

Australian Synchrotron Development Plan Project Submission Form

Section A: Summary and Proponent Details

Project Title

A High-coherence Nanoprobe Facility for the Australian Synchrotron

Spokesperson

Name	Andrew Peele	
Institution	La Trobe University	
Email	a.peele@latrobe.edu.au	
Phone	(03) 9479 2651	

Executive Summary (approx. 100 words)

A nanoprobe beamline will provide a unique facility capable of spectroscopic and full-field imaging at sub-30 nm resolution. Operating in the range 2 - 22 keV the nanoprobe beamline will use an undulator source and a very long beamline, of order 100 m, to deliver the highest brightness x-rays possible to an experiment.

While providing access to materials and environmental samples, the system will also provide the ability to probe frozen hydrated biological samples using a cryogenic sample mount, imaging and identifying cellular substructures that are critical components in biological machinery but are far smaller than current beam spots can resolve.

other proponents (uuu h	iore retub ir necessarj)	
Name	Institution	Email address
Keith Nugent	University of Melbourne	keithan@unimelb.edu.au
Hugh Harris	The University of Adelaide	hugh.harris@adelaide.edu.au
Chris Ryan	CSIRO	chris.ryan@csiro.au
David Paterson	Australian Synchrotron	David.Paterson@synchrotron.org.au
Martin de Jonge	Australian Synchrotron	Martin.deJonge@synchrotron.org.au
Leann Tilley	La Trobe University	l.tilley@latrobe.edu.au
Eric Hanssen	La Trobe University	e.hanssen@latrobe.edu.au
Garth Williams	University of Melbourne	garthw@unimelb.edu.au
Mike Ryan	La Trobe University	m.ryan@latrobe.edu.au
John Clement	University of Melbourne	johngc@unimelb.edu.au
David Thomas	University of Melbourne	cdthomas@unimelb.edu.au
Ian McNulty	Advanced Photon Source	mcnulty@aps.anl.gov
Abid Khan	Monash	Abid.Khan@nano.monash.edu
Sally McArthur	Swinburne	SMcArthur@groupwise.swin.edu.au
Matteo Altissimo	CSIRO	Matteo.Altissimo@csiro.au
Brett Sexton	CSIRO	Brett.Sexton@csiro.au

Other proponents (add more rows if necessary)



Will Gates	Monash	Will.Gates@eng.monash.edu.au
Bill Skinner	University of South	William.Skinner@unisa.edu.au
	Australia	
Paul Pigram	La Trobe University	p.pigram@latrobe.edu.au
Paul Dastoor	Newcastle	Paul.Dastoor@newcastle.edu.au
Phil Moriarty	Nottingham	Philip.Moriarty@nottingham.ac.uk
Chris Hall	Monash	Chris.Hall@sync.monash.edu.au
Greg Giles	Otago	gregory.giles@otago.ac.nz
Simon James	CSIRO	simon.alex.james@gmail.com
Daniel MacDonald	ANU	daniel.macdonald@anu.edu.au
Frank Reith	CSIRO	frank.reith@csiro.au
Terence Turney	Monash	Terry.turney@sci.monash.edu.au
Giuseppe Ciccotosto	University of Melbourne	j.ciccotosto@unimelb.edu.au
David Thurrowgood	National Gallery of	David.Thurrowgood@ngv.vic.gov.au
	Victoria	
Robert Hough	CSIRO	Robert.Hough@csiro.au
Mel Lintern	CSIRO	Mel.Lintern@csiro.au
Paul Wright	RMIT	paul.wright@rmit.edu.au
Stuart Ramsay	James Cook University	stuart.ramsay1@jcu.edu.au
James Camakaris	Melbourne University	j.camakaris@unimelb.edu.au
Peter Barnard	La Trobe University	p.barnard@latrobe.edu.au
Michael Parker	St Vincent's Institute of	mparker@svi.edu.au
	Medical Research	
Craig Marshall	University of Kansas	cpmarshall@ku.edu
Heather Wright	Monash	Heather.Wright@sci.monash.edu.au
David Wacey	University of Western	david.wacey@uwa.edu.au
	Australia	
Hugh O'Neill	ANU	hugh.oneill@anu.edu.au
Jade Aitken	University of Sydney	j.aitken@chem.usyd.edu.au
Peter Lay	University of Sydney	p.lay@chem.usyd.edu.au
Carolyn Dillon	University of Wollongong	carolynd@uow.edu.au
Barbara Etschmann	Adelaide University	barbara.etschmann@adelaide.edu.au
Joel Brugger	South Australian Museum	Joel.Brugger@samuseum.sa.gov.au
Sola Ajiboye	Adelaide University	sola.ajiboye@adelaide.edu.au
Nicolas Voelcker	Flinders University	nico.voelcker@flinders.edu.au
Andrew Stevenson	CSIRO	andrew.stevenson@csiro.au
Balwant Singh	University of Sydney	b.singh@usyd.edu.au
Paul Witting	University of Sydney	pwitting@med.usyd.edu.au
Louis Rendina	University of Sydney	rendina@chem.usyd.edu.au
Damian Myers	University of Melbourne	damianem@unimelb.edu.au
Alexander Fink	La Trobe University	a.fink@latrobe.edu.au
Hans Riesen	University of New South	h.riesen@adfa.edu.au
	Wales, ADFA	
John Webb	La Trobe University	John.webb@latrobe.edu.au
Sherry Mao	CSIRO	Sherry.Mayo@csiro.au
Eric Reynolds	University of Melbourne	e.reynolds@unimelb.edu.au
Marian McKenzie	The New Zealand Institute	McKenzieM@crop.cri.nz



