



# 2007 ANNUAL REPORT

ARC Centre of Excellence for Coherent X-ray Science



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ARC Centre of Excellence for  
COHERENT X-RAY SCIENCE

CXS would like to acknowledge the support of the Australian Research Council. We would also like to acknowledge the financial and in-kind support provided by our collaborators – The University of Melbourne, La Trobe University, Monash University, Swinburne University of Technology and the Australian Commonwealth Scientific and Research Organisation (CSIRO). We are grateful for the financial support received from the Science, Technology and Initiative coordinated by the office of Science and Technology in the State Government of Victoria.

CXS would like to thank the School of Physics at the University of Melbourne, Ms Norma Hayes of Monash University, Ms Emmanuelle Duglas of La Trobe University and Ms Tatiana Tchernova of Swinburne University of Technology for their support.

Finally, CXS would like to thank the CRC Biomedical Imaging Development, David Cohen and Ms Janet Carlon for the images contributed to this report.

## **CXS**

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Front cover illustration based on Associate Professor Andrew Peele's technical drawings.

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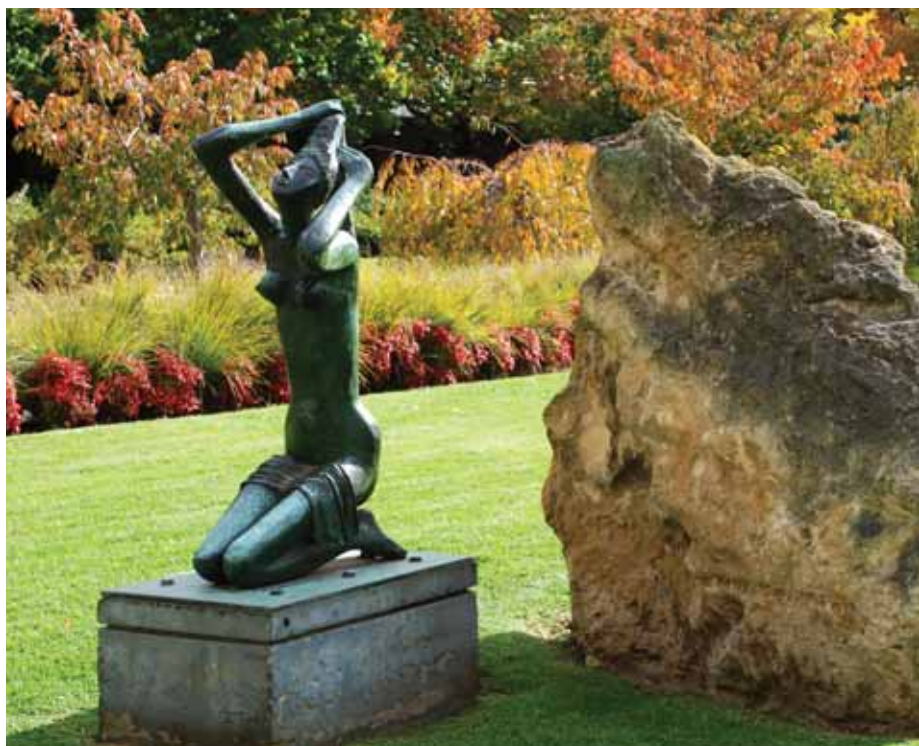
# ABOUT CXS

The Australian Research Council (ARC) Centre of Excellence for Coherent X-ray Science (CXS) brings together leading Australian researchers in the fields of X-ray physics, the design and use of synchrotron radiation sources, and the preparation, manipulation and characterisation of biological samples.

Its aim is to open a new frontier in biotechnology: the non-crystallographic structural determination of membrane proteins. These proteins mediate the activity of pharmaceuticals in human medical therapies. Their structures, however, are still mostly unknown because they do not form crystals suitable for analysis using the conventional crystallographic techniques that have driven almost all the progress in structural biology. A breakthrough in this area would revolutionise rational drug design through the insight gained into the function of membrane proteins. This would have far-reaching consequences for the pharmaceutical industry. CXSs' research is driven by its access to existing third-generation synchrotron light sources and to the Australian Synchrotron. We are also exploring the application to imaging problems of short wavelength high-harmonic generation sources and free-electron X-ray lasers that are under development worldwide.

When combined with non-crystallographic diffractive imaging techniques, the brightness and intensity of these sources gives us the opportunity to take snapshots of biomolecules. We are exploring the fundamental issues in the use of these light sources, including the nature of the interaction between intense coherent X-rays and electronic matter. The efficiency of diffraction processes in these highly coupled light-matter systems and the detection of the scattered light, the preparation and handling of suitable biological samples, the management of radiation damage throughout the interaction, and the design of algorithms to extract structural information from diffraction data is also under exploration.

It is an ambitious interdisciplinary program of research.





*Mr Gavin Jennings MLC and Professor Keith Nugent at the official opening of the Femtosecond High Power Laser Facility Opening at Swinburne University of Technology.*

# DIRECTOR'S REPORT

**The ARC Centre of Excellence for Coherent X-ray Science (CXS)** is a complex multi-institutional organisation dedicated to the exploration of scientific problems that cross traditional disciplinary boundaries. As such, the establishment of CXS requires continuing communication across these boundaries and a staged development of the necessary scientific programs and infrastructure.

The first year of CXS operation, 2006, was considered to be the year of establishment. Organisational structures were developed and put in place, communication between all members was developed and we undertook a program of finding and recruiting the very best people. Spending priorities were established and the process of ordering some major purchases began – specifically the laser and the synchrotron end-station.

The large infrastructure began to arrive in 2007 and we made excellent progress with the commissioning. We let the contracts for the X-ray end-station to the company Xradia, with an expected delivery in 2008, and we have had extensive discussions with them on refining and optimising the design.

We also took delivery of the very high power laser for the development of the high harmonic generation light source program. The facility is now up and running and we have already observed the production of soft X-rays by this process. Preliminary experimental work with this source has also commenced. This laser facility was largely funded by the contribution from the Victorian State Government and so we were delighted to have the Victorian Minister for Innovation, Gavin Jennings, declare it open in September.

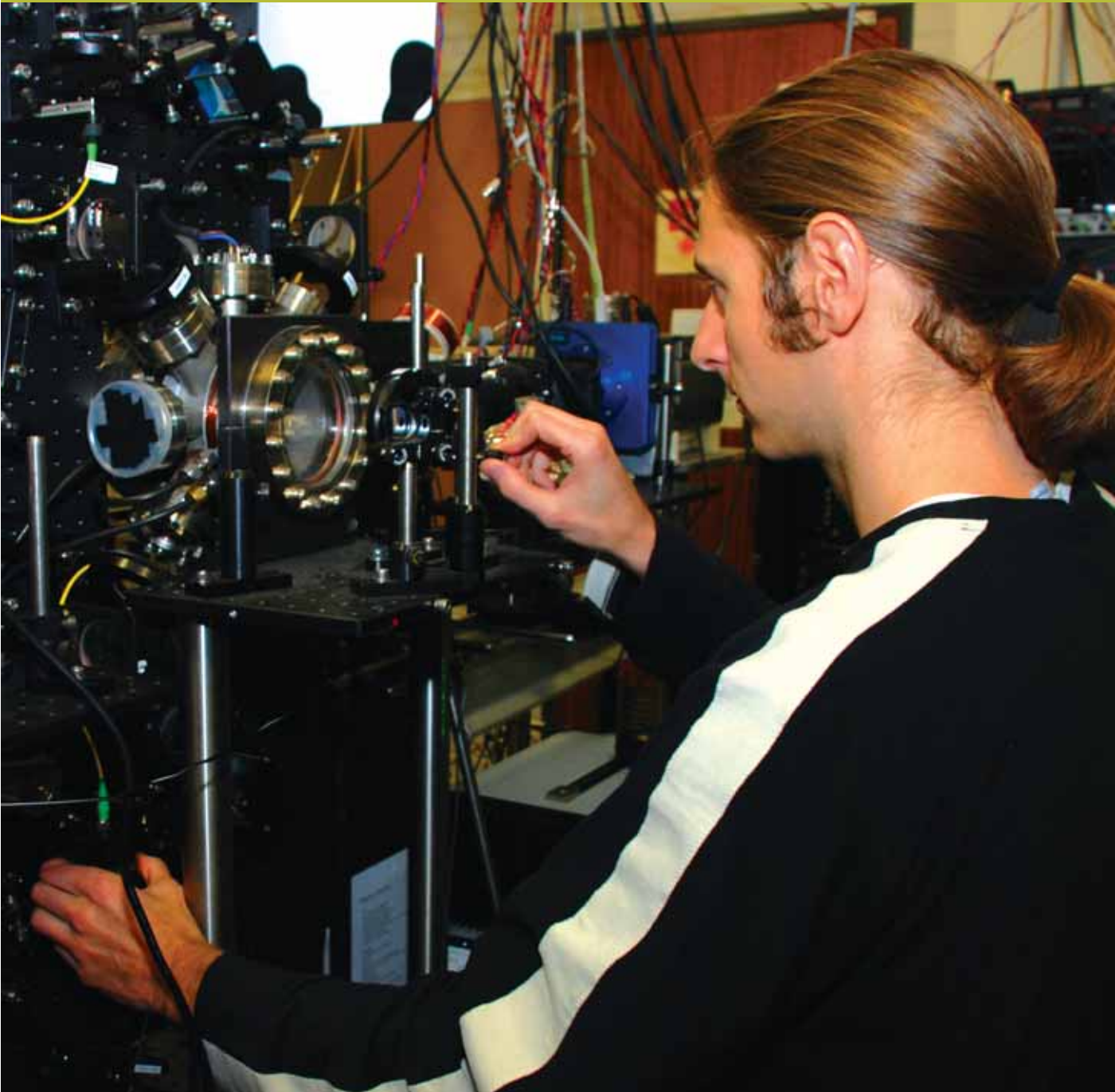
My renewed Federation Fellowship started in 2007 and it brought with it significant further support from the University of Melbourne. The proposal to the ARC incorporated establishment of a program using ultracold plasmas as an electron source to produce coherent X-rays. As a result, I was delighted to welcome Associate Professor Rob Scholten and his students into CXS as the new Ultra-Cold Plasma Source Group.

CXS is determined to embed itself deeply within the Australian scientific community and so we have made significant efforts to establish linkages. This has included a very stimulating workshop with the ARC Centre of Excellence for Matter - Anti Matter Science, and detailed discussions with the CRC for Biomedical Imaging Development that we hope will lead to an exciting collaborative project on the development of X-ray detector technology. We have also signed the Memoranda of Understanding with the Australian Synchrotron and the National Synchrotron Radiation Research Centre in Taiwan.

CXS held a major international workshop with a wide range of participants from across the world. This event turned into a significant international conference and CXS members have received many complimentary comments about the quality of the program and the organisation. CXS continues to develop well and has had considerable national and international exposure. I believe that we are seen as a major force in the rapidly growing field of coherent X-ray science and 2008 is shaping up to be an even busier and more productive year.



**Professor Keith Nugent**  
Director



*To be the world leader in the development of coherent X-ray diffraction for imaging biological structures.*

# THE YEAR IN SUMMARY: RESEARCH

**The establishment of an interdisciplinary project** such as CXS requires careful planning and coordination for the appropriate development of resources and the establishment of strong scientific relationships. Our strategic plan for CXS denoted that 2006 should be the year in which we consolidate the scientific collaborations and complete our planning for the infrastructure that is needed to achieve our long-term scientific goals.

The year 2007 was the year in which the scientific infrastructure was commissioned and delivered, and we began the process of learning how to use it most effectively. And there can be no doubt that 2007 has been a very successful year.

The Short-Wavelength Laser Source Program, led by Professor Lap Van Dao saw the commissioning of the new femtosecond laser system and the first observation of fully coherent X-rays in the Southern Hemisphere. While claiming that anything is the “first in the Southern hemisphere” always seems a bit weak, we were absolutely delighted that the team based at Swinburne University and at the School of Chemistry at the University of Melbourne were able to achieve this goal so rapidly and so successfully. As a result, with the Experimental Methods Program, the Short-Wavelength Laser Source Program has already started to obtain very promising experimental diffraction data. The Theory and Modelling Program has established a very successful interaction with the Laser Program and has begun its program of theoretical work looking at the physics of the generation of high harmonic laser light.

The Experimental Methods Program, led by Associate Professor Andrew Peele, continued its program of experimental work, and its interaction with the Biological Science Program working towards the goal of high-resolution imaging of a malaria-infected red blood cell. This is a challenging problem but one in which we continue to make excellent progress. The Experimental Methods Program, with excellent support from the Detector & Beamline Development Program, has also been very active in the design of our microscope endstation, a facility that will be of value across a wide swathe of Australian science. We have also been active in developing an Australia-wide collaboration in scanning X-ray microscopy that will use this facility over the coming years, and which will ultimately see this facility relocated as a national resource at the Australian Synchrotron.

The Biological Science Program and the CSIRO Program have also been working closely on the structure of natural haemozoin and have obtained some very promising results. In 2007, CXS met all its milestones and has continued to develop as a cohesive interdisciplinary team determined to work together on challenging but important problems. CXS has established a high profile national and international presence and, through our specialist workshops – notable in the level of attendance by non-CXS members – has nucleated important new national programs, the impact of which will be felt over the next few years. CXS has done the groundwork, in both facilities and relationships that will lead to the delivery of high impact science for Australia. The next few years are going to be exciting, and a great deal of fun.



# RESEARCH PROGRAMS

## Biological Sciences Program

The **Biology Sciences Program (BSP)** in CXS involves the participation of biochemists and structural and cellular biologists who are undertaking specific research in the area of biomedicine. These groups conduct world-class research in the areas of malaria and mitochondrial biology. As part of work undertaken within CXS, BSP members collaborate closely with members of the Experimental Methods Program (EMP) in the development and implementation of novel imaging techniques with the aim of furthering these and other biological research programs.

### Goals:

- Prepare and optimise cellular samples for use as test-beds for X-ray coherent diffraction imaging and for other pioneering imaging techniques.
- Use X-ray imaging and other imaging modalities to gain novel insights into cellular architecture and function.
- Prepare samples of soluble and membrane proteins and determine their structural characteristics using both conventional X-ray crystallography techniques and novel X-ray-based approaches.

## OVERVIEW OF ACTIVITIES AND OUTCOMES

We are using the malaria parasite *Plasmodium falciparum* as a test system for X-ray coherent diffraction imaging (CDI), and are correlating the data with other imaging modalities, including light and electron microscopy and scanning X-ray microscopy. In addition, the group has performed pioneering efforts in the development of electron tomographic imaging, X-ray tomographic imaging and fluorescence imaging. The work has involved visits to a number of synchrotrons, including the Advanced Photon Source in Chicago, the Advanced Light Source in Berkeley and the Australian Synchrotron.

Work in 2007 focused on analysing the architecture of the malaria-infected red blood cells using novel fresnel coherent diffraction imaging and comparing this with other established imaging techniques. This involved extensive optimisation of sample preparation and significant data analysis. The malaria parasite was also used as a test-bed for both X-ray and electron

tomography techniques and has led to important findings into understanding the organisation of the Maurer's cleft organelles found between the parasite and the red blood cell membrane. Analysis of other biological samples has also been undertaken – including analysis of mitochondria using electron tomographic techniques.

Our studies into structural analysis and the production of protein samples continue. We solved the structure of malaria hemozoin using X-ray powder diffraction techniques. Membrane protein complexes have been purified and a range of conventional and novel approaches are being employed to study their molecular architecture. The respiratory complexes of the mitochondria inner membrane and their supercomplexes were isolated for future structural analysis. Other membrane proteins have also been reconstituted after their expression by recombinant means and subsequently employed in structural studies.

## Experimental Methods Program

**The Experimental Methods Program (EMP)** develops imaging methods using coherent and partially-coherent light sources. The research profile of EMP includes the design of experimental systems, sample handling and nano-fabrication techniques, tomographic imaging of three-dimensional objects, the detailed characterisation of radiation sources and the development of novel imaging methodologies using diffraction data. Currently developing is the imaging program within the Short-Wavelength Laser Source Program (SWLP), in collaboration with EMP. Already developed are several new imaging schemes in collaboration with the Theory and Modelling Program (TMP), including Fresnel Coherent Diffractive Imaging (FCDI) and its recent extension, Keyhole FCDI, which is a promising new form of Scanning Transmission X-ray Microscopy.

### Goals:

Beyond its scientific goals within CXS, the main goals of EMP in 2007 were to finalise infrastructure development.

**These infrastructure goals, which were all met, include:**

- Commissioning of the fabrication laboratory;
- Commissioning of the optics laboratory; and
- Finalisation of the design and procurement of the end-station project.

## OVERVIEW OF ACTIVITIES AND OUTCOMES

Pending the commissioning of the end-station, when the longer term goal of high resolution Fresnel Coherent Diffractive Imaging (FCDI) will be attainable, the scientific aim of the EMP is to explore the scope for FCDI at synchrotron sources and to demonstrate the technical feasibility of the method. Other aims included the continued exploration of the interaction of coherence in the imaging process and the continued development of fabrication and tomographic methods of relevance to the EMP activities.

In pursuit of these scientific goals the EMP expanded its interaction within the CXS undertaking major projects with each of the Biological Sciences Program, the Theory and Modelling Program, the Detector and Beamline Development Program and the Short Wavelength Laser Source Program. This work also saw the EMP lead six synchrotron experiments – one at the National Synchrotron Radiation Research Centre in Taiwan, one at the Swiss Light Source and four at the Advanced Photon Source in the USA. This, and work from previous visits, has led to the successful completion of a number of pieces of analysis – resulting in publications in 2007 and some accepted for 2008. The major publication outcomes from work undertaken in 2007 include results in FCDI, Coherence and Imaging

and in ancillary work such as refining sample fabrication methods and in tomographic methods.

