and biologists in the Organising Committee to enhance the multidisciplinary aspect of the annual workshop in line with the Centre's aims. (Mike, Leann and Andrew noted that their involvement would only be possible if additional Professional help were obtained).

- Also, to be discussed: when to hold the 2008 Annual Workshop.

## **The Centre of Excellence for Coherent X-ray Science (CXS) Annual Workshop 2007: *Facilitating X-ray Biophotonics - Physicists and Biologists Working Together.***

Report by Mike Ryan, Andrew Peele and Leann Tilley

The ARC Centre of Excellence in Coherent X-ray Science (CXS) Annual Workshop 2007 was held at the Bio21 Institute, in Melbourne, Australia, 11<sup>th</sup>-14<sup>th</sup> April 2007. The workshop aimed to bring physicists and biologists together at a very exciting time for X-ray (and other novel) imaging techniques. The workshop participants included most of the members of the CXS as well as other members of the physics, biology and chemistry communities. There were a total of 140 registrants including 12 international speakers from the US, Japan, China and Europe as well as prominent local speakers from the CXS and other premier institutions in Australia. It was a fantastic opportunity to meet within and across disciplines and countries.

Professor Keith Nugent opened the meeting explaining the goals of the workshop. He gave an overview of the activities within CXS, in particular some of the successes for 2006. Some of the recent CXS results in coherent diffractive imaging were previewed including the exciting notion that reconstructions of large samples may be possible using a focussed X-ray beam to zoom in on regions of interest.

### ***Coherent Diffraction Imaging***

Dr Ivan Vartaniants is a scientist at the HASYLAB at DESY in Hamburg. He has made extensive study of the methods of coherent diffractive imaging (CDI). His previous research includes examination of partial coherence in CDI and he participated in the first experiments using CDI concepts in Bragg geometry from a crystalline sample. In his talk he reviewed these methods and gave us an insight into the potential for CDI to probe nanosystems. The vexed question of radiation damage was also addressed and simulations showed a way to quantify the problem.

Dr Harry Quiney leads the Theory and Modelling Program in CXS. His work has demonstrated the benefits of using a focused beam to illuminate samples in an approach followed in CXS known as Fresnel Coherent Diffractive Imaging (FCDI). Harry examined CDI from the theoretical viewpoint demonstrating how the iterative schemes used to reconstruct samples can be seen as a problem in optimisation theory. This characterises nicely the particular advantages and disadvantages of the different iterative schemes currently in use. Harry explained the theoretical and computational advantages in using FCDI and then went on to explore the possibility of direct analytical solutions to the problem. This creates the intriguing possibility that a close to complete inversion of the diffraction pattern may be obtained in a single step and then refined using the iterative schemes.

Dr Qun Shen is the leader of the X-Ray Science Division at the Advanced Photon Source, Chicago, USA. His work has examined the possibility of using iterative methods to phase Fresnel diffraction images. Qun demonstrated recent results that provide a way to remove parasitic scatter in X-ray experiments. This work will be of great benefit as CDI data is particularly susceptible to corruption from scatter. Qun also gave a review of the current scientific interests at the APS, in particular as they relate to CDI. The possible future upgrade to the APS was described along with its possibilities for CDI.

Mr Jesse Clark is a PhD student in the Experimental Physics Group in CXS at La Trobe University. Jesse presented recent FCDI results showing that quantitative recovery of information about the thickness of a sample is possible.

Dr Garth Williams is a post-doctoral fellow in the Experimental Physics Group at the University of Melbourne in CXS. Garth explained the methods of image formation in x-rays and delivered a clear exposition of the interpretation of the complex exit surface wave for both simulated and experimental data. He showed the phase and intensity profiles of series of malaria parasite-infected red blood cells that have been successfully reconstructed revealing the major features of the cells. The CDI images were compared with X-ray fluorescence micrographs of the distribution of different metals in the cells.

Professor Peter Coleman is head of the Structural Biology Research Division at the Walter and Eliza Hall Institute of Medical Research. During his career Peter has crossed the boundaries between Physics and Biology and his group has solved the crystal structures of a number of very important biological molecules. In his talk Peter reviewed the rich crystallographic history of attempts to derive phase information for the X-ray diffraction of crystals. In an entertaining and informative discussion he described the origins of the concepts used today in coherent diffractive imaging and demonstrated to the audience the wealth of interactions that have led to the development of this promising field.