	for Plant and Food	
	Research Limited	
Enzo Lombi	University of South	Enzo.Lombi@unisa.edu.au
	Australia	
Paul Wright	RMIT	paul.wright@rmit.edu.au
Nathan Cochrane	University of Melbourne	n.cochrane@unimelb.edu.au
Tony Hollencamp	CSIRO	Tony.Hollenkamp@csiro.au
Markus Grafe	CSIRO	Markus.Grafe@csiro.au
Antony Cooper	Garvan Institute of	a.cooper@garvan.org.au
	Medical Research	
Mike McLaughlin	Adelaide University	michael.mclaughlin@adelaide.edu.au
Chris Pakes	La Trobe University	c.pakes@latrobe.edu.au
Steve Wilkins	CSIRO	Steve.wilkins@csiro.au
David Williams	University of Auckland	david.williams@auckland.ac.nz
Gareth Moorhead	CSIRO	Gareth.Moorhead@csiro.au
John Thornton	DSTO	John.Thornton@dsto.defence.gov.au
Jim Metson	Auckland University	j.metson@auckland.ac.nz
Mike Austin	RMIT	michael.austin@rmit.edu.au
Stephen Kidd	Adelaide University	stephen.kidd@adelaide.edu.au
Daniel Riley	University of Melbourne	driley@unimelb.edu.au
Cassandra Schefe	DPI	Cassandra.Schefe@dpi.vic.gov.au



Section B: Detailed Description

B1: Description of Proposed Beamline/Development Project B1.1 Introduction

We propose a long beamline at the Australian Synchrotron suitable for Scanning X-ray Microscopy at the nano-scale (SXM). The high coherence properties of such a beamline and the commonality of equipment also make the beamline suitable for emerging techniques in full-field imaging using so-called coherent diffractive imaging (CDI). The combination of the two methods will usher in a unique capability in imaging spectroscopy.

The beamline will be capable of 5 nm resolution 3D full field imaging coupled with 25 nm resolution spectroscopy of biological and materials samples. The beamline will operate in the 2 - 22 keV range, optimized to a narrower range that will overlap a portion of the tender x-ray range (1 - 4 keV).

B1.2 Beamline Design Features

The conceptual design for the beamline will utilize lessons learned from recent nanoprobe designs worldwide. This will include the SXM/CDI endstation designs at the Advanced Photon Source (to be relocated on the soft x-ray branchline at the AS) and for ELETTRA, the Hard X-ray Nanoprobe at beamline 26-ID of the Advanced Photon Source, the nanoprobe at beamline 2-ID-E of the Advanced Photon Source, the designs for the Nanoprobe beamline at NSLS-II, and the cryogenic and sample loading design for the soft x-ray microscope system at the Beijing Synchrotron Radiation Facility.

B1.2.1 Experiment schematic and nanoprobe outline

Figure 1 shows a schematic for the 2 modes of operation for a combined SXM/CDI system. The transition is effected by a small translation in the longitudinal sample position and by switching detectors thus enabling ready transition from full-field imaging mode in CDI to spectroscopy mode in SXM. The transition will allow the morphology of a sample to be correlated with its chemical and state information.



Figure 1: Schematic of (a) the experimental arrangement for FCDI and (b) illustrating use of the instrument for scanning x-ray microscopy.

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The nanoprobe will employ diffractive optics (Zone-Plates or Multilayer Laue Lenses, if sufficiently developed by the time of construction) and will reference the focusing optic to the specimen with sub-nm error using laser-encoded referencing. Extremely low run-out (aided by correction algorithms) will enable multi-elemental nano-XANES to be performed in-situ and at a single location on a specimen. The optics, stages, and specimen mount will all be in vacuum. Scanning will be extremely fast, using piezo stages. High-accuracy tomographic capabilities will be enabled by adding appropriate rotation stages. Cryo-compatibility is demanded by the biological community to mitigate the effects of radiation damage at high-resolution and will be implemented. There are at least two functioning solutions: that implemented by the Larabell group at the Advanced Light Source and that implemented by Xradia Inc.