In the FCDI work, in conjunction with the Biological Sciences Program, we obtained data allowing us to demonstrate the capacity of FCDI to obtain images of biological samples using existing synchrotron sources and methods. In parallel with this qualitative work we obtained data from test samples demonstrating that it is possible to obtain a quantitative reconstruction of a fabricated sample using FCDI. We also undertook experiments that have allowed us to demonstrate that FCDI can be used like a microscope to obtain images of the region of a larger sample that is within the beam illumination. This is an important result that will facilitate the use of the FCDI technique as a high resolution survey tool.

In conjunction with the Theory and Modelling Program and the Short Wavelength Laser Source Program synchrotron experiments measuring coherence, the interaction of coherence and beam curvature and laboratory experiments demonstrating coherent diffraction were successfully undertaken. These have produced a number of publications and signal some exciting developments for laboratory-based FCDI.

## Short Wavelength Laser Source Program

The Short Wavelength Laser Source Program (SWLP) is involved in developing tabletop short wavelength sources in facilitating their application to coherent diffractive imaging. This approach complements the activities of the Experimental Methods Program, who are mainly engaged in the use of partially-coherent synchrotron sources, and forms the foundation for future research using highly-coherent X-ray free-electron laser (XFEL) sources that are currently under international development. The Theory and Modelling Program strongly supports this research. The program is currently developing theoretical descriptions of the high-harmonic generation (HHG) processes that form the basis of the source technology, as well as the non-linear interaction physics involving strong electromagnetic fields and electronic matter.

### Goals:

The goals for SWLP in 2007 were:

- To observe HHG from the interaction between our new laser system and a gas jet.
- To optimise the output from the HHG source to provide maximum power at the shortest possible wavelength.
- To utilise the HHG source in imaging experiments, in collaboration with the EMP and TMP groups.

### OVERVIEW OF ACTIVITIES AND OUTCOMES

In the first quarter of 2007, the Femtosecond High Power Laser Facility and ancillary equipment were installed. The femtosecond laser system combines a femtosecond oscillator (FemtoLasers) and a two-stage multi-pass amplifier (Quantronix). This is the first system in this energy range in Australia.

Using a semi-infinite gas cell significant enhancements in the efficiency of HHG have been achieved. An XUV beam with a high photon flux, high coherence and good spatial beam profile can now be generated routinely, and involves only a small number of harmonics in the short-wavelength region. This is the first experimental realisation of HHG in Australia.

Our studies in collaboration with the TMP and EMP groups have demonstrated that it is possible to use a few harmonics in the XUV region of the HHG spectrum as the source for coherent diffraction imaging. In collaboration with TMP a new method for extraction of the HHG power spectrum from the Young double slit interference fringes has been developed. This spectral information is fed into a new algorithm that recovers images using diffraction data

obtained using the optimised, narrow bandwidth HHG source, eliminating the large losses incurred through the use of a grating monochromator. This is a significant achievement in the context of the broad aims of CXS.

Development of a non-interferometric form of Fourier transform spectroscopy in collaboration with TMP, was achieved in 2007. Time resolved spectral intensity measurements are used to deduce the complete time evolution of the complex molecular third-order polarisability using an inversion technique adapted from phase retrieval imaging algorithms. This approach promises to be useful in spectroscopic studies of biological molecules involved in photosynthesis as well as coherent dynamics studies of quantum dot arrays. This was an unexpected research outcome that was achieved through the collaborative structure of the research programs within CXS, and may find application in, for example, the future design of quantum computing devices or of biomimetic technologies to enhance our utilisation of solar energy.

## Theory and Modelling Program

The Theory and Modelling Program (TMP) is responsible for developing the theoretical physics underlying the Experimental Methods Program (EMP) in CXS, and designs many of the computational algorithms that all nodes of the Centre currently use. Our current interests include the solutions of inverse problems in all forms of coherent diffractive imaging, the relativistic formulation of molecular electronic structure and quantum electrodynamics, the dynamical description of non-linear interactions between molecules and strong laser fields, and the design of computational algorithms.

### Goals:

The Theory and Modelling Program provides theoretical and computational leadership and support to the experimental program across the Centre, mainly in the fields of:

- Image reconstruction from experimental X-ray diffraction data.
- Development of detailed quantum electrodynamical models of the interaction between matter and strong external laser fields.

### OVERVIEW OF ACTIVITIES AND OUTCOMES

In 2007 TMP focused its efforts to engage closely with the experimental activities of the Short Wavelength Laser Source (SWLP) Program at Swinburne while maintaining our already close connection with the Experimental Methods Program (EMP).

One of the key aims of the HHG project included the use of the raw output from the short wavelength source as the illumination in a diffractive imaging experiment. We adopted the Maximum Entropy Method (MEM) to characterise the power spectrum of the HHG source from Young's double-slit data and other *a priori* information about the experiment. Preliminary results on simple samples suggest that this approach will provide a powerful imaging technique that makes maximal use of the available XUV flux from the HHG source.

Work continued on the development of computational methods in relativistic molecular many-body theory and quantum electrodynamics. This work represents an essential progression in the theoretical description of inner-shell electrodynamics that is required to assess the potential use of XFEL sources in imaging applications. Several approaches are now in place to model the time-dependent evolution of molecules interacting with strong external electromagnetic fields.

The development of detailed models of partially coherent light sources based on modal and spectral expansions of their mutual optical intensity distributions was completed. This work now forms the theoretical foundation of experimental work within EMP to characterise the spatial coherence properties of partially-coherent, quasi-monochromatic synchrotron sources and of polychromatic HHG sources that exhibit high spatial coherence. The approach also lends itself to phase retrieval algorithms in which the spatial coherence properties known to us can be utilised in the recovery of images from diffraction data.

The program also contributed to the development of a non-interferometric form of Fourier transform spectroscopy based on the solution of an inverse problem constrained by intensity measurements and *a priori* information about the temporal structure of the laser-molecule interaction. This promises new insights, in particular, into the role of quantum coherence in energy transfer processes.

## Structure Determination Methods Program

The Structure Determination Methods Program (SDP) comprise CSIRO researchers working broadly within the fields of X-ray and electron crystallography. It has as one of its main aims the development of novel experimental techniques and data analysis methods for extracting structural information from 2-D crystals and 3-D nanocrystals, especially relating to the determination of the structure of the pharmaceutically very important class of proteins known as integral membrane proteins (IMP). This Program brings with it internationally recognised expertise in the preparation, purification, crystallisation and handling of these samples.

### Goals:

This Program has produced 2-D crystalline samples of the membrane protein Bacteriorhodopsin, which is a well-studied system selected to serve as the prototype for method development. The goal across this Program in 2007 was to extend existing theoretical methods relating to diffraction from single-crystals and powders to the characterisation of molecular structures using 2-D samples.

### OVERVIEW OF ACTIVITIES AND OUTCOMES

The program has been involved in the development of techniques which facilitate the growth of 2-D arrays of membrane proteins using novel methods. It also includes the exploitation of grazing incidence X-ray diffraction (GIXD) methods to obtain high sensitivity structural information for thin samples. A powerful aid to the development of these techniques is simulation software developed in order to help better understand the nature of the diffraction data on such systems, including the influence of structural disorder.

A key component of the program in 2007 has seen a departure from traditional, empirical approaches towards physical modelling-based approaches in the analysis of diffraction data from 2-D crystals. This requires the development of 2-D single-crystal and powder diffraction theory as it applies to biological samples of interest, in particular, fully or partially ordered nano and micro-arrays of integral cell membrane proteins. The theoretical framework is to be put into practice by

assembling a suite of computational tools used to process and fit diffraction data to a comprehensive physical model. Further methods of data analysis proposed for implementation include Bayesian and MaxEnt methods that seek to incorporate both experimental data and *a priori* information.

The initial system we continue to study is *Purple Membrane*, a naturally occurring 2-D crystal of the membrane protein *Bacteriorhodopsin* that serves as a useful test case because there is also high-resolution structural information available from 3-D X-ray crystallography and 2-D cryo-electron microscopy that we can use for comparison.

A long-term aim of the program is to develop novel techniques and instruments for the structure determination of integral membrane proteins, especially with a view to implementation at the Australian Synchrotron.

## Ultra-Cold Plasma Source Program

The Ultra-Cold Plasma Source Program (UCP), formed within CXS in 2007, exploits the potential advantages of a bright, coherent source of high-energy electrons in the imaging of single molecules. The program is designed to utilise many of the theoretical and experimental techniques already being developed in the EMP and TMP programs, while exploiting the enhanced probe-molecule interaction strength that a coherent electron source offers, compared with any existing coherent short wavelength light source. This approach offers an improvement of four orders of magnitude in brightness over existing sources.

### Goals:

The primary goals of the UCP Program are:

- To build a bright, coherent ultra-cold plasma source of high energy electrons.
- To use this source to perform coherent diffractive imaging experiments.

While an ultra-cold plasma source has already been constructed in Eindhoven, UCP will pursue a different and innovative design based on a quasi-mirror-magneto-optical trap architecture. This approach allows for a much more compact accelerator structure and, consequently, much lower electric potentials for a given field strength. This will reduce the technical requirements and should enable a smaller energy spread in the electron beam.

## OVERVIEW OF ACTIVITIES AND OUTCOMES

The UCP Program commenced midway 2007. They expended most of their efforts on the design of the experiment and the purchase of equipment. The various components will begin to function before the middle of 2008, with the first electrons following before the end of the year.

The transverse coherence length of the existing UCP source is too small to observe useful diffraction, except from crystalline materials with periodicity of no more than  $\sim 0.5\text{nm}$ . To image larger crystal units, such as biomolecules, with a cell periodicity of a few nm or more, the coherence length must be increased proportionally. For diffractive imaging of a single molecule, the coherence length must be similar to the target size (again, a few nm), but the effective source size (the focused beam radius) must be small, not much larger than the molecule.

To appreciate the significance of the new source in the context of proposed imaging applications, it is informative to estimate its

likely transverse coherence. Starting with a cold-atom density of  $10^{12}\text{cm}^{-3}$ , extracting  $10^7$  electrons in a cigar-shaped pulse of  $80\mu\text{m}$  radius and 1mm length, the normalised emittance would be around  $3\mu\text{m mrad}$  and the coherence length  $23\text{nm}$  when focused to a  $0.2\text{mm}$  spot. That is not only large enough for diffractive imaging from biomolecules but also for atomic-scale imaging of small viruses.

In a further design refinement, the magneto-optical trap (MOT) will be loaded from a Zeeman slower rather than a thermal vapour, to reduce background collisions and increase the loading rate, thus obtaining more trapped atoms in the steady-state. More atoms in the MOT allows for larger charges in each bunch, or a higher pulse rate: this will be a second-generation improved source. The program has already commenced rebuilding the existing MOT at the University of Melbourne into the UCP system.

## Detector and Beamline Development

The **Detector and Beamline Development Program (DBD)**, based at Monash University has undertaken the design and construction of an optimal detector for X-ray coherent diffractive imaging. In collaboration with the EMP Program, DBD is also involved in the design and delivery of the high-technology end-station, which will control the optics, sample and detector positioning for coherent X-ray diffractive imaging experiments. The end-station is due to start in mid 2008.

### Goals:

The cost of building a detector means that extensive modelling is necessary including in the physics of the X-ray interactions, the critical demands of the imaging algorithms and the performance of the circuits. Goals that must be satisfied before fabrication of a detector include:

- Characterisation of the detector's sensitivity and dynamic range requirements for successful coherent diffractive imaging.
- Development of the data acquisition system.
- Specification, design and commissioning of the CXS imaging end-station.
- DBD has undertaken a detailed program of modelling to address these issues.

### OVERVIEW OF ACTIVITIES AND OUTCOMES

Work in progress for other projects within the Monash Centre for Synchrotron Science (MCSS) has led us to believe that a new technology for a medical imaging detector will be applicable to CXDI. A dual layer hybrid pixel X-ray detector, which is progressing well in design, could provide the capabilities that are sought after for efficient and precise Fresnel CXD imaging. A significant amount of modelling and design work needs to be undertaken before silicon fabrication is considered. Two PhD projects, development of a data acquisition system, and a training project have all been set running this year in order to underpin this work.

The CXS project addresses the limitations of the current CCD based X-ray imaging devices for CXDI. If the precise number of photons which hit a pixel must be known precisely for successful CXDI, the estimate provided by an integrating detector such as a CCD may not be good enough. Noise and other detector artefacts increase the error in the data especially when there are only a few photons measured as is the case in the large angle regions of the image.

A better alternative is to count individual X-ray photons as they arrive at the detection plane. In this case the measurement of flux is accurate with almost no noise. A limitation with this technique arises when the flux is high. In this case the electronic circuits can struggle to keep up with the rate of arrival of the photons. However if the area for which the counting is taking place is very small this reduces this limitation. Using very large scale integrated circuit (VLSI) technology the circuitry can be made very small. It is feasible to place all the readout circuitry for an individual X-ray detector in an area of less than 100 microns square. It is also possible to reproduce this many times and devise a means to multiplex the outputs into a few electronic channels.

Using this technique a matrix of readout nodes can be fabricated which may extend to 25 mm by 25 mm. If an X-ray sensitive material is placed above this matrix circuit given electrically connected, a versatile detector can be made. The general name given to such a device is a hybrid pixel detector (HPD), or simply 'pixel detector'. These HPD devices possess characteristics that are superior to CCD detectors for imaging applications.



❖ *Mr Andy Berry (Senior Electronics Design Engineer), and Dr George Jung (CXS post-doctoral fellow) inside the X-ray absorption spectroscopy (XAS) hutch on the Australian Synchrotron. The synchrotron beam was being used to investigate the non-linearities in the X-ray detection capabilities of certain room temperature semi-conductor materials.*

[04] RESEARCH REPORTS



*Mr Andy Berry examining a solid-state device at Monash University.*

# RESEARCH REPORTS

## Biological Sciences Program

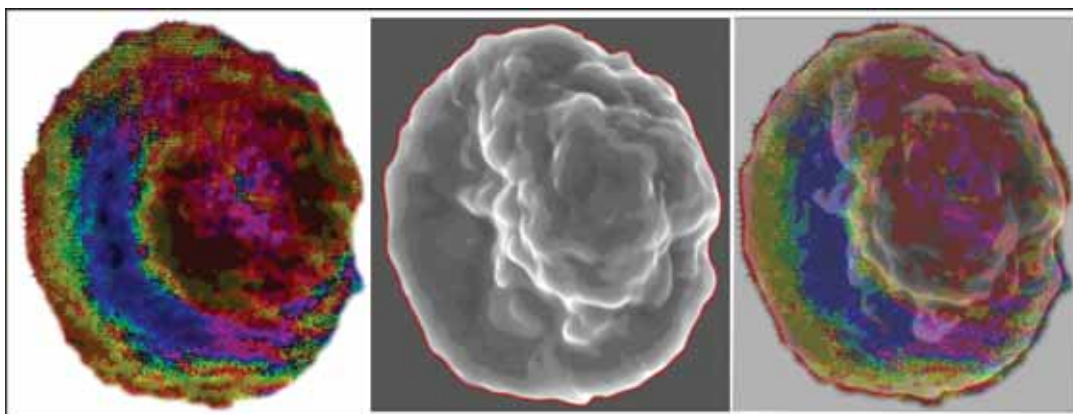
The **Biology Sciences Program (BSP)** involves the participation of biochemists as well as structural and cellular biologists from La Trobe University and the Walter & Eliza Hall Institute for Medical Research. These groups conduct world-class research in the areas of malaria and mitochondrial biology. In 2007, members of the BSP continued to work closely with members of the Experimental Methods Program, the Structure Determination Methods Program as well as outside collaborators to develop and implement novel imaging techniques and to continue with structural studies. The year 2007 also saw the relocation of the CXS biology groups at La Trobe University into new state-of-the-art laboratories.

- ❖ *One of the new laboratories for the BSP at La Trobe University.*



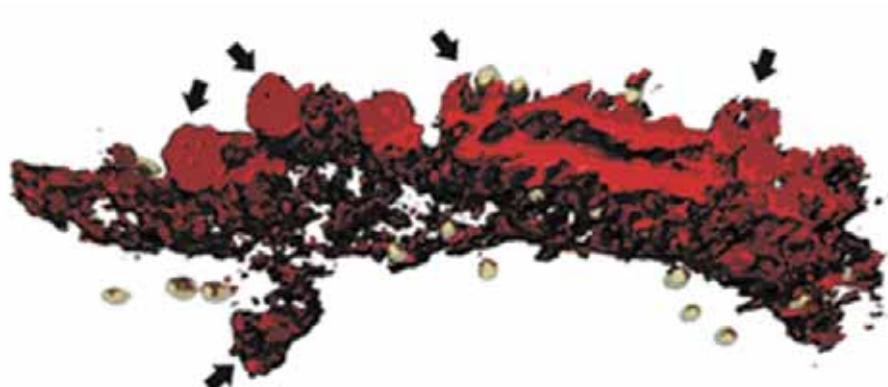
### Sample preparation and imaging

Malaria parasite-infected red blood cells have been prepared using different fixation and staining conditions for analysis using Fresnel coherent diffraction imaging (CDI). CDI images were viewed in comparison with data obtained from the same cells using scanning electron microscopy, light microscopy and scanning X-ray fluorescence microscopy. The work provided information about both the elemental content and the structure of the host red blood cell and the intracellular parasite at a spatial resolution of approximately 30 nm.



- ❖ *Coherent X-ray diffraction image, scanning electron microscopy image and overlay of images of a malaria parasite-infected erythrocyte.*

A research visit was made by BSP members (Leann Tilley, Eric Hanssen and Nick Klonis) to the laboratory of Carolyn Larabell, University of California, National Center for X-ray Tomography, Advanced Light Source, Berkeley, USA, where X-ray tomographic imaging of malaria parasite infected red blood cells was undertaken. The group also visited the laboratory of John Sedat, (University of California) and analysed their samples using Structured Illumination Microscopy. CARS imaging was also performed in Steve Lane's Facility, NSF Center for Biophotonics, University of California.