### ***Advances in X-ray Sources and Detectors***

Prof. Tetsuya Ishikawa is Chief Scientist of the Coherent X-ray Optics Lab at RIKEN Harima Institute and is the project leader for the Japanese XFEL project. In an exciting talk he reviewed the progress of the Japanese XFEL project and reviewed crucial developments in X-ray optics required to take advantage of these new sources.

Dr Ian McNulty is a senior scientist at the Advanced Photon Source, USA. Ian reviewed the challenge that optical singularities, or vortices, present for CDI. He showed the progress made recently in the controlled production of vortical light in X-ray beams and speculated on future prospects in this area.

Dr Chris Hall is a senior research fellow with Detector Group at Monash University in CXS. In a comprehensive presentation Chris reviewed detector developments at the Monash group and explained the potential for development of a photon counting detector for CDI. Chris then expertly backed up and stood in for Ralph Menk who was unable to attend and reviewed progress in single photon counting and integrating devices.

Dr Sven Teichmann is a PhD student in the Laser Group at Swinburne University of Technology in CXS. Sven presented progress in production of coherent X-ray flux using High-order Harmonic Generation (HHG). Alternative approaches, such as the use of a capillary guide, were also outlined.

Dr John Tisch is a Reader in the Physics Department and an experimental physicist working in the QOLS Group within the Blackett Laboratory Laser Consortium (BLLC). John presented exciting work in the use of HHG light sources for ultrafast imaging, demonstrating molecular structure and dynamics.

### ***Advances in X-ray Imaging Techniques***

Dr Andrzej Krol is at the Department of Radiology, SUNY Upstate Medical University. In a comprehensive address, Andrzej reviewed phase contrast micro-CT using a laser-based source. Imaging capabilities of the method were reviewed and expansion for clinical use was outlined.

Dr Burkhard Kaulich is with Dr Maya Kiskinova responsible for the TwinMic project at ELETTRA in Trieste. This combines scanning and full field microscopy into a single instrument. Burkhard outlined the current status of the instrument and gave an excellent presentation on the research applications possible.

Professor Ziyu Wu is the Research Director at the Beijing Synchrotron Radiation Facility. Ziyu reviewed the great strides forward taken in diffraction enhanced imaging at BSRF. Advances in the analysis of DEI images were also shown and developments into hard X-ray nanotomography were discussed.

Dr Connie Darmanin and Dr Steve Homolya are CXS-associated Research Fellows at CSIRO, Molecular Health and Technology and Manufacturing and Materials Technology respectively. In an entertaining two-hander they outlined the challenges and possibilities for 2-D crystal formation and structure determination.

Professor Janos Hajdu is at the Laboratory of Molecular Biophysics, Institute of Cell and Molecular Biology, Uppsala University and the Stanford Synchrotron Radiation Laboratory. Janos is at the forefront of biological applications using Free Electron Laser (FEL) sources. Janos gave an entertaining and fascinating account of recent *tour de force* experimental work at the FLASH facility at DESY. This was the first demonstration of CDI using an FEL. Results on the imaging of live phytoplankton were also presented.

### ***Alternative Technologies for Cellular Imaging: the Biologists View***

Coherent diffraction imaging needs to compete against a number of very powerful imaging technologies that have been under development for many years as well as some exciting new techniques that are emerging. To examine some of these competing technologies we invited talks from several experts in state-of-the-art imaging methods. Their preferred techniques ranged from transmission X-ray imaging, through light microscopy and fluorescence imaging to electron tomographic imaging.

Professor Carolyn Larabell is the principal investigator, at the National Center for X-ray Tomography (NCXT) at the U.S. Department of Energy's Lawrence Berkeley Laboratory. She has worked with colleagues to commission an X-ray tomographic microscope at the Advanced Light Source (ALS). The microscope is the first soft X-ray transmission microscope to be designed specifically for biological applications. It is capable of imaging whole, hydrated cells at a resolution of about 35 nanometers. This is made possible by a combination of the high brightness of the X-rays produced from an ALS bend magnet beamline and nanofabricated zone plate optics. Caroline showed us some fantastic 3D reconstructions of yeast cells and lipid vesicles that relied on the natural contrast in biological samples in the water window as well as exploring methods for specific labelling of particular cellular components.

Dr Sherry Mayo, a CXS-associated Senior Scientist at CSIRO Manufacturing and Materials Technology, has been a significant contributor to the development of the X-ray ultramicroscope, a scanning electron microscope-hosted projection X-ray microscope. This instrument allows phase-contrast imaging of microscopic samples at resolutions down to 60 nm. She demonstrated the potential of the microscope for a wide variety of applications in both X-ray phase-contrast microscopy and micro-tomography of biological and material science samples.