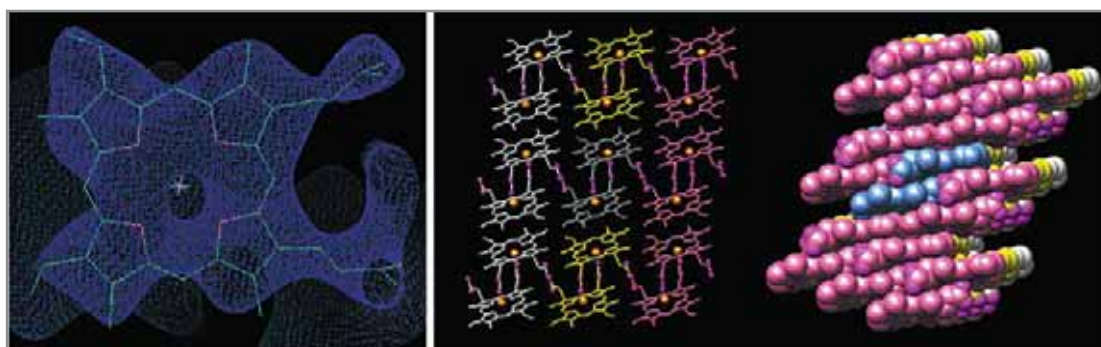


❖ *Rendering of an electron tomogram of Maurer's clefts from the malaria parasite.*

In addition, Eric Hanssen has developed the methodology for electron tomographic imaging of the Maurer's cleft organelles of malaria-infected red blood cells. These experiments have revealed novel structural features and led to a publication on the front cover of *Molecular Microbiology*. Members of the BSP are also undertaking the analysis of different biological samples. This includes the tomographic analyses of mitochondria from a number of different cell types including from patients with mitochondrial disease.

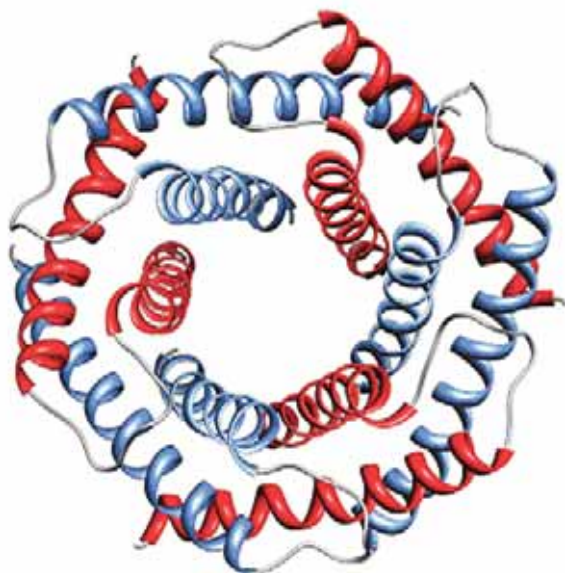
■ **Structural studies**

In conjunction with the Structure Determination Methods Program (SDP), we solved the structure of parasite hemozoin using X-ray powder diffraction data. The structure reveals the presence of two previously undescribed modes of hemozoin self-association involving  $\pi$ - $\pi$  interactions. These  $\pi$ -bonding interactions may initiate crystal formation and stabilise the extended structure.



❖ *Structure of haemozoin pigment from the malaria parasite.*

We have now successfully isolated the large membrane protein complexes of the mitochondrial respiratory chain. We are optimising methods to isolate their supercomplex forms for future structural analysis using 2-D crystallisation. In addition, we have expressed a number of protein domains and purified for structural analysis. This includes the structural characterisation of the Tim9-Tim10 complex of mitochondria that chaperones membrane proteins across the mitochondria intermembrane space. As disulfide bonds brace the subunits, we have been assessing their potential to act as scaffolds for the stabilisation of protein-protein interactions. This has potential novel applications in future structural studies of membrane receptor domains.



❖ *Structure of the Tim9-Tim10 chaperone complex.*



❖ *Laura Osellame and Michael Baker in the Mitochondria Biogenesis and Disease Ryan Laboratory.*

## Experimental Methods Program

The **Experimental Methods Program (EMP)** met all its milestones in 2007. These involved the development of research infrastructure and the successful analysis of Fresnel Coherent Diffractive Imaging (FCDI) data. The program is tracking well against the longer term goals of CXS, especially with regard to the imaging of biological samples. There are no apparent “show stoppers” that might undermine the strategy of EMP, which is based primarily on the further development of the FCDI technique. The results obtained in 2007 regarding the characterisation and role of spatial coherence in imaging applications and our research into fabrication methods (process modelling) and tomographic techniques will also become important enablers towards the ultimate goal of high-resolution imaging in biological samples.

### Optics Laboratory

The optics laboratory, developed by Garth Williams, is located at the University of Melbourne. It includes a light-tight optical bench enclosure and a visible light analogue of the X-ray FCDI experiment. In 2007 the facility was used to perform proof-of-principle experiments for several CXS researchers and was used to produce the results for a 4th year project.



❖ *View inside the hutch of the Optics Laboratory.*

### Fabrication Laboratory

The fabrication laboratory, developed by Eugeniu Balaur and Kaushal Vora, is located at La Trobe University. It includes a lithography facility with fume-hood capability, electron beam lithography using a JEOL 840 scanning electron microscope modified with pattern generation software, as well as reactive ion etching and sputtering. In 2007, the facility has produced samples for several CXS imaging experiments.

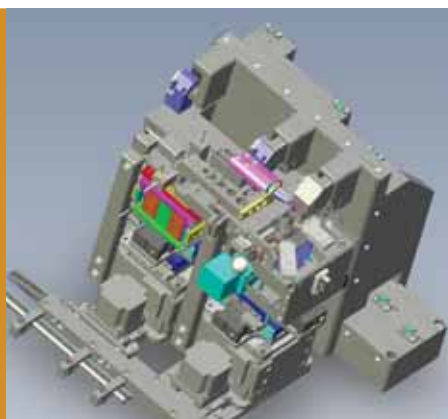


❖ *Corey Putkunz undertaking sample preparation in the fume-hood of the Fabrication Laboratory.*

## Endstation Project

Mark Pfeifer manages the Endstation Project that is designed to be located at a synchrotron source when completed. It involves the close collaboration of members of the Detector and Beamline Development Program (DBD). After an extensive design and review process, we commissioned Xradia Inc to build a vacuum endstation, which incorporates the optics and stages necessary for FCDI and tomography. The initial plan was to build the system in two stages, with the second stage incorporating a feedback system for stability as well as high-precision tomographic stages. We have now been able to accelerate this project to deliver the full system by mid 2008.

❖ *Solid model of the optics stages inside the endstation.*

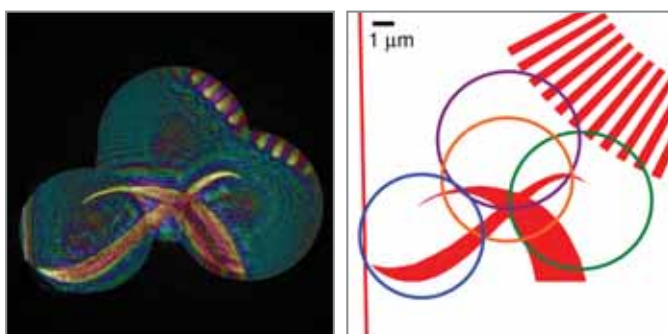


## Fresnel Coherent Diffractive Imaging

Three of the challenges for the FCDI method are:

- (i) demonstrating that biological samples can be imaged,
- (ii) demonstrating that the results obtained by FCDI are quantitative; and
- (iii) identifying any advantages that the FCDI method has compared to conventional plane wave CDI.

We achieved significant progress in addressing each of these challenges in 2007. Garth Williams led experiments and analysis of FCDI data from malaria parasite infected red blood cells, which has resulted in a publication submitted between the EMP and the Biological Program within CXS. Jesse Clark undertook an analysis resulting in a paper accepted for publication, which demonstrates that you can obtain quantitative results for the thickness of gold samples using FCDI. Brian Abbey led work in the development of a variant on the FCDI method that has been accepted for publication in *Nature Physics*. The work has shown that knowledge of the beam in the plane of a sample can be utilised to define a region of illumination that can be scanned across a sample that is larger than the beam. This removes the standard constraint in coherent diffractive imaging – that the sample be isolated – while retaining the advantages of image recovery based on iterative methods. The new method has been termed “Keyhole” FCDI. It offers great promise as a fast and improved method of Scanning Transmission X-ray Microscopy.



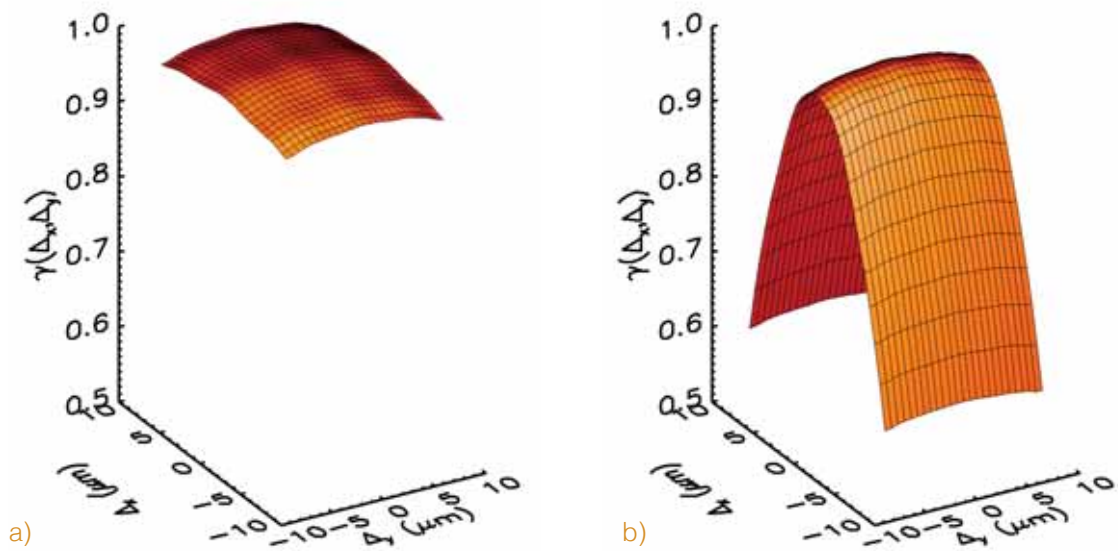
❖ *The panel on the left shows an image of the large test sample shown in the panel on the right.*

## Coherence and Imaging

Lachlan Whitehead and Garth Williams, in collaboration with Harry Quiney in the Theory and Modelling Program, produced publications demonstrating that the curvature of the beam in FCDI can be optimised with respect to the degree of transverse spatial coherence in the illumination.

In work led by Chanh Tran, techniques enabling the characterisation of the coherence properties of a synchrotron beam resulted in a publication in *Physical Review Letters*. Work continues to develop coherence in analysis methods based on the coherent mode expansion of the mutual optical intensity distribution for imaging light sources.

In work led by Bo Chen, and in collaboration with the Short Wavelength Laser Physics Program the first spatial coherence measurements of the HHG spectrum were taken, together with measurements of the HHG power spectrum. This work is ongoing in 2008, during which the continuing goal is to demonstrate laboratory-based FCDI at wavelength below 10 nm.



- ❖ *Two experimental measurements of the complex degree of coherence of a synchrotron beam. These data show the reduction in the transverse spatial coherence due to changes in the experimental arrangement.*

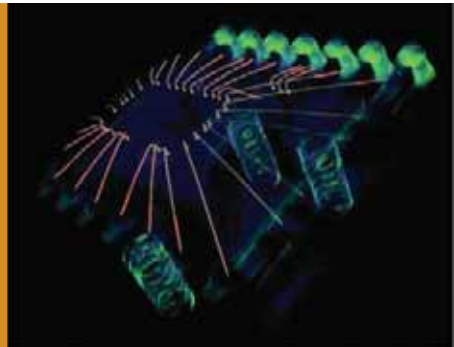
## Process Modelling and Tomographic Methods

Our fabrication program has investigated difficult process areas for the types of samples and sample mounts we need. Work undertaken by Kaushal Vora as part of his PhD studies has definitively modelled elements of the X-ray lithography process for high aspect ratio structures and has produced a number of publications in 2007, including one chosen by the Institute of Physics editors for inclusion in a special collection of articles – IoP Select. Our tomography program, led by Benedicta Arhatari, has also enjoyed research success and produced a publication in 2007. This program pursues the development of experimental methods to be used in FCDI as well as seeking to clarify broader issues of principle in phase tomography.

### Program Goals for 2008:

- Further work on the Beamline Advisory Panel for the soft X-ray branchline at the Australian Synchrotron to develop the plan for location of the CXS endstation at the Australian Synchrotron and to apply for LIEF funding to support this.
- Development of FCDI at the Swiss Light Source.
- Development of FCDI at the Centre for Nanomaterials at the Advanced Photon Source.
- Development of research linkages in Taiwan.
- Commissioning of the endstation.
- Demonstration of proof of principle imaging at the HHG laser source at Swinburne University of Technology.
- Demonstration of improved quality in FCDI using the CXS endstation.

❖ *Example of a tomographic image produced in the Tomography Laboratory.*



## Detector and Beamline Development Program

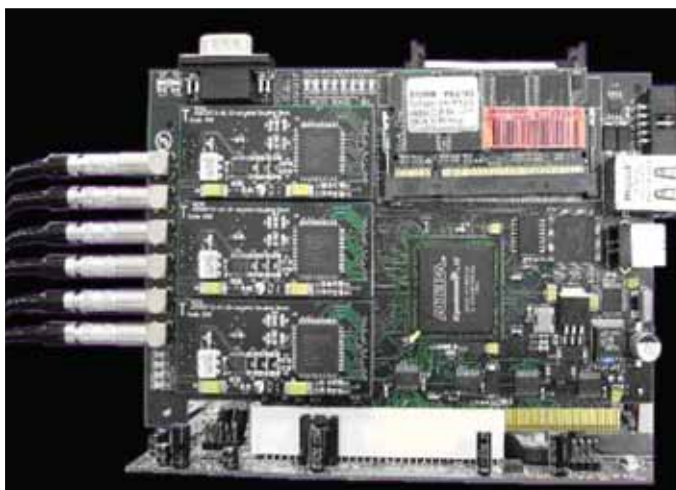
The **Detector and Beamline Development Program (DBD)** works closely with the Experimental Methods Program (EMP) in the design and commissioning of the CXS endstation project which contains the optics, detector and positioning instrumentation that are necessary to perform the Fresnel coherent diffractive imaging (FCDI) experiments that form a key part of the program of CXS. The program is placing particular emphasis in 2007 on the investigation and development of the various X-ray detector systems that are available for imaging work. This has involved the detailed modelling of the characteristics of these devices, and an appraisal of the relative merits of existing and cutting edge technologies.

### Detector Readout Systems

A significant part of the DBD group detector program concerns development of the readout systems for 2-D X-ray detectors. Starting with the front end electronics, understanding the intimate interactions between X-ray produced charge and the front end electronics is crucial for successful operation. Every X-ray that interacts in the detector material releases a very small charge. These have to be measured and amplified, avoiding noise and any other errors that might perturb the measurement. Further down stream in the chain of signal processing high interaction rates imply high bandwidths in both the analogue and digital side of the circuitry. This demands very carefully screening and noise management from the first amplification stages onwards to avoid generating errors. Until we obtain a digital signal in multi-channel devices with strict space constraints, the management of the data stream until storage is also a

design challenge. A data acquisition system, designed with the help provided by the CXS, now successfully incorporates these functions. The Generic Data Acquisition (GDAQ) system has completed the first phase of its development with a high versatile unit made in the format of a PCI card to function from a standard PC. The front end of this card is designed to be altered to suit the particular detector which it is reading out from. We also completed the testing and production of several versions of the daughter card this year.

As a test bed a 2-D gas proportional detector has been coupled to the acquisition system and is now being trialed in a small angle X-ray scatter instrument. The GDAQ will feature strongly in the stages of testing of the Hybrid Photon Detector (HPD). It will be able to collect, assemble and present data from all stages of the detector from the analogue output of the detector layer through to the serial streams post digitisation.



- ❖ *The Generic Data Acquisition system (GDAQ) card. Based around a powerful field programmable gate array (Altera chip in the centre of the card). GDAQ is designed to interface with many detectors. It uses the popular tried and trusted PCI bus to interface with a controlling computer. In the configuration shown here, the daughter card has digitisation capability. Six channels of analogue signal can be accepted allowing pulse timing and shape to be made digital for storage.*

## Gas Electron Multiplier Detectors

As part of our training program, a detector project based on gas electron multipliers (GEM) has been progressed this year. This device might be useful for CXDI since it is a photon counting detector, and we believe can be made to work at X-ray energies close to those currently used for CXDI. Although the spatial resolution would be inferior to the standard CCD detector, the sensitivity would be high. GEMs were developed for high energy physics detectors, so the principles and technologies for working with minimum ionising particles are well understood. Less understood is their behaviour for lower energy

X-rays, so we plan to undertake some studies to trial the prototype in this regime. The primary purpose of this project is for training researchers in X-ray detection issues. All the skills required for a basic understanding of X-ray interactions, and electronic readout of detectors are encompassed in this project. These skills are rare and so it is essential that DBD put in place an in-house training scheme. A GEM device designed, produced and tested by Dr George Jung, has been proven to be stable, and capable of detecting 6 keV X-ray from a  $^{55}\text{Fe}$  isotope. The next step in this project is to design the 2-D readout electrode structure, then using the GDAQ system produce a GEM based soft X-ray imaging detector system.