Dr Nick Klonis, La Trobe University, uses confocal fluorescence microscopy to study cell architecture. He described techniques such as fluorescence photobleaching, fluorescence correlation, spectral imaging and 3D reconstructions that allow quantitative imaging of cellular processes. He explained the advantages of using green fluorescent protein as an endogenously encoded specific label of different cellular compartments for live cell imaging. These studies provide evidence for novel sub-compartments and highly unusual trafficking pathways in malaria parasite-infected erythrocytes. He noted the limitations in resolution associated with light microscope-based techniques (~200 nm) but pointed out new developments in fluorescence microscopy (eg patterned illumination) that allow practitioners to break the diffraction limit of light.

Dr Eric Hanssen, CXS Postdoctoral Fellow, La Trobe University, and Dr Brad Marsh, Institute of Molecular Bioscience, Queensland, gave us some insights into the wonderful world of tomographic imaging using the electron microscope. Thanks to advances in electron beam energies, sample preparation and acquisition hardware and software it is now possible to collect high-resolution data on tilted samples and reconstruct it into a 3D tomogram at ~4-5 nm resolution in a few hours. Eric and Ben have used these techniques to image malaria parasite-infected erythrocytes and insulin-secreting pancreatic beta cells. Their reconstructions are mesmerising.

### ***Current approaches to solving structures of membrane proteins***

Membrane proteins are difficult to isolate and to retain in their native forms. A number of speakers focused on these problems and what can be done to alleviate them. Two sessions on protein structure techniques and their relevance to membrane proteins were conducted.

Ben Hankamer, Institute of Molecular Bioscience, Brisbane, discussed his research into the study of algal proteins involved in methanol production. He presented work on determining protein structure using cryoelectron microscopy using molecules such as photosystem II of thylakoid membranes and the model protein ferritin. He also pointed out future technologies to reconstitute proteins into membrane arrays by using fluorinated lipid monolayers.

Jacqueline Gulbis, a CXS Principle Investigator, at the Walter & Eliza Hall Institute, Melbourne, elegantly covered the scope of membrane proteins and the intrinsic difficulties associated with using them in crystallographic approaches to determine protein structure. She used the structure of the potassium channel as an example of what can be done. (She solved this structure in the lab of Rod MacKinnon, which helped him to earn a Nobel Prize).

Michael Parker, St Vincent's Hospital, Parkville, spoke about his efforts to crystallise different proteins and focussed on the pore-forming streptolysins which exist in both soluble and membrane forms. The structure of the soluble complex has been used to model how the pore might form.

Bonnie Wallace, a CXS International Advisory Board member, from Birkbeck College, University of London, UK, showed us the wonders of synchrotron radiation circular dichroism (SRCD) techniques to determine the secondary structures of soluble and membrane proteins alike. The potential of this technique puts it on structural biologists' wish-list for a future experimental end-station at the Australian Synchrotron.

Interactions continued in very lively discussions and hypotheticals during breaks and over the poster sessions. There was a palpable buzz of excitement about the possibilities in the field. The conference dinner was held in convivial if somewhat unusual surroundings at the Melbourne Zoo. A series of toasts in approximately 20 different languages ensured that everyone left with their thirst well quenched.

The Organizing Committee for the workshop (Andrew Peele, Mike Ryan, Steve Wilkins, Emma Douglas, Tania Smith and Leann Tilley) thank all of the participants for contributing to such an excellent program. We hope you enjoyed the event and found it to be a worthwhile experience and are now getting back to work with renewed enthusiasm and vigour knowing that there are great things happening in the Centre.

The feedback we have received so far suggests that everyone, from students to PIs, agreed that it was a terrific workshop. This was due to the extremely high standard of presentations and the friendly, interactive spirit of all involved. We thank everyone who made oral and poster presentations, initiated discussions in the sessions and continued those discussions between the sessions.

We value your feedback on how it met your expectations and are interested to hear any suggestions you have for next year's conference. Please let us know if there are speakers, sessions or themes you would like us to pursue.

Many of the attendees have asked if copies of the talks will be available. We have made some of these available on our web site. Photos from the workshop are also available at <http://www.coecxs.org/workshop2007.html>.

Planning is already underway for the next Annual Workshop. So we hope to see you there!