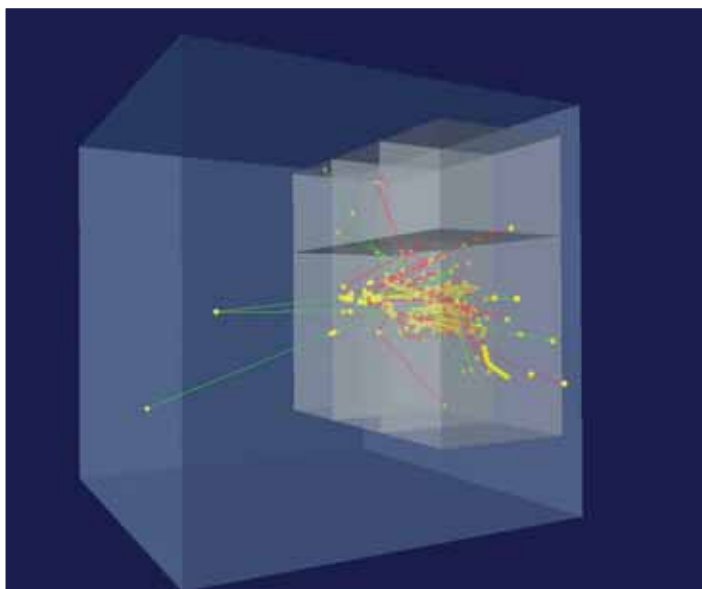


- ❖ *This CAD drawing shows the arrangement of the components of the low energy detector test system. From left to right: the detector (grey), the central cube (blue), an extension tube and cross piece for distant mask positioning (magenta and cyan) and a pair of vacuum isolation valves, one incorporating an X-ray transparent window (yellow). The items to the right are designed to allow interfacing of this apparatus to either beam line or X-ray set transfer tubes.*

## Device Modelling

The DBD team focused some of its work in 2007 on background research on modelling potential X-ray detector configurations. One of our PhD students, Evan Curwood, has embarked on building a Monte Carlo model of two layers of a HPD. He is using a tried and trusted code developed at CERN for modelling high energy physics detector

systems. The GEANT4 code is complex, but comprehensive. It will allow the DBD group to model the movement of charges generated by X-rays in the detection layer, subsequently providing prediction of the size and shape of signals from electrodes placed on the surface. This is crucial information to provide for the electronic design team, who will use this to design the amplification, digitisation and digital data management circuitry.



- ❖ *Results from a Monte Carlo simulation of one layer of a proposed CXDI detector. The model shows several 4 keV photons interacting in a pixelated silicon block. Photon paths are shown in green, interaction points in yellow and electron paths in red. Modelling such as this will allow us to predict signal shapes and sizes as input into the design of the electronics.*

### Testing Existing Detector Technologies

Detailed tests of commercially available detectors will allow the assessment of the limitations of these devices against the demands of CXDI. Two HPD detectors have been marked as a potential interest. One of them, the Pilatus 100K, started its testing program late last year. Our second research student, Guido Cadenazzi, has undertaken the task of understanding the intricacies of the functioning of this detector. Results have been encouraging so far. Noise assessment shows that the detector will certainly provide efficient data collection at 6 keV. The prospect of working at 4 keV and lower is highly promising. Signal to noise ratio at 6 keV is sufficient; however, assessment of the impact of dropping thresholds to allow lower energy photon detection at 4 keV is a future goal.

An evacuable detector test system designed and the parts procured this year by the DBD group post-doctoral research fellow Dr. Linda Feketeova. This instrument will enable precise testing of soft X-ray detectors using both conventional and synchrotron X-ray sources. We can position masks and other test objects in front of the detection plane and manipulate them within the evacuated volume. Soft X-rays will illuminate the detector down a vacuum flight tube. A double valve isolator with one valve including a thin X-ray transparent window will ensure vacuum compatibility with external equipment such as a synchrotron or conventional X-ray source beam pipe. The port which interfaces with the detector has been designed for the current Princeton Instruments CXS detector but will easily provide mechanical and vacuum compatibility with the Pilatus and other detectors for future testing.

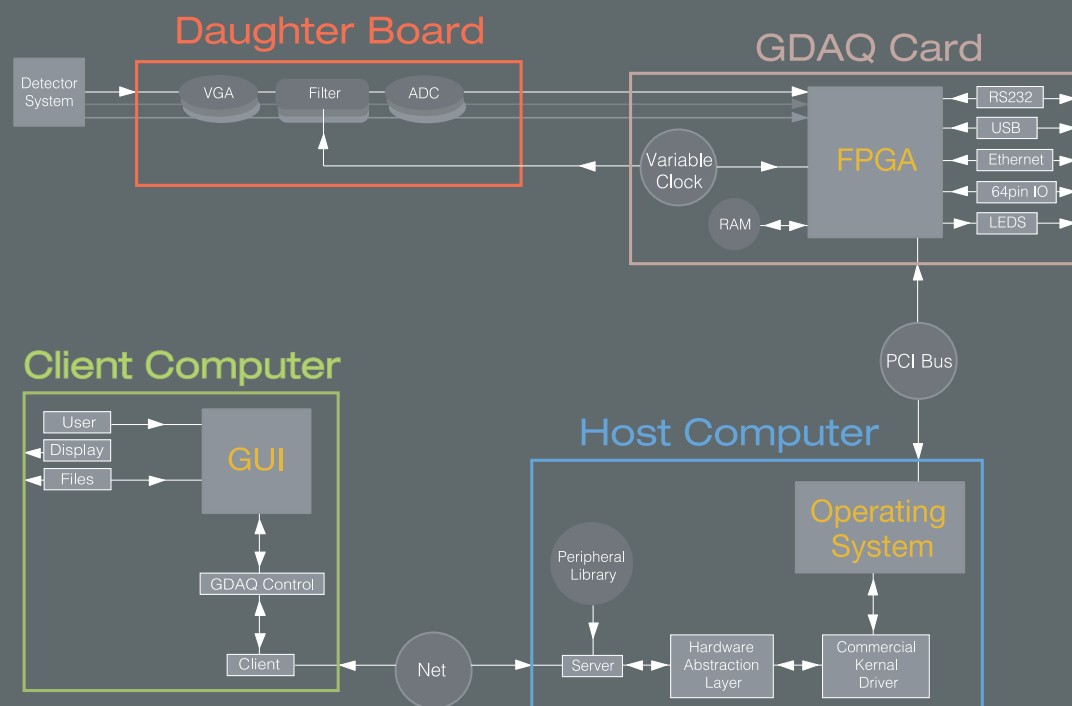


- ❖ *An engineering drawing of the central part of the low energy detector test apparatus. Manipulators will allow in-vacuum positioning of masks and collimators in front of the detector.*

## Hybrid Photon Detector Development

Progress in the design and development of the HPD electronics layer made this year was on track. CXS and the partners in the medical HPD project (CRC) share the effort in this area. Some effort has been put into defining a Systems Engineering model of the design. This approach has made the interface with the industrial partners more secure and supportable. Our senior engineer Andrew Berry has drawn up a comprehensive project plan. This incorporates tasks for all the DBD teams to allow them to predict costs and timescales in an efficient manner, even in a rapidly changing environment.

## Functional Diagram of the GDAQ System



❖ A functional diagram of the GDAQ system, showing how it interfaces to a controlling computer via the PCI bus. In this case the detector signals are accepted by a daughter card which carries digitisation capability. The analogue signals are converted to a series of numbers which are passed on to the next stage for processing.

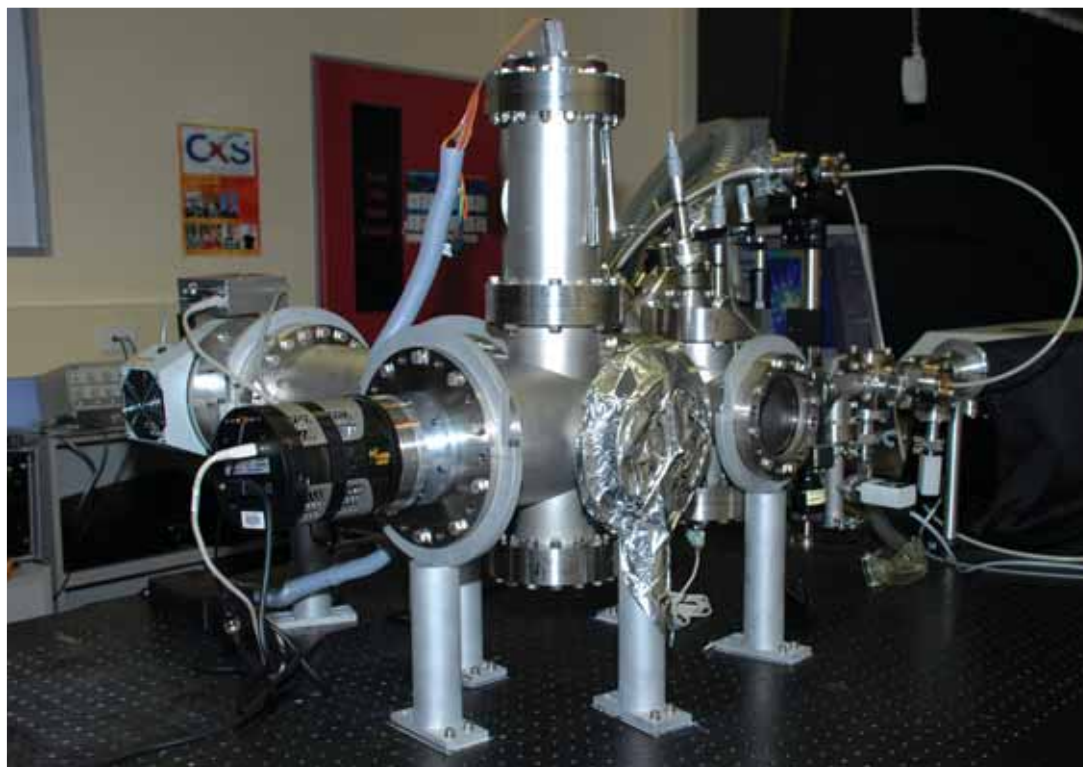
At the heart of the unit is a powerful field programmable gate array (FPGA). This can be rapidly programmed to process the signals depending on the demands of the detection task. An extension to the control application allows the use of remote control via a network connection. A client graphical user interface (GUI) has been coded to allow ease of control of the system.

## Short Wavelength Laser Source Program

The Short Wavelength Laser Source Program (SWLP) took delivery of the key components of the Femtosecond High Power Laser Facility in the first quarter of 2007; and in November, the facility had its official opening. There is no system of comparable power currently within Australia in this energy range and it has enabled the production of short wavelength light by High Harmonic Generation (HHG), fulfilling one of the key goals of SWLP for 2007. This establishes the research infrastructure required for the laboratory-based imaging technologies CXS will be developing in coming years, and has already generated a considerable amount of experimental and theoretical activity involving the Theory and Modelling (TMP) and Experimental Methods (EMP) Programs.

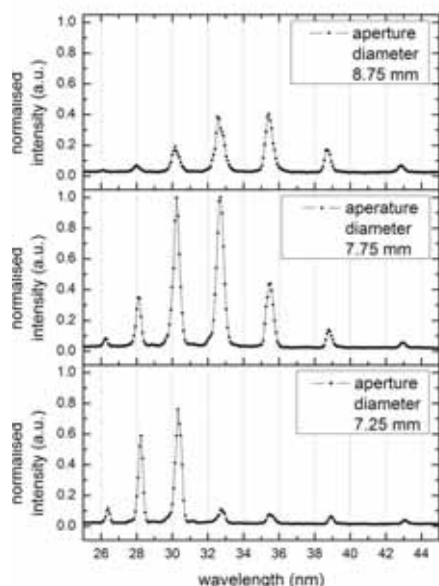
### Generation of High Flux, Highly Coherent, Small Bandwidth Extreme Ultraviolet Radiation

Using a semi-infinite target gas cell, we were able to achieve significant enhancements in the efficiency of HHG. An XUV beam can now be generated within the apparatus shown below, with a high photon flux, high coherence and good spatial beam profile.



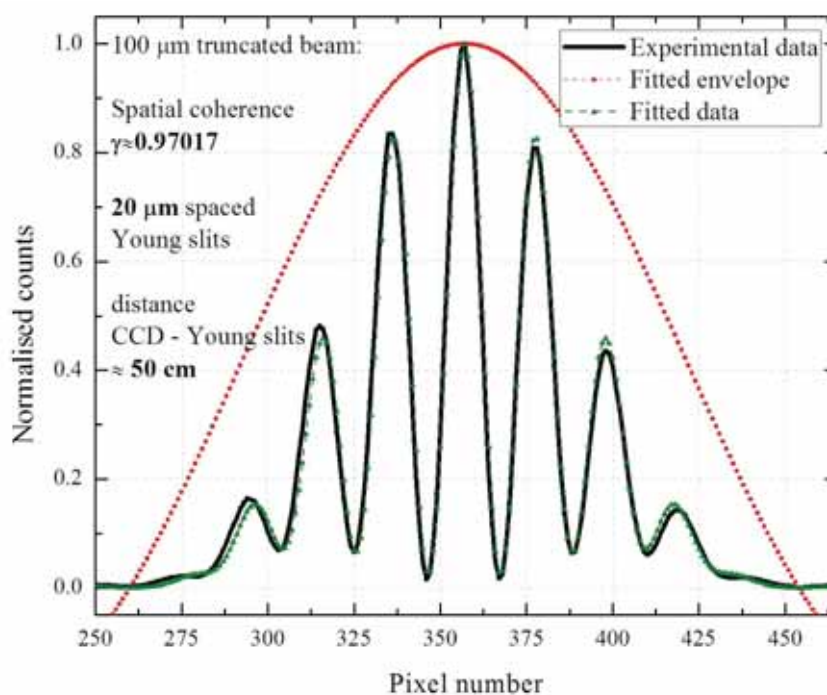
❖ *Experimental setup for generation, detection and diffraction of XUV radiation.*

The spectral distribution of the HHG output may be restricted, for example, to the energy region spanning from the 27th to the 33rd harmonic in argon (a wavelength range spanning 22 nm to 32 nm), from the 51st to the 63rd harmonic (12 nm – 17 nm) in neon, and from the 59th to the 81st harmonic in helium. By careful selection of experimental conditions such as the geometry and gas pressure, we are able to generate just a few harmonics (in some cases just two main harmonics) in argon gas.



- Phase matching for generation of few harmonics in Ar gas by variation of the size of the laser beam.

By considering the contrast in the interference fringes obtained from a Young's double slit experiment shown below, the degree of spatial coherence for HHG radiation in an argon gas cell is estimated to be about 0.95.



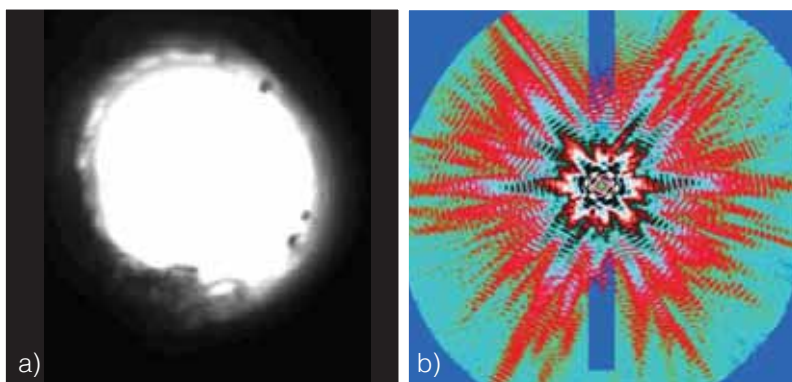
- Measurement of the coherence of HHG source with 20 μm spaced Young double slits.

In collaboration with members of TMP, a new method for obtaining the HHG power spectrum from Young's double slit interference fringes has been developed, based on a maximum entropy recovery of the exit wave at the slits under illumination by the source. This is an important component of our strategy for coherent diffraction imaging because it allows us to obtain accurately the HHG power spectrum during the coherent diffraction imaging process. This knowledge of the spectrum may be used to perform imaging experiments using the complete output from the HHG source, rather than suffering the very significant loss in flux that would occur if the source were first passed through a grating to render it monochromatic.

## Coherent Diffraction Imaging with Few Harmonic-Orders Beam

In collaboration with members of TMP, we have shown that it is possible to use the 'bare' HHG source in coherent diffraction imaging experiments without filtering out a single frequency component using a grating monochromator, provided that the source is composed of a small number of high-harmonic contributions. The high photon flux of such a 'harmonically-restricted' source generated in argon gas is used for this study. The images below shows a 25  $\mu\text{m}$  pinhole as an optical microscope image (left); this pinhole was used as the first test sample. The diffraction obtained using this pinhole and the HHG source as illumination is shown on the right.

Illumination shown below in sample (b) displays a complicated diffraction pattern that is characteristic of diffraction from an imperfectly-formed circular pinhole, but which is not strongly blurred by the polychromatic composition of the HHG beam. The data included a sufficient signal in high-angles of scattering to enable the reconstruction of the pinhole to be performed.



- ❖ (a) Image of a 25  $\mu\text{m}$  diameter pinhole under optical microscope and (b) diffraction data obtained using HHG source.

## Future Generation of Radiation in the Water Window

Using helium gas we are able to obtain HHG in the water window but the flux is very low. One solution for the generation of a high flux in the 4 nm range is to ionize the atomic targets prior to the non-linear HHG interaction, thereby significantly increasing the ionization potential of the nonlinear medium without changing the reaction cross section. We are exploring different configurations to achieve this. These investigations include the use of an ionizing pre-pulse or an electric discharge to ionize the atoms as well as the use of the ionized atoms in an optical waveguide or self-guiding configuration.

## "Deep UV" fluorescence microscopy

We have also investigated the potential of directly exciting the dominant amino acids in biological samples, in particular tryptophan, by multiphoton absorption. We have also concentrated on developing fluorescence microscopy techniques that we can use in the "deep UV" region of the spectrum, directly exciting the intrinsic fluorophores within a sample, using the second or third harmonics of an ultrafast laser. We have developed a scanning UV confocal microscope that is capable of time-resolved emission imaging. Most recently, we have adopted the rapidly developing technique of structured illumination microscopy (SIM) and extended this, for the first time, to UV excitation. In addition to unstained imaging, this approach offers the potential for improved spatial resolution. We have shown the feasibility of this direct UV excitation approach for a range of samples. Craig Lincoln is conducting this work in conjunction with an Honours student, Peter Wichta and a visiting intern student, Niels Zijlstra, from University of Twente in The Netherlands (11/7-23/11).

Our goals for the near future are to make UV SIM measurements of malaria infected red blood cells and other biological samples. We also hope to perform more time-resolved UV confocal measurements of appropriate samples using SIM.

## Femtosecond High Power Laser Facility

In the first quarter we installed the Femtosecond High Power Laser Facility and ancillary equipment, in the first quarter of 2007 at a cost of approximately one million dollars. It consists of a multi-pass femtosecond amplifier system, a vacuum spectrometer equipped with an XUV CCD camera and vacuum chambers for different experiments using the HHG source. The femtosecond laser system combines a femtosecond oscillator (FemtoLasers) and a two-stage multi-pass amplifier (Quantronix). This laser system has an output pulse energy of ~6 mJ and pulse duration of ~30 fs at 1 kHz pulse repetition rate. This is the first system in this energy range in Australia.

The spectrograph is equipped with four different XUV gratings that allow detection of wavelengths in the range of 80 nm - 4 nm and a soft X-ray CCD camera that can detect photons in a very broad range of energies (10 eV to 5 keV). The new laser system and experimental vacuum chambers, are located at Swinburne University of Technology (Hawthorn campus). On 27 November 2007 the Victorian Minister for Innovation Minister Gavin Jennings opened this Femtosecond High Power Laser Facility with approximately 60 people in attendance, including visitors from overseas.



❖ *High Harmonic Vacuum Chamber.*

The Theory and Modelling Program (TMP) provides theoretical and computational support and leadership to the experimental programs within CXS, and particularly to EMP and SWLP. A goal of the TMP throughout 2007 has been the development of theoretical models for non-linear opticals that are applicable to complex molecular targets containing any element of the periodic table and to a wide range of electromagnetic field strengths and frequencies. These conditions include both the laboratory strength infra-red sources that are used in high-harmonic generation studies as well as the short wavelength X-ray free electron laser (XFEL) sources that will become available within the next few years. The second research theme has involved the ongoing development of novel techniques to obtain images from X-ray diffraction data.

### XFEL-Molecule Interactions

The availability of XFEL sources will bring with them new challenges and the likely occurrence of unexplored electronic phenomena. In the case of intense infra-red radiation sources, it has been observed that in almost all cases a single active valence electron, promoted into the continuum, precipitates a chain of events that leads to highly non-linear processes such as high-harmonic generation. In the case of an intense short wavelength source, the ponderomotive energy is unlikely to be sufficient to cause a similar chain of events unless the intensity of the source is many orders of magnitude greater than existing infrared laboratory sources.

However, unexpected inner shell excitation processes may occur due to strong field collisional excitation. These are likely to lead to core or inner valence ionization, and the consequent rearrangement of the electronic structure that will cause the breaking of bonds in any molecular target, and its inevitable explosion under the residual Coulomb forces of its ionic fragments. This will manifest itself as severe damage or disintegration in any target or optical component used in an XFEL imaging experiment, though the mechanisms that define these events are not well-described by the usual low-order perturbative approaches that are enshrined in existing molecular dynamics procedures. Moreover, these events will not be well-described by the one-electron mean-field models that have served so well in the description of, for example, high harmonic generation, in which a single active electron is almost the sole

participant; a many-electron description is required.

Theory and Modelling are pursuing a promising approach that assembles several existing strands of research. In our recent work, a particularly efficient and general scheme has been developed that enables us to construct a finite-dimensional representation of the electronic structure of complex molecules containing heavy elements, using an implementation of relativistic density functional theory.

As part of our work in HHG, we have developed several methods to propagate electronic structures in time when atoms or molecules are exposed to very strong time-dependent electromagnetic fields. It is natural to combine these two approaches to devise a scheme that provides a general, time-dependent, relativistic, many-body description of these strongly interacting systems. There has been considerable recent activity in the field of time-dependent density functional approaches, but the so called "real time" propagation approach is the most appealing. This approach propagates only the one-particle electron density matrix by explicit solution of the Liouville equations of motion, rather than the complex amplitudes of quantum mechanical wavefunctions, which are further complicated in a relativistic formalism by the Dirac spinor structure. While this is a computationally intensive approach, it is simple to implement, utilises many of our existing computational resources, and is physically transparent in its interpretation.

## Algorithms for Coherent Diffractive Imaging

In the field of diffractive imaging, a particularly appealing direction for development is the generalisation of the Maximum Entropy Method for the reconstruction of arbitrary object of finite extent, rather than rely on the assumption of a real electron density or of a binary diffracting object. The power of the MEM, already demonstrated in the development of methods to characterise the power spectrum of HHG sources, is that the scheme less frequently encounters the troublesome stagnation problems that continue to plague other iterative methods that are based on the many variants of the Gerchberg-Saxton-Fienup prescription. If we could develop a robust MEM based scheme that was applicable directly to arbitrary complex scattering objects it would represent a great advance in the field of diffractive imaging.

Using a variant of existing MEM resources, Rouben Dilanian has developed a scheme to analyse diffraction obtained using the first-generation HHG source at Swinburne, taking into account its spectral structure, which is also deduced by an application of MEM methodology to a measurement of diffraction from a well-characterised Young's slit experiment. This unconventional approach has enabled TMP to recover images from the diffraction of simple objects, such as apertures. It is expected that further refinement will yield a robust imaging scheme that makes the fullest possible use of the output from a harmonically-restricted HHG source.

Also of continuing interest to the group is the role played by discontinuities in the phase on the performance of phase reconstruction algorithms. It was established by Fienup and his collaborators that stagnation in iterative reconstruction algorithms is accompanied

## Partially Coherent Fresnel Diffractive Imaging

Following our earlier work that investigated the role of partial coherence in conventional iterative reconstruction algorithms, phase retrieval algorithms we based our design on the coherent mode expansion theory of Wolf. In the new scheme, the mutual optical intensity at the exit surface is constructed as an eigenfunction expansion of the wavefield at the entrance surface of the object. The modal eigenfunctions are modified by the transmission function of

by the formation of phase vortices in the detector plane that do not coincide with the zeros of the measured intensity data. These zeros in the intensity and their local morphology are characteristic of the true zeros in the wavefield and of propagating phase vortices, and carry critical information about the finite support of the diffracting object. No existing phase recovery algorithm makes any use of this information, declaring that iterative stagnation is characteristic of a non-convex optimisation problem. While this diagnosis is correct, the only remedies offered to date are only partially successful, at best, and rely on empirical relaxation parameters that appear in, for example the Hybrid-Input Output algorithm of Fienup or its elaboration, the Difference Map of Elser. A treatment that identifies the distribution of vortices in the propagated wavefield with the measured distribution of zeros in the intensity offers a new direction which we will pursue in the coming year.

A wholly satisfactory general solution to the diffractive imaging problem using a single set of intensity data and support constraint information alone remains elusive. A step in this direction has, however, recently been accepted for publication in which it is shown that a solution of the Transport of Intensity Equation may be obtained solely from a knowledge of intensity distribution and the experimental geometry. The approach is based on the use of a known functional relationship existing between the intensity distribution of the illuminating beam and its paraxial derivative in the detector plan, as well as a knowledge of the finite support of the diffracting object. In that regard, it bears some resemblance to the formulation of the Hohenberg-Kohn Theorems of density functional theory in quantum many-body theory, which served as the model from which we devised the scheme.

the object and propagated independently to the detector; the modal eigenvalues correspond to occupancy numbers. An iterative scheme has been devised in which the measured intensity data are used to update the modal amplitudes, which are back-propagated to the exit surface, and constrained to satisfy the support constraints. The use of modal expansions in refining Fresnel diffractive imaging analysis is currently under investigation as a PhD project within EMP and is reported elsewhere as part of their program.

## Source Coherence Studies

The coherent mode expansion that was implemented to reconstruct images in the presence of well-characterised partially coherent sources was extended to serve as a tool to characterise the partially-coherent character of X-ray sources using well-controlled experimental data obtained from pin-hole diffraction. This approach is currently under development as a PhD project within EMP and is reported elsewhere as part of their program.

## Relativistic Molecular Quantum Electrodynamics

Work continued on the development of relativistic methods for electronic structure problems based on conventional many-body theory and on relativistic current-density functional theory. This work involves a long-term collaboration with a leading molecular science group based in Perugia, Italy. It is leading towards the development of methods for relativistic molecular quantum electrodynamics. A major development in 2007 has been the implementation of a particularly efficient scheme to represent molecular charge-current densities in complex molecules containing heavy elements. This is based on a density fitting scheme that is transformed by the use of the Poisson equation into a representation that involves simple overlap integrals rather than more computationally expensive quantities that evaluate electrodynamic contributions directly. The representation of these charge-current densities has recently been extended to include contributions in the high orbital angular momentum limit,  $l > 3$ .

## High-harmonic Generation

Theory and modelling assigned a large part of its 2007 activities to the support of the experimental high-harmonic generation project at Swinburne. This involved the development of theoretical methods to describe the time-dependent dynamics of atomic and molecular systems in strong laser fields, and the design and control of experimental conditions required to affect quasi-phase matching. These methods involved the direct numerical time-dependent propagation of molecular wavefunctions under the influence of strong external laser fields.

Some preliminary work was performed on recovering images from diffraction data obtained from the Swinburne Light Source, which is described elsewhere, in the program report by SWLP. Our goal is to provide detailed quantum dynamical models of complex biological molecules in laboratory laser sources and, ultimately, in the fields generated by X-ray free-electron lasers.

## Time-resolved Fourier Transform Spectroscopy

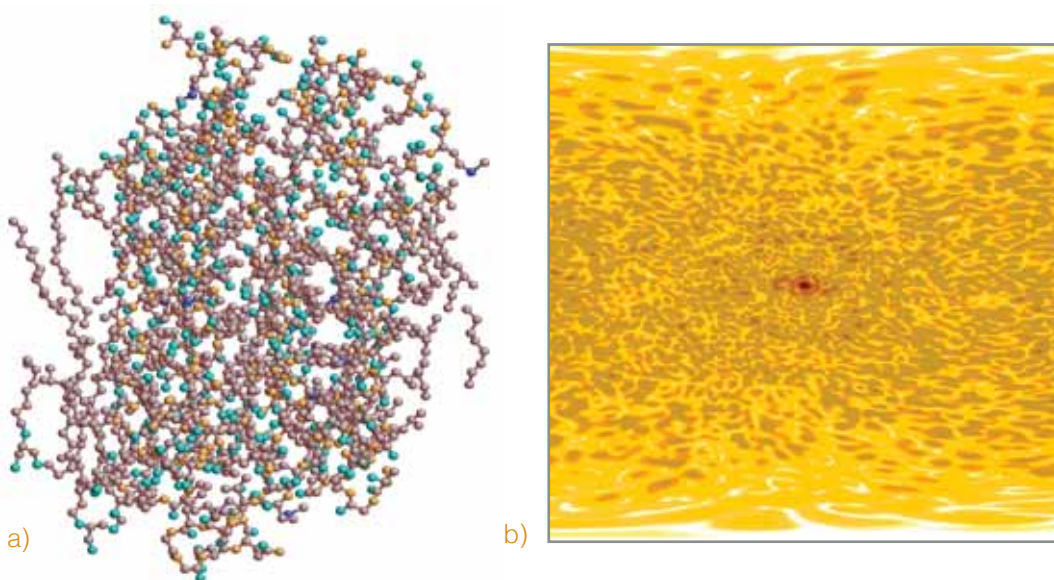
Time resolved polarisation spectroscopy reveals the electrodynamic phenomena in the biological molecules involved in photosynthesis. In a fusion between the imaging and electrodynamic branches of our research programme, a non-interferometric form of Fourier transform spectroscopy was developed in collaboration with Swinburne. This enabled the determination of the complete complex molecular polarisability solely from intensity measurements of the molecular emission and temporal constraints on the incident pulse sequences. The availability of this approach potentially opens a new window on our understanding of energy capture and energy transfer in the antenna molecules that play an important role in photosynthesis, since these experiments provide a direct and detailed probe of the electrodynamic of, for example, carotenoids. A publication describing both the theory and simulation of this non-interferometric form of Fourier Transform Spectroscopy been accepted for publication in *Physical Review Letters*.

## Structure Determination Methods Program

### Mathematical Methods and software for the analysis of powder diffraction from 2-D crystals of Integral Membrane Proteins

Development has begun of novel experimental and related theoretical methods for the preparation and analysis of powder samples and related X-ray diffraction data for Integral Membrane Proteins. These techniques include preparation of and data collection from various 2-D crystal powders, a little explored line of approach. They offer the exciting possibility of providing alternative and easier paths to the X-ray structure determination of this very important class of proteins that have mostly resisted the efforts of conventional 3-D single-crystal methods of structure determination.

On the CMHT side, work has progressed on the preparation of a number of different types of powder samples of integral membrane proteins, including 2-D oriented and randomly oriented samples.



- ❖ *Bacteriorhodopsin molecule (a) in real space, shown here as a ball and stick model, and (b) in diffraction space, as seen in the far field under illumination by a hypothetical high-energy X-ray source. Detailed diffraction space maps such as this one are available in practice only by combining X-ray diffraction data from a very large number of molecules arranged in highly ordered structures in two- or three-dimensional protein crystals.*

## Theoretical Models and Computational Methods

CMSE has focused the bulk of its research effort on the development of a detailed and computationally tractable theoretical model of the scattering process in order to understand how biological systems investigated respond to synchrotron radiation under experimental conditions. The level of detail included is down to atomic level, and the model is based on novel applications of a well established atomic scattering theory.

Systems considered include 2-D nano- and micro-arrays (2-D crystals) of large molecules, i.e., typical integral membrane proteins containing several thousand atoms or more, as well as random or partially ordered assemblies of such arrays. The latter types of systems are used to describe the interaction between synchrotron X-rays and various types of 2-D crystal powders.

The physical description of the scattering process forms the basis for the analysis of X-ray diffraction data from single 2-D crystals and powders. The analysis utilises a parameterised physical model that describes the X-ray scattering from the biological sample under a range of different experimental conditions (X-ray wavelengths, scattering angles, sample and detector orientations).

The physical model is used to predict theoretical diffraction patterns, while the model parameters serve as fitting parameters to relate theory back to experiment by using standard non-linear least squares techniques. The fitting parameters provide direct insight into the structure of the biological systems under study. This is the key advantage of the physical modelling based approach to data analysis being developed in this program, over empirical-based data fitting that has been used to analyse similar data elsewhere.

The necessary software tools are being developed with the aim of achieving efficiency without compromising accuracy. To accomplish this aim a range of custom tailored techniques are being used including: i) adaptive sampling of diffraction space, ii) the use of an efficient transformation between Cartesian and polar coordinate systems as appropriate for sampling and numerical integration, and iii) the explicit inclusion of the semi-discrete nature of 2-D crystal diffraction patterns in both the theoretical model and in the computational code.

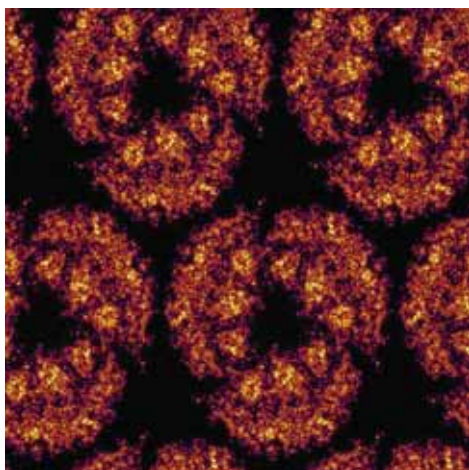
These methods are now being implemented on actual data obtained both at the Advanced Photon Source (ChemMatCARS) and the Australian Synchrotron.

### Current challenges in the program are as follows:

- To extract high quality 2-D and 3-D structure factors from powder diffraction data recorded for Integral Membrane Proteins.
- To improve the model used, so as to extract as much information as possible from the data, including information on the 3rd dimension in the case of 2-D crystal samples.
- To optimise signal-to-noise in the 2-D-crystal powder diffraction experiments.
- To develop essentially *ab initio* methods for phasing 2-D-crystal powder data (i.e. methods not depending on electron microscopy data).
- To develop improved methods of sample preparation of IMPs suitable for high quality structure determination from powder diffraction experiments.

### Some targets for future activity are:

- Development of a proposal for a low X-ray energy beamline or station at the Australian Synchrotron especially suited to diffraction from 2-D crystals of IMPs, both single crystals and powders. The design of this beamline should be able to exploit anomalous scattering from sulfur and phosphorus.
- Development and implementation of Bayesian and MaxEnt methods for analysis of 2-D crystal data.
- Consideration of opportunities that will be afforded 2-D and 3-D powder diffraction by intermediate energy XFELs.

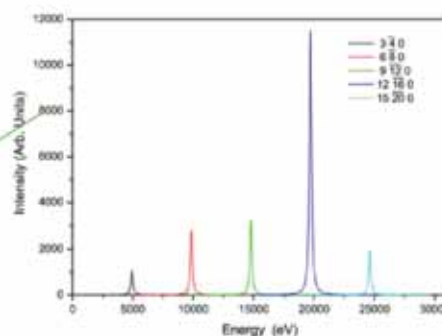
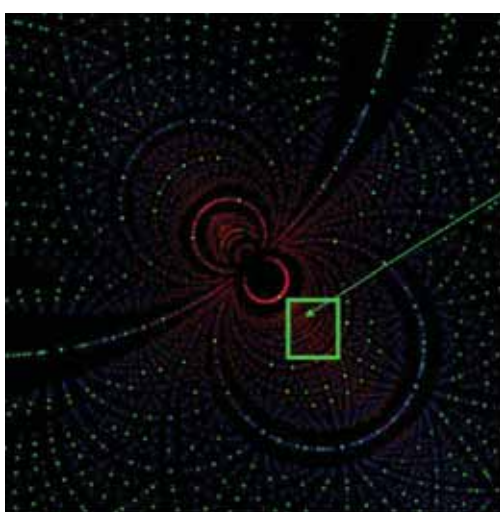


- *Theoretical atomic resolution electron density projection map for bacteriorhodopsin molecules in a two-dimensional hexagonal crystal.*

### Improved Methods for Micro-diffraction Studies on Proteins

Laue photographs represent the oldest X-ray diffraction technique for the characterisation of crystalline materials. In recent years there has been resurgence in the use of the technique for a variety of reasons, including the advent of synchrotron sources, the desire to perform structural studies of dynamic systems and processes in real-time, advances in detector technology, and so on. The CSIRO team have been actively developing the technique in the laboratory and at overseas synchrotron facilities for the purposes of studying, for example, polycrystalline light-metal alloy systems, via microdiffraction. The laboratory-based system utilises a microfocus X-ray source, with a single capillary optic to focus the beam to a spot of a few microns on the sample.

The detector group at CMSE has recently made some exciting developments in the area of energy-sensitive X-ray area detectors and with such technology considerably more information can be extracted from Laue data. Of particular interest are the possibilities for improving protein-structure determination methodology. CMSE have been developing in-house software for the simulation and analysis of Laue patterns, including the possible use of quite general (non-conventional) experimental geometries, investigation of multiple spots. The figure below shows an example of a Laue simulation for a typical protein structure, with spots binned according to 3 ranges of X-ray energy, together with an analysis of the energy contributions to one particular multiple spot. This approach opens up new possibilities for diffraction data collection on 2-D and 3-D protein nanocrystals.



X-ray energies  
 5 → 8keV  
 8 → 14keV  
 14 → 30keV

- *Laue simulation of a typical protein (HEWL lysozyme) structure, with diffraction spots binned according to energy and an analysis of a “multiple-energy” spot.*

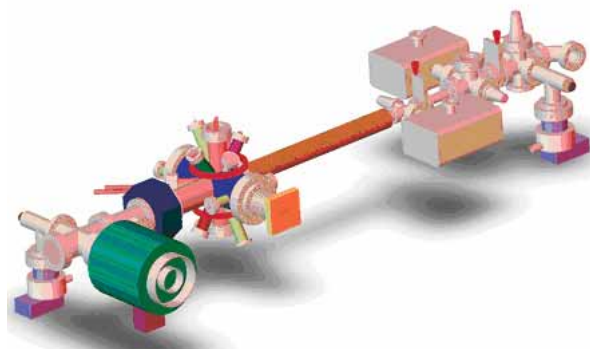
## Ultra-Cold Plasma Source Program

**Many forms of X-ray production**, from dentistry to synchrotrons, depend on bright sources of electrons. Electrons are also inherently useful for imaging directly, as in electron microscopes. Conventional electron sources have limited brightness – we cannot focus intense beams to very small dimensions because electrons repel each other. The Ultra Cold Plasma Source Program is developing an entirely new source of electrons, in collaboration with leading groups in the Netherlands and Germany, to enable ultrafast, single-shot, diffractive imaging of biologically relevant molecules.

The source begins with atoms laser-cooled to micro-Kelvin temperatures. The cold atoms will then be photoionised, to create an ultra-cold plasma (UCP). A UCP has a very large electron charge in a very small volume at a very low temperature. In combination, these provide much higher brightness than is possible with conventional pulsed electron sources, sufficient to enable diffractive determination of structures down to 10nm, the typical size of a protein molecule.

### Novel Ultra-Cold-Plasma Accelerator

**High-flux atom source:** We are building a second-generation UCP system, starting with an innovative cold atom source. Hot rubidium atoms are slowed to cm/s using a novel single-layer tapered coil Zeeman slower which will produce very large samples of cold atoms in a very short time (10<sup>10</sup> atoms per second), while maintaining a very long lifetime of the rubidium charge and very low vacuum pressure in the main chamber.



❖ *Engineering drawing of second-generation ultracold plasma electron source. Rubidium atoms will be Zeeman-slowed and projected into the central chamber where they will be cooled and trapped in a quasi-mirror MOT. The cold atoms will be photoionised, and electrons extracted using conventional electrostatic, electromagnetic and radio-frequency charged particle optics.*

**Mirror-Mot accelerator:** The central ultra-high vacuum chamber contains the electrostatic electron accelerator, numerous feed-throughs and vacuum windows to allow access for the laser beams which cool and trap the atoms, the photoionisation laser beam, imaging access, and high-voltage supplies for the accelerator and charged particle (electron and ion) detectors.

The atom trap is a new variation of a mirror-MOT design. Four laser beams in two parallel pairs are incident on a mirror inside the vacuum system. The pairs are displaced so that they intersect a significant distance from the in-vacuum mirror, where they also intersect with the remaining two laser beams of the MOT. The mirror is conductive, to form one plate of an electrostatic accelerator. The second plate will be ITO (indium tin oxide) coated transparent glass, to allow the beams through to the trap centre. A third electrode will accelerate the electrons to high energy (e.g. 1 to 10kV) for applications.

## Electron Generation

The electron generating sequence will proceed as follows:

1. Load MOT from source (108 atoms, < 1 second). Density  $\sim 10^{10}$  to  $10^{12}$   $\text{cm}^{-3}$ .
2. Optional: Compress MOT, further cooling, to reduce source size (few milliseconds).
3. Extinguish MOT beams and MOT coils.
4. Excite atoms to 5P state using 780nm laser, spatially profiled using an SLM.
5. 480nm photoionisation pulse, pulse energy tens of  $\mu\text{J}$ .
6. Apply low field and extract electrons into static high-field second-stage accelerator.
7. Detect with microchannel plate (MCP) + phosphor + CCD camera.
8. Replenish MOT and repeat.

For pulse energies of 10 – 100 $\mu\text{J}$ , the ionisation will typically only ionise  $\sim 1\%$  of the atoms, allowing rapidly eject a series of diminishing pulses. Alternately, continual loading, with only a very short off-time while the MOT coils are damped (< 1ms), will allow a higher repetition rate. Higher 480nm pulse energies have shown to increase the ionisation fraction to 90% for producing very large electron bunches.

### Ionisation and Rydberg Atoms

The “ionisation” of the cold atom cloud is not necessarily a simple process as implied above. For near-threshold ionisation, desirable to obtain low electron temperatures, there is substantial excitation of atoms to high-lying Rydberg states through, for example, electron collision and recombination. Those atoms can then self-ionise through long-range dipole interactions. Indeed, intentionally exciting the cloud to Rydberg states may be preferable in terms of the electron temperature.

Disorder-induced heating (also called correlation heating) arises from random spacing between the cold atoms. Immediately after photoionisation, the ultracold plasma is not in thermal equilibrium. The ions and electrons have very little kinetic energy, but the ion-ion and electron-electron distances are random. Coulomb repulsion tends to

distribute the particles far from each other. Some separation distances are shorter than average and thus there is initially an excess of potential energy, which is converted into kinetic energy, giving rise to heating. The temperature can increase by two or three orders of magnitude in a fraction of a microsecond and this could be the major limitation on achieving sub-Kelvin electron temperatures. A potential solution would be to trap the atoms into an optical lattice prior to ionisation to control the interatomic spacings.

Understanding these excitation and heating processes will be an important part of optimising the beam characteristics. Our collaborators in Freiburg, led by Professor Weidemüller, are at the forefront of frozen Rydberg gas dynamics and will play an important role in these aspects of the research.



David Sheludko, Ultra Cold Plasma Source Program.

## Source Emittance, Coherence and Brightness Characterisation

Commonly-used parameters to define the source are the reduced emittance, brightness, and angular intensity, and for dynamic processes, the pulse duration. The reduced emittance is the phase space occupied by the beam, the reduced angular intensity is the current per unit angle, and the reduced brightness provides a useful measure of how much you can focus current into a spot. Simply speaking, you can increase the brightness by producing more electrons from a smaller area with a smaller divergence. These can be measured with a current detector and a scanning aperture, or with a “pepperpot” method, in which an image of the electrons is acquired after they pass through an array of small apertures.

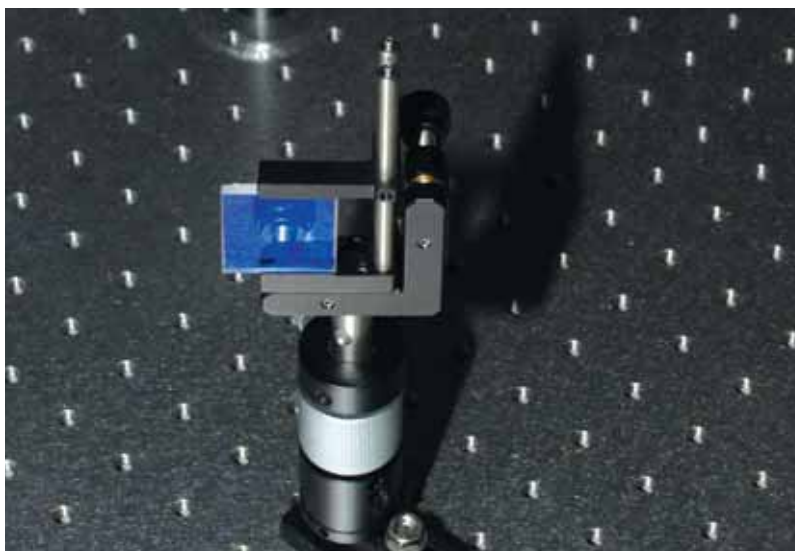
We have used a propagation-based method for measuring phase curvature in neutral atom and optical beams. The concept has been applied to electron microscopy by CXS Director Keith Nugent and colleagues at the University of Melbourne, and a more complete phase-space tomography approach to measure the spatial coherence of a synchrotron X-ray beam, which will be applied for the UCP source. The method provides more information without requiring the placement of an aperture in the beam.

## High Resolution and Ultrafast Pulses: Space-Charge Repulsion and Bunch Shaping

Space-charge expansion of electron bunches cannot be avoided but is irrelevant if we can re-compress the bunch. That is possible if the bunch is initially ellipsoidal, with a uniform charge density inside. The initial charge

distribution is defined by the combination of the excited-state atom distribution, which can be controlled with the excitation laser profile, and by the photoionisation laser profile. Pulses can be “pancake” shaped for very short pulses, or “cigar” shaped for very high spatial resolution. Our Eindhoven collaborators have recently described how the bunches can be re-compressed using RF cavities and focussed with DC solenoids. A spatial light modulator (SLM) will control the excitation laser profile to modulate the phase and/or amplitude of the beam. A Gaussian profile laser beam can be deflected from the SLM, and with appropriate settings of the phase retardance at every pixel, will propagate and diffract into, say, a parabolic profile. Intersecting with a Gaussian distribution atom cloud, will produce a half-circle density profile of excited atoms to first approximation. A slice of atoms can then be ionised with a pulse from the 480nm laser propagating orthogonally to the excitation laser, cylindrically focused into a sheet of light at the atom cloud. Only atoms within the intersection volume of the two lasers will be ionised, for three-dimensional electron-bunch shaping.

We have developed optical diffraction code for determining the SLM pattern needed to obtain a desired light-field. In general, the forward problem is easy to solve, given the phase shift from the SLM, i.e. it is straightforward to calculate the diffracted field intensity pattern. We use an iterative technique, comparing the diffracted field to the desired field, to calculate a modification to the SLM pattern, cycling until convergence. With two SLMs the phase and amplitude can both be controlled to achieve maximum efficiency and resolution.



Detail of an experimental system used in CXS research.



*CXS Annual Workshop 2007 – Physicists and Biologists Working Together.*

# KEY PERFORMANCE INDICATORS

## Awards and Honours

We congratulate the following CXS members on the recognition of their achievements during 2007.

- Professor Keith Nugent was awarded his second Australian Research Council Federation Fellowship.
- Lahiru Gandoda and Rebecca McEwan were awarded the CXS Protein Structure Analysis Prize 2007.
- Gregory Barbante was awarded first prize in the Student Research Poster Awards at the Aurora Symposium.
- Claudia Leidhold was awarded a Deutscher Akademischer Dienst German Academic Exchange Service (DAAD) Fellowship 2007.
- Michael Baker and Laura Osellame were awarded a Poster prizes at the Melbourne Protein Group Meeting, 2007.
- Corey Putkunz was awarded the Rio Tinto OTX cash prize and the AXAA Bursary for Best Presentation in Bundoora, September 2007.



• Professor Leann Tilley presents the Student Research Poster Award to Gregory Barbante at the Aurora Symposium 2007.

## Scholarships and Studentships

We would like to congratulate the following students for their successful applications in 2007:

- Ms Cherrine Chan, CXS Summer Cadetship– Biological Science Program, La Trobe University.
- Mr Tom Payten, CXS Summer Cadetship– Experimental Methods Program, La Trobe University.
- Mr Niels Zijlstra, University of Twente, Netherlands – Intern student with the Short Wavelength Laser Source Program, University of Melbourne.
- Mr Simon Bell, six month studentship at the University of Eindhoven, Netherlands.

## Research Training and Professional Education

The Centre met all of its recruitment and Professional Education targets for 2007, and exceeded expectations in the areas of Postgraduate Recruitment and Presentations to Schools and/or Teaching Communities. An increase in CXS member awareness was also a focus in 2007 with a number of media sources being utilised to educate members.

- The *Media in Focus* series of articles appeared in the CXS newsletter *In Coherence*, educating members on dealing with the media, appearing on radio or television and what to do when dissatisfied with the outcome of an interview.
- *IP@ CXS – Knowing it when you see it* – this seminar was held at the University of Melbourne on 23rd July, 2007, coordinated by Tania Smith.
- International participants in the *2nd CXS Annual Workshop* participated in a tour of the Australian Synchrotron facility.
- *CXS Commercialisation Workshop*, concentrated on the protection and exploitation of commercially valuable IP, August.
- *CXS IP Show and Tell Forum*, program teams presented their IP ideas to the CXS IP Committee, October.

### Target Breakdown

Postgraduates recruited	7
Postgraduate completions	7
Honours students	5
Professional courses	2
Presentations to schools or teaching community	7
Overseas visits by CXS members	25

## Workshops Conducted by CXS

### CXS conducted the following interdisciplinary workshops in 2007:

- *CXS Biophysics Seminar*, University of Melbourne, hosted by CXS and the School of Physics, February.
- *Synchrotron Seminar Series*, University of Melbourne 's School of Physics, March – June.
- *Imaging and Spectroscopy of Biological Materials Workshop*, hosted by the Short Wavelength Laser Source Program, Swinburne University of Technology, March.
- *The 2nd Annual CXS Workshop: Facilitating X-ray Biophotonics – Physicists and Biologists Working Together*, University of Melbourne, Bio21, April.
- *International Consortium of Coherent X-ray Diffractive Imaging (I<CCXD>I) Meeting*, Australian Synchrotron, April.
- *Scattering, Structure and Dynamics in Electronic Systems Workshop*, University of Melbourne, May.
- *Grazing Incidence X-ray Techniques for 2-D Crystal Workshop*, University of Melbourne, July.
- *IP@ CXS Workshop*, University of Melbourne, July.
- *CXS Commercialisation Workshop*, University of Melbourne, August
- *Synchrotron Seminar Series*, La Trobe University, February – September
- *CXS IP Show and Tell Forum*, October.
- *Imaging Workshop and Fluorescence Microscopy Facility Opening*, La Trobe University, October.
- *2nd Advanced Optical Imaging Workshop*, University of Melbourne, November.
- *ARC COE Members at University of Melbourne Group Meetings*, monthly.



❖ CXS Annual Overview 2007 poster viewing.

## Visitors to CXS

1. **Dr Julian Adams**, Australian Synchrotron
2. **Dr Anton Barty**, Lawrence Livermore National Laboratory, USA
3. **Dr Andrew Boston**, Liverpool University, UK
4. **Mr. Frederic Bouly**, Ecole Nationale Supérieure de Physique, Grenoble, France
5. **Professor Igor Bray**, ARC Centre of Excellence for Antimatter-Matter Studies
6. **Dr John Burns**, University of Hawaii, Manoa, USA
7. **Dr Angnieszka Chacinska**, University of Freiburg, Germany
8. **Professor Peter Colman**, Walter & Eliza Hall Institute
9. **Dr Katherine de Villiers**, Department of Chemistry, University of Cape Town, SA
10. **Professor Yadin Dudai**, Weizmann Institute, Israel
11. **Professor Peter Dyson**, Acting Deputy Vice Chancellor (Research), La Trobe University
12. **Prof David Ferguson**, Nuffield Department of Pathology, University of Oxford, UK
13. **Dr Michael Feser**, Xradia Ltd, California, USA
14. **Professor Andrew Flitman**, Pro-Vice Chancellor of Swinburne University of Technology
15. **Dr Dmitry Fursa**, ARC Centre of Excellence for Antimatter-Matter Studies
16. **Dr Enrico Gratton**, Laboratory of Fluorescence Dynamics, UC Irvine, USA
17. **Dr Jacqui Gulbis**, Walter & Eliza Hall Institute
18. **Associate Professor Ben Hankamer**, University of Queensland
19. **Professor Janos Hajdu**, Uppsala University, Sweden
20. **Ms Silvia Haase**, Bernhard Nocht Institute for Tropical Medicine, Hamburg, Germany
21. **Ms Stephanie Hoppe**, student from Marburg University, Germany
22. **Professor Daren Huang**, Sun Yat-Sen University, People's Republic of China
23. **Professor Ikeda**, Aerospace Exploration Agency, Japan
24. **Professor Tetsuya Ishikawa**, RIKEN Spring-8 Center, Japan
25. **Dr Ken Jacobsen**, University of California, USA
26. **Dr David Jameson**, Swinburne University of Technology
27. **The Hon. Mr Gavin Jennings**, Victorian Minister for Innovation
28. **Dr Alisher Kadyrov**, ARC Centre of Excellence for Antimatter-Matter Studies
29. **Dr Burkhard Kaulich**, ELETTRA, Italy
30. **Dr Anatoli Kheifets**, ARC Centre of Excellence for Antimatter-Matter Studies
31. **Associate Professor Andrzej Krol**, State University of New York, USA
32. **Professor Carolyn Larabell**, University of California, USA
33. **Mrs. Kris Laurie**, The Office of the Nobel Laureates, Australia
34. **Ms Claudia Leidhold**, Freiburg, Germany
35. **Dr Andrey Lugovskoy**, ARC Centre of Excellence for Antimatter-Matter Studies
36. **Dr Brad Marsh**, University of Queensland
37. **Professor Barry Marshall**, The Office of the Nobel Laureates, Australia
38. **Dr Ian McNulty**, Argonne National Laboratory, USA
39. **Dr Ralf Menk**, ELETTRA, Italy
40. **Professor Oscar Moze**, Università di Modena, Italy
41. **Dr Fujio Nakano**, Advanced Mision Research Centre, Aerospace Exploration Agency, Japan
42. **Mr. George Pappas**, Chair of Management Advisory Board, Monash Institute of Medical Research
43. **Professor Michael Parker**, St Vincent's Institute of Medical Research
44. **Senator The Hon. Kay Patterson**, Senator for Victoria
45. **Professor Krithi Ramamritham**, Indian Institute of Technology, Bombay, India
46. **Associate Professor Vassilios Sarafis**, University of Queensland
47. **Dr Qun Shen**, Argonne National Laboratory, USA
48. **Professor Andris Stelbovics**, ARC Centre of Excellence for Antimatter-Matter Studies
49. **Professor Takahasi**, Aerospace Exploration Agency, Japan
50. **Professor Peter Thorsness**, Wyoming State University, USA
51. **Dr John Tisch**, Imperial College, USA
52. **Dr Ivan Vartaniants**, HASYLAB at DESY, Germany
53. **Dr Russell Walker**, Department of Innovation, Industry and Regional Development
54. **Dr Nils Wiedermann**, Freiburg, Germany
55. **Professor Ziya Wu**, Director, Beijing Synchrotron Radiation Facility, China
56. **Mr Xiao Yaqing**, Chalco Aluminum Cooperation of China, People's Republic of China

[06]

CXS MANAGEMENT AND GOVERNANCE



# CXS MANAGEMENT AND GOVERNANCE

**CXS is a collaborative research program** between the University of Melbourne, La Trobe University, Monash University, Swinburne University of Technology and CSIRO, funded under the Australian Research Council (ARC) Centre of Excellence program and the Victorian Government Science, Technology and Innovation program (STI).

As the lead administrative institution, the University of Melbourne manages the grants and distributes funds in accordance with the signed funding agreements. These agreements cover CXS management, collaborator and intellectual property arrangements.

All collaborating organisations are embedded in CXS boards. Commercial expertise is represented on the CXS Intellectual Property Committee and Sub Committee. A Scientific Advisory Board and a General Advisory Board have been established and meet annually. The CXS Annual Report was published for 2006.

## Centre Management

The CXS Management team is responsible for the following areas as they pertain to the centre policy, performance, financial matters, research output, research training and professional education of members, partnerships, national and international liaison, commercialisation and outreach.

**The management team is:**



**Professor Keith Nugent**  
Director of Research



**Professor Leann Tilley**  
Deputy Director of Research



**Ms Tania Smith**  
Chief Operating Officer

## Executive Committee

During 2007, CXS administration was overseen by the Executive Committee comprising the following members:

- Professor Keith Nugent, Research Director
- Professor Leann Tilley, Deputy Research Director
- Ms Tania Smith, Chief Operating Officer
- Associate Professor Mike Ryan, Biological Sciences Group Leader
- Dr Chris Hall, Detector and Beamline Development Group Member
- Associate Professor Andrew Peele, Experimental Methods Group Leader
- Professor Lap Van Dao, Short Wavelength Laser Source Group Leader
- Associate Professor Trevor Smith, Short Wavelength Laser Source Group Member
- Dr Steve Wilkins, Structure Determination Methods Group Leader
- Dr Jose Varghese, Structure Determination Methods Group Member
- Dr Harry Quiney, Theory and Modelling Group Leader
- Ms Rosslyn Ball, Executive Officer to Committee
- Ms Emma Douglas, Administrative Officer

## Advisory Board

The CXS Advisory Board met in April 2007 as part of the 2nd Annual CXS Workshop – *Physicists and Biologists Working Together*. The meeting focused on key areas such as papers and articles, patent possibilities, linkages, the ARC review, management and outreach.



**Professor John McKenzie (Chair)**  
Deputy Vice Chancellor (Research), University of Melbourne



**Dr Stephen Lane**  
Chief Science Officer, NSF Centre for Biophotonic, Science & Technology UC Davis



**Professor Andrew Flitman**  
Pro Vice-Chancellor (Research), Swinburne University of Technology



**Dr Michael Barber**  
Executive Director, Science Planning CSIRO



**Professor Edwina Cornish**  
Deputy Vice Chancellor (Research), Monash University



**Mr David Krenus**  
CEO, Cyclotek



**Professor Bonnie Wallace**  
Professor of Crystallography, Birkbeck College



**Professor Erich Weigold**  
Deputy Vice Chancellor (Research), La Trobe University



**Dr Bruce Whan**  
Chairman of INNOVIC (Victorian Innovation Centre Ltd) & Director, Swinburne Knowledge



**Professor John Helliwell**  
Professor of Structural Chemistry, University of Manchester

### The Scientific Advisory Board members are:

- Dr Stephen Lane
- Professor John Helliwell
- Professor Keith Nugent
- Professor Leann Tilley
- Professor Bonnie Wallace

## Professional Staff



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## Research Teams

### Biological Sciences Program



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## Detector and Beamline Development Program



**Professor Rob Lewis**  
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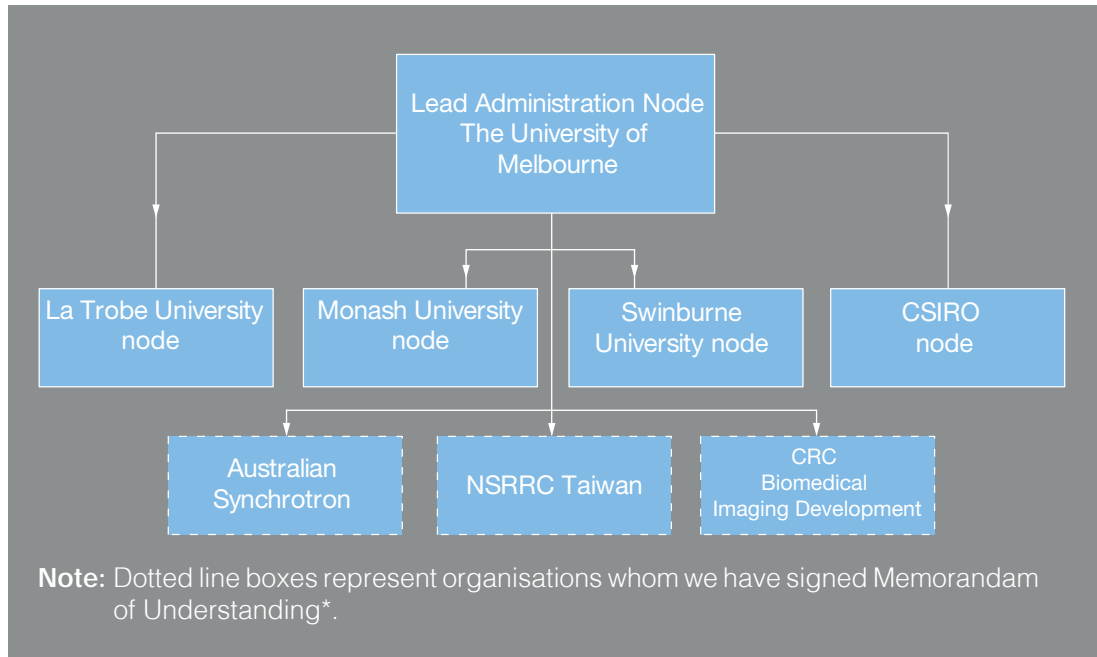
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## Member Departures

The following members farewelled CXS in 2007:

- Ms Imogen Colton – Ultra Cold Plasma Source Program, University of Melbourne
- Chandni Dosh – Experimental Methods Program, La Trobe University
- Dr Linda Feketeova – Detector and Beamline Development Program, Monash University
- Mr Pawan Kashyap – Experimental Methods Program, University of Melbourne
- Dr Danielle Smith – Biological Sciences Program, La Trobe University
- Mr David Stroud – Biological Sciences Program, La Trobe University
- Ms Emma Douglas – Administrative Officer, La Trobe University

# ORGANISATIONAL CHART



\* As at June 2007

## SCIENTIFIC LINKAGES

CXS is pleased to announce **Memorandum of Understanding** with the Australian Synchrotron and National Synchrotron Radiation Research Center of Taiwan.

A number of ongoing collaborations were also developed with the following groups:

- Centre for High Performance Computing, Perugia Italy (developing the Theory and Modelling Program's earlier work on relativistic heavy element chemistry, magnetic effects in molecules, and molecular quantum electrodynamics).
- Dr Clemens Schultz of the Swiss Light Source (investigating radiation damage in crystals).
- Blakett Laboratory, Imperial College London (investigating relativistic methods in electron scattering).
- Tohoku University of Japan (investigating X-ray generation from thin liquid films).
- ARC Centre of Excellence for Antimatter-Matter Studies (CAMS) from Curtin University of Technology (to work on non-linear atomic processes).
- ARC Centre of Excellence for Quantum Computing Technology and the Theory (developing computational tools for designing configurations of phosphorus donors in silicon).
- The Theoretical Condensed Matter program in the School of Physics at the University of Melbourne (developing methods of imaging inverse problems).

Also, CXS is leading discussions with other interested parties to form a Beamline Advisory Panel for the development of the branch line at the soft X-ray beamline at the Australian Synchrotron.

**Photo courtesy of David Cohen.**



❖ *Internal view of the Australian Synchrotron.*

# PRESENTATIONS

## Dr Benedicta Arhatari

Tomography Workshop,  
**Canberra, December 2007.**

## Dr Jacqueline Gulbis

Gordon Research Conference on Protein  
Transport across Cell Membranes- II  
Ciocco, **Italy, May 2007.**

## Dr Chris Hall

SmartPET Collaboration Meeting, Monash  
University, **Melbourne, March 2007.**

3rd Italy-Australia Workshop on Imaging  
and Spectroscopy, **Melbourne,  
April 2007.**

Monash Institute for Medical Research,  
**Clayton, August 2007.**

Medical Applications of Synchrotron  
Radiation 2007, University of  
Saskatchewan, **Canada, August 2007.**

Engineering and Physical Sciences in  
Medicine 2007, **Fremantle,  
October 2007.**

## Dr Eric Hanssen

University of Montpellier, **France,  
July 2007.**

## Professor Rob Lewis

SmartPET Collaboration Meeting,  
**Monash University, March 2007.**

MCSS Detector Group Retreat,  
**Marysville, April 2007.**

The Perinatal Society of Australia &  
New Zealand 11th Annual Congress,  
**Melbourne, April 2007**

Bernard O'Brien Institute of Microsurgery,  
St Vincent's Hospital, **Melbourne,  
May 2007.**

## Professor Keith Nugent

Energy Recovery Linac Optics Workshop,  
Argonne National Laboratory, Chicago,  
**USA, March 2007.**

Properties and Applications of Random  
Electromagnetic Fields Workshop,  
Florida, **USA, March 2007.**

APS Users Meeting Workshop on  
Coherent X-ray Imaging, Chicago,  
**USA, March 2007.**

Lawrence Livermore National Laboratory,  
USA, Invited Speaker, **April 2007.**

Launch of Australian Synchrotron  
Decadal Plan, **Canberra, June 2007.**

Erice Summer School, Invited Speaker,  
Erice, **Italy, June 2007.**

ICMAT 2007, **Singapore,** Keynote  
Speaker, **July 2007.**

Classification Workshop at SLAC,  
Invited Speaker, San Francisco,  
**USA, September 2007.**

2nd Advanced Optical Imaging Workshop,  
Melbourne, **November 2007.**

2nd Asia-Oceania Forum for Synchrotron  
Radiation Research, NSRRC,  
**Taiwan, November 2007.**

## Associate Professor Andrew Peele

3rd Italian-Australian Workshop on  
Imaging and Spectroscopy,  
**Melbourne, April 2007.**

APS User' Meeting Coherence  
Workshop, USA, **May 2007.**

HARMST 2007, France, **June 2007.**

Soft X-ray Workshop, Australian  
Synchrotron, **Melbourne, July 2007.**

## Dr Mark Pfeifer

Université Paul Cezanne Seminar,  
France, **December 2007.**

ESRF Seminar, France, **December 2007.**

## Mr Corey Putkunz

AXAA/VEMAS Student Seminar,  
**September 2007.**

**Dr Harry Quiney**

Blackett Laboratory, Imperial College  
**London, February 2007.**

Coherence 2007, Asilomar, **USA,**  
**July 2007.**

**Associate Professor Mike Ryan**

Lorne Protein Structure and Function  
Conference, Chair of Young  
Investigations, **Lorne, February 2007.**

FASEB Summer Research Conference,  
Tuscon, **Arizona, August 2007.**

**Associate Professor Trevor Smith**

International Conference on  
Photochemistry, Cologne,  
**Germany, August 2007.**

**Professor Leann Tilley**

Lorne Protein Structure & Function  
Conference, **Lorne**, Victoria, Chair  
of Novel Imaging Technologies,  
**February 2007.**

FABLS Workshop, **Melbourne,**  
Chair of Fluorescence Techniques,  
**February 2007.**

MacFarlane Burnet Institute for  
Medical Research and Public Health,  
**Melbourne, July 2007.**

ComBio 2007, **Sydney,**  
**September 2007.**

Aurora Symposium,  
**Melbourne, September 2007.**

**Professor Lap Van Dao**

3rd Asian and Pacific Rim Symposium  
on Biophotonics and Biophotonics  
Downunder II, **Cairns, July 2007.**

**Dr Stephen Wilkins**

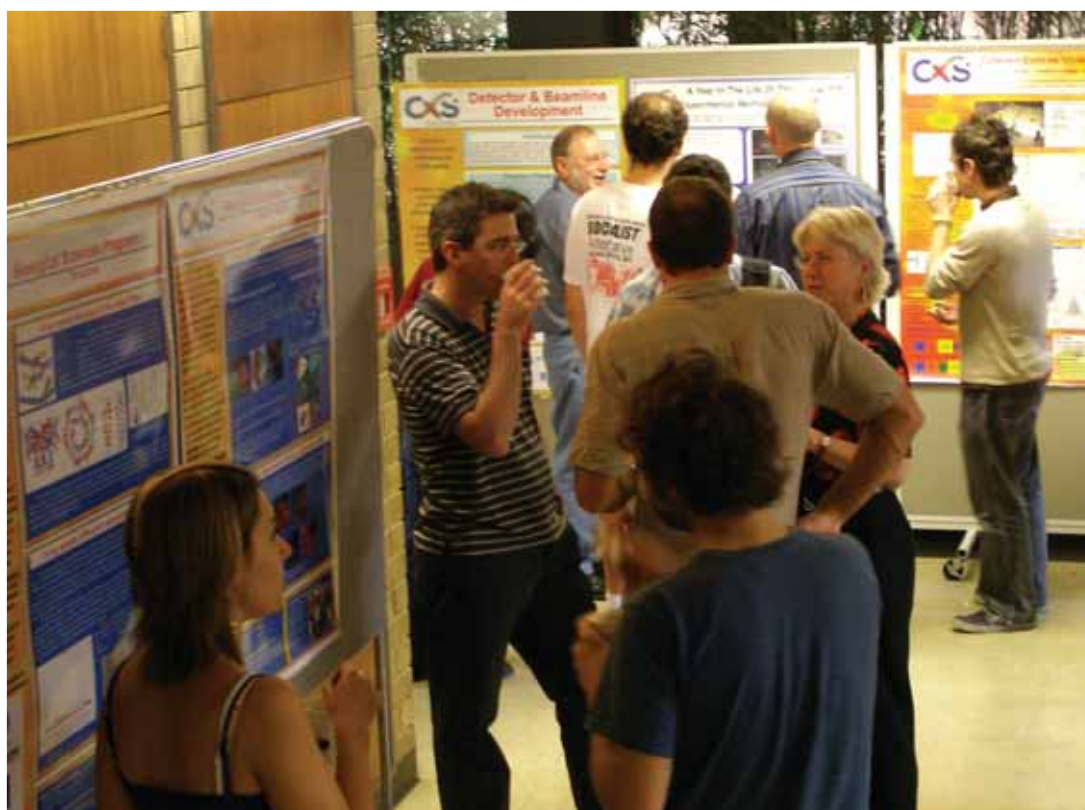
AIP Conference Proceedings 2007,  
Ritsumeikan University, **Japan,**  
**January 2007.**

Application of Synchrotron  
Radiation to Medical Clinical  
Diagnosis, Shanghai, **China, June 2007.**

**Dr Garth Williams**

Coherence 2007, Asilomar,  
**USA, July 2007.**

HASYLAB Seminar, Hamburg,  
**Germany, October 2007.**



## COMMERCIALISATION

**Professor Keith Nugent** continued to serve on the Board of Directors of Iatia Ltd. Using their globally patented QPI technology, Iatia has continued to expand into life sciences, nanotechnology, ophthalmology and defense markets, with customers including GE Healthcare, Columbia University, Oxford University, the Federal Bureau of Investigations (FBI) and the Australian Defence Force.

Associate Professor Robert Scholten and colleagues developed the MOGLabs range of external cavity diode laser (ECDL) controllers. Each MOG unit provides everything needed to run an ECDL and lock it to an

atomic transition. Marketing material has been produced and a targeting marketing strategy will be developed in 2008. All revenue derived from this activity will be the property of the University of Melbourne and one student inventor. There are no sales or license agreements to date.

A number of other activities were undertaken in 2007 to provide CXS members with training in the areas of intellectual property and commercialisation. The success of the Commercialisation Workshop and the IP Show and Tell Forum resulted in this activity becoming a yearly event.



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## OUTREACH

**In December 2007, the executive committee endorsed the CXS Outreach Program proposal, focusing on:**

- Lessons and Resources for Educators
- Professional Development for Educators
- Project Opportunities for Students
- Open Days and Expos
- Tours and Demonstrations
- Community Linkage Program
- Internship Opportunities
- A Lecture Series

As part of the program a number of factors were considered including trends in the arts, community and the Centre end-user links, which are required by the ARC.

Presentations to schools and media exposure have also added to the public's awareness of CXS. The following community outreach and work experience engagements were made with outside organisations in 2007:

- Professor Keith Nugent chaired the BHP Billiton Science Prize Selection Committee, Scienceworks Melbourne.
- Professor Keith Nugent is an ongoing member of the School of Chemistry & Physics Advisory Board, University of Adelaide.
- Professor Keith Nugent is a member of the Creative Victoria Roundtable, Melbourne.
- Professor Keith Nugent lectured at a Summer School on X-ray Imaging, Erice, Italy.
- Ella Bourne from Apollo Bay undertook work experience with the La Trobe University node.
- Visitor, Dr Agnieszka Chacinska, gave a seminar at La Trobe University on protein import and folding in the mitochondrial intermembrane space.
- Part sponsorship of the Melbourne Protein Group Symposium at the Institute for Advanced Study.
- Associate Professor Mike Ryan and Prof Leann Tilley organised and spoke at the School of Molecular Science Postgraduate Career Development Forum, La Trobe University.
- Information Day for undergraduate students at Swinburne University of Technology.
- Short Wavelength Laser Source Program conducted an information talk for Honours students at Swinburne University of Technology.
- Open Day at the University of Melbourne.
- Visiting Professor Ian McNulty, gave a number of seminars at La Trobe University and the Australian Synchrotron, and gave advanced undergraduate lectures on X-ray techniques at La Trobe University.
- Associate Professor Mike Ryan gave a number of seminars at St Vincent's Institute for Medical Research and Bio21.
- Associate Professor Andrew Peele presented a show of Physics demonstrations at the La Trobe University Open Day.

- Part sponsorship of the poster prizes at the Aurora Symposium, La Trobe University.
- Dr Chris Hall lectured at Cheiron Summer School at Spring I, Hyogo, Japan.
- Dr Stephen Wilkins gave a talk at the Royal Children's Hospital.
- Mr. Gavin Jennings MLC, Victorian Minister for Innovation, conducted the official opening of the CXS Femtosecond High Power Laser Facility, Swinburne University of Technology

## Media Commentaries

The following articles relating to CXS were published or appeared in 2007:

- *New frontiers in imaging*, Research in Action, LaTROBE BULLETIN, **p11 (Nov/Dec 2006)**
- *"Bob Rosner and Rob Lewis"*, 774 ABC MELBOURNE RADIO **(21 Mar, 2007)**
- *Shattering the crystal lattice*, 5th World Conference of Science Journalists, SCIENCE STORIES, **p11 (April 2007)**
- *A certain synching feeling leaves scientist beaming*, THE AGE **(20 April, 2007)**
- *Nanotechnology*, Australian Capability Report, INVEST AUSTRALIA, **p11 (May 2007)**
- *Synchrotron Expansion Plans Unveiled*, News in Science, ABC SCIENCE ONLINE **(24 May, 2007)**
- *La Trobe University in new synchrotron partnership*, LaTROBE BULLETIN **(Sept/Oct 2007)**
- *Scientists get close to malaria bug*, LaTROBE BULLETIN **(Sept/Oct 2007)**
- *So what does a synchrotron do?*, Postgraduate Study, THE AGE, **p6 (6 Oct, 2007)**
- *Seeing the light in femtoseconds*, AUSTRALIAN LIFE SCIENTIST ONLINE **(Nov 2007)**
- *World Class Laser Facility for Victoria's X-ray Scientists*, MEDIA NEWSWIRE ONLINE **(Nov 2007)**
- *Australia's first laser facility to investigate global disease structure based at Swinburne*, SWINBURNE NEWS ONLINE **(Nov 2007)**
- *Power Failure!*, AUSTRALIASIAN SCIENCE, **p20 (Dec 2007)**
- *MITOCHONDRIA: The Good, The Bad & The Ugly!*, AUSTRALIASIAN SCIENCE, **p22 (Dec 2007)**
- *World Class Laser Facility for Victoria's X-ray Scientist*, BIOTECHNOLOGY VICTORIA, **p1 (Dec 2007)**



On the 7th December, Victorian Parliament's HANSARD recorded the CXS Femtosecond Laser Facility being discussed at length, as part of the world-class research and development infrastructure in Victoria.

**Mr LEANE** — President, I thought that with the removal of time limits for questions one could take a bit more time. I ask Minister Jennings if he could inform the house how the Brumby government is working to deliver world-class research and development infrastructure in Victoria?

**Mr JENNINGS (Minister for Innovation)** — I note that Mr Leane is almost off his P-plates, so in fact his licence will be more permanent in the years to come. I thank him for his question and the opportunity to share with the house, and indeed with the Victorian community, a great event that I had the good fortune to take part in last week at Swinburne University in Hawthorn when I officially launched a fantastic new scientific facility that we have established through a collaboration between Swinburne University, University of Melbourne, Monash University, the CSIRO and the Australian Synchrotron. It is a state of the art X-ray machine. In fact the full title — and here is one for Hansard — is the high-power laser facility at the Australian Research Council Centre of Excellence Coherent X-ray Science machine. I would have thrown Hansard if the first words I used in describing this machine — which is an indication of the capacity of this X-ray machine — had been to describe it as a Femtosecond High-Power Laser Facility.

**An honourable member — How do you spell that?**

**Mr JENNINGS** — It is f-e-m-t-o-second. The reason the femtosecond is very important is that it is a very short period of time. In terms of the equivalent of a second it is 10 to the power of minus 15 — that is how short it is. It is that short that it is even quicker than the time it took Joe Hockey to dump WorkChoices after the federal election. That is how quick it is! It is extremely quick. The importance of being able to undertake scientific research which is that quick is that it undertakes electro-chemical processes that take place very, very quickly. We are in the order of 10 to the power of minus 15 of a second — a very short period of time.

These are very important pieces of technology that enable protein imaging, because membrane proteins are an essential part of the medicinal drug processing chain. In fact 70 per cent of all medicines that are currently available across the globe have membrane proteins as part of their molecular structure. This piece of equipment will be able to measure chemical effects within that time frame, which will enable great breakthrough developments of scientific endeavour in the Victorian community that can lead to great benefits through pharmaceutical products being established in Victoria in the years to come. We are very fortunate to have that capacity in Victoria.

The Brumby government recognises the value of providing key infrastructure such as the femtosecond high-powered laser facility at the Australian Research Centre. I was very happy to meet Keith Nugent, who is a scientist of the highest calibre in the Victorian community and indeed the international community. He is a previous Victoria prize winner who has expertise in protein imaging. We are very pleased to provide support of \$1.8 million, which will drive the capacity of scientific endeavour across our universities in collaboration with the CSIRO and the synchrotron to take this further.

It will lead to real and lasting benefits for our citizens and for global citizens through the medicines we will be able to establish and through our scientific endeavour generally. It builds on the capacity of the Bio-21 facility, the synchrotron and the Australian Centre for Neuroscience and Mental Health Research. We have great capacity in Victoria and great scientific endeavour, and we are very pleased to support that great collaborative effort which will benefit the Victorian community in the years to come.

<sup>1</sup> Victorian Parliamentary Debates, Legislative Assembly, Book 17, 6 December 2007, pp 3969

## PUBLICATIONS

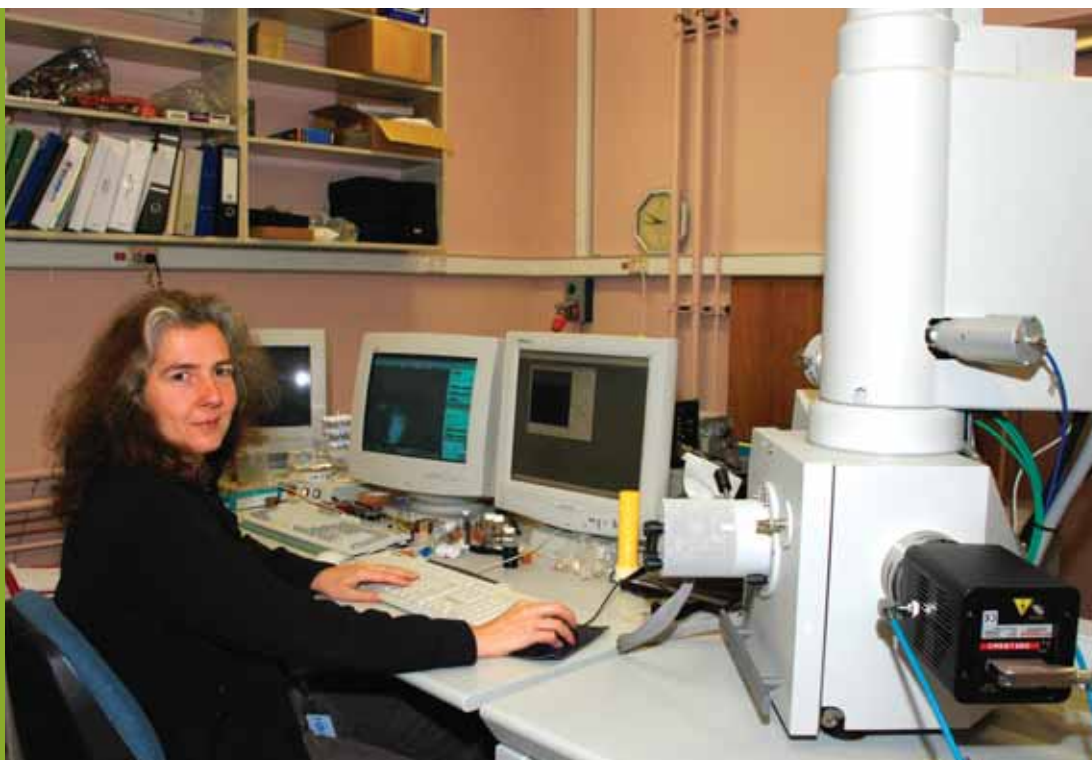
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2. **Arhatari, BD; Carlo, F De; Peele, AG**, *Direct quantitative tomographic reconstruction for weakly absorbing homogeneous phase objects*. Review of Scientific Instruments, 2007, 78(5): p. 053701/1-5.
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4. **Bell, SC; Heywood, DM; White, JD; Close, JD; Scholten, RE**, *Laser frequency offset locking using electromagnetically induced transparency*. Applied Physics Letters, 2007, 90(17).
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8. **Bird, DK; Schneider, AL; Watkinson, A; Finnin, B; Smith, TA**, *Navigating Transdermal Diffusion with Multiphoton Fluorescence Lifetime Imaging*. Microscopy (in press), 2007.
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12. **Cooper, RJ; Turk, G; Boston, AJ; Boston, HC; Cresswell, JR; Mather, AR; Nolan, PJ; Hall, CJ; Lazarus, I; Simpson, J; Berry, A; Beveridge, T; Gillam, J; Lewis, RA**, *Position sensitivity of the first SmartPET HPGe detector*. Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2007, 573(1-2): p. 72-75.
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# TRENDS IN CELL BIOLOGY



- ❖ Trends in Cell Biology journal cover featuring CXS work.

# GRANTS

## CXS members attracted \$1,059,500 in additional support in 2007:

Grant scheme, title, CIs	
Australian Research Council, Linkage Infrastructure, <i>Equipment and Facilities, X-Ray Facility for 3-D High Resolution Diffraction Imaging of Nanostructures</i> , Associate Professor Nikulin, Dr Muddle, Associate Professor Peele	\$350,000
Australian Research Council, Linkage Projects, <i>Industrial-strength X-ray Phase Tomography</i> , Associate Professor A. G. Peele, Dr W. B. Yun, Dr. B. D. Arhatari	\$340,000
Australian Research Council, Linkage Infrastructure, <i>Equipment and Facilities, X-ray Diffraction Microscope</i> , Associate Professor Peele, Professor Tilley, Associate Professor Ryan, Professor Nugent, Associate Professor Smith, Professor Dao, Professor Lewis	\$290,000
ATSE International Science Linkages <i>Support of CXS Annual Workshop 2008: Biophotonics: Physicists and biologists working together</i> , Professor K. Nugent and Professor L. Tilley	\$22,000
ARC/NMRC Research Network <i>Fluorescence Applications in Biotechnology and Life Sciences</i> , Professor L. Tilley	\$10,000
<i>Fluorescence Applications in Biotechnology and Life Sciences</i> , Dr N. Klonis, Dr E. Hanssen	\$10,000
Australian Synchrotron Research Program, <i>Tomographic survey of a human femur</i> , Associate Professor A. G. Peele	\$10,000
Australian Synchrotron Research Program, <i>Fresnel coherent diffractive imaging</i> , Associate Professor A. G. Peele	\$9,000
Australian Synchrotron Research Program, <i>Diffractive imaging using soft x-rays</i> , Associate Professor A. G. Peele	\$6,000
Australian Synchrotron Research Program, <i>XRL for Lobster III</i> , Associate Professor A. G. Peele	\$4,000
<i>Research Network for Parasitology Support of research visit to Light and X-ray Imaging Facilities in California</i> , Professor L. Tilley	\$3,500
Australian Research Council, Linkage International, <i>Diffractive Imaging using Soft X-rays and Electrons</i> , Professor K. A. Nugent, Associate Professor A. G. Peele, Associate Professor L. J. Allen, Dr K. S. Liang, Professor F. Chen	\$3,000
<i>Researcher Exchange</i> , Professor L. Tilley	\$2,000

# CXS LOCATIONS

## Parkville Campus

### Location

Corner of Swanston Street and Tin Alley  
(running off Elgin Street), Parkville, Vic 3010

### School of Physics (David Caro Building)

CXS Head Office - Room 260  
The Experimental Methods Program  
(also at La Trobe University)  
The Theory and Modeling Program  
The Ultra Cold Plasma Source Program

### Parking

'Scratch & Display' car parking permits are available for the use of official visitors to the campus and nearby University parking areas. Upon notification, CXS staff can arrange permits in advance.



## Bundoora Campus

### Location

Kingsbury Drive, Bundoora, Vic 3086

### Physical Sciences buildings 1 and 4

The Biological Sciences Program  
The Experimental Methods Program  
(also at University of Melbourne)

### Parking

Parking for visitors is on a fee-paying basis. Tickets can be purchased at car parks from the ticket machines. Upon notification, CXS staff and visitors can arrange daily temporary permits in advance.



## Clayton Campus

### Location

Wellington Road, Clayton, Vic 3186

### Physics Building

Detector and Beamline Development Program

### Parking

Parking permits are required during weekdays and short-term parking zones are also available. Parking without a permit is available in the blue, red and yellow zones after 5pm on weekdays and all weekend.



## Hawthorn Campus

### Location

John Street, Hawthorn, Vic 3122

### Centre for Atomic Optics and Ultrafast Spectroscopy

The Short Wavelength Source Program

### Parking

Parking in university car parks is on a fee-paying basis only. Tickets can be purchased in car parks from the ticket machines or from multi deck car park. This campus is also situated a couple of minutes walk from the Glenferrie Train Station & Tram Stops.



## Clayton

### Location

Normanby Road, Clayton, Vic 3186

### Manufacturing and Infrastructure Technologies

The Structure Determination Methods Program  
(Gate 5)

### Parkville

343 Royal Parade, Parkville  
Molecular and Health Technologies



# FINANCIAL STATEMENT

## Financial and In-kind Contributions

### A. CXS FINANCIAL REPORT YEAR ENDING 2007

Current Reporting Period 2007 (\$)		Next Reporting Period 2008 (Estimated) (\$)	
Carry Forward	\$1,432,044		\$ 2,092,399
STI Allocated Funds	\$ 400,000		\$ 200,000
Other Funds	\$1,800,000	ARC	\$1,800,000
	\$ 980,000	Node contribution	\$ 980,000
<b>TOTAL INCOME</b>	<b>\$4,612,044</b>		<b>\$5,072,399</b>
Expenditure	\$ 574,541	Salaries	\$ 160,000
	\$ 38,774	Consumables	\$ 50,000
	\$1,728,307	Node distribution	\$ 1,717,526
	\$ 4,293	Conferences	\$ 10,000
	\$ 39,867	A/node equipment	\$ 400,000
	\$ 79,881	Travel	\$ 150,000
	\$ 14,919	Scholarships	\$ 240,000
	\$ 4,545	Sponsorship	\$ 15,000
	\$ 34,518	Marketing	\$ 50,000
	\$ 0	Education Program	\$ 60,000
	<b>\$ 2,519,645</b>		<b>\$2,852,526</b>
<b>BALANCE</b>	<b>\$2,092,399</b>		<b>\$2,219,873</b>
<b>IN-KIND REPORT - YEAR ENDING 2007</b>			
University of Melbourne			\$1,528,376
La Trobe University			\$700,746
Monash University			\$387,919
Swinburne University of Technology			\$338,881
<b>TOTAL</b>			<b>\$2,955,922</b>

## CONTACT US

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ARC Centre of Excellence for  
COHERENT X-RAY SCIENCE