B1.2.2 Detectors and Experiment Hutch

For SXM fluorescence and transmission detectors will be chosen to optimize scan speeds while ensuring full coverage of the desired energy range. The Maia detector currently implemented on the XFM beamline will allow fast acquisition rates for energies above 3.6 keV and future development should enable acquisition of lower energy fluorescence; in the interim other detectors can be used at lower energies. There is strong evidence to suggest that commercial detector technologies will deploy fast readout within 3 years, and the instrumentation will anticipate this development. In scanning transmission mode the use of segmented detectors^{1,2} will also be pursued for differential phase contrast, and larger pixel array detectors will be used to extend this to super-resolution CDI / ptycography. In imaging mode photon counting detectors, such as the Pilatus or Medipix, will be used. Due to larger pixel sizes than convention CCD detectors longer sample to detector distances may be required to reach comparable resolution. This will require a long end hutch – probably of similar dimensions to the existing SAXS hutch.

B1.2.3 Long Beamline

The use of a long beamline – of order 100 m – will maximize the coherent flux available at the sample. In SXM mode this will allow optics limited resolution while accepting a larger portion of the source, which will improve sensitivity. In CDI mode the transverse coherence length will be long enough to allow large (> 100 μ m) samples to be imaged. It also means that the zone plate used to provide the sample illumination will be coherently illuminated – improving reconstruction quality.

B1.2.4 Insertion Device

The chosen energy range is feasible based on experience from other beamlines. In-vacuum undulators with small gap and short period (~20 mm) are now routinely used at existing 3 GeV machines and planned to be used at the latest storage rings being constructed, such as NSLS-II. We would optimise the undulator design in collaboration with colleagues at APS, NSLS-II and SLS to produce maximum brightness across the energy range. In addition the benefits of a variable polarization insertion device will be explored.

B2: Applications and Potential Outcomes to Australian Scientific Community

The summaries below give examples of research projects in a range of areas that could benefit from the nanoprobe. We have listed the names of proponents associated with each project. It should be noted that not all the proponents listed for each project are necessarily collaborators. A strength of the nanoprobe is that it can provide outcomes for a diverse range of researchers – including competitors!

B2.1 Biological applications

New information on biological structures at the nanoscale, in terms of morphological, elemental and chemical makeup, has the potential to revolutionise our understanding of processes that occur in healthy cells and those challenged by disease or disease treatment. The biological sciences



community in Australia currently provides almost half of the demand for beamtime on XFM at the AS. The capability to image elemental and chemical distribution in nanoscale biostructures is extremely limited worldwide and its development would provide a huge scientific advantage to our community. A non-exhaustive selection of projects that would only be possible with the proposed beamline is described below.

B2.1.1 Cellular architecture

L Tilley, E Hanssen, AG Peele (La Trobe University), GJ Williams, KA Nugent (University of Melbourne)

The malaria parasite (Figure 2) leads to more than two million deaths per year, mainly in the young. It spends part of its lifecycle inside human red blood cells where it establishes a system of membranes within the host cell cytosol and induces changes in the host cell membrane. These changes are critical to the disease pathology. The cellular architecture of infected erythrocytes has previously been studied by electron and optical microscopy. X-ray wavelengths allow imaging at high spatial resolution in 3D of the intracellular structures



Figure 2: CDI image³ of a malaria parasite within a red blood cell.

of *P. falciparum* infected erythrocytes that will assist in the study of the development of the parasite and in the morphological response to different treatments. SXM methods have already been shown to be of benefit in assessing elemental concentrations within different regions of the parasite; using the nanoprobe this can be coupled with CDI full-field³ and 3D imaging.

B2.1.2 Sub-cellular imaging

M Ryan, L Tilley, E Hanssen, AG Peele (La Trobe University), GJ Williams, KA Nugent (University of Melbourne), N Voelcker (Flinders University)

Using recent advances in CDI^4 – the ability to image a specific region within a larger host environment with high spatial resolution – we can examine important aspects of mitochondrial organization as a test of our ability to image sub-cellular structures in mammalian cells. In most cells, mitochondria form a dynamic, branched reticulum that extends throughout the cytoplasm. Their diversity in shape reflects a multiplicity of roles in cell development and differentiation. Alterations in mitochondrial morphology often result as a secondary consequence of disruptions in mitochondrial function, which includes a wide variety of important cellular processes, including energy generation, metabolism, cell death, and aging. High resolution diffractive imaging methods

have the potential to unravel some of the questions underlying mitochondrial fusion and fission.

B2.1.3 Intracellular disease processes and their treatment

PA Lay, JB Aitken, PK Witting, LM Rendina (The University of Sydney), MW Parker (St Vincents Institute), P Barnard (La Trobe University), G Giles (Otago), CT Dillon (Wollongong), HH Harris (The University of Adelaide), K.M. Munro, S. Ralph (UOW), J. Aldrich-Wright UWS)

Microprobe XRF imaging of single mammalian cells has been a cornerstone of research into fundamental science on normal metabolic functions and the molecular and cellular differentiation of normal and diseased tissues. However, identification of individual organelles beyond the nucleus has been



20 µm

Figure 3: Elemental distribution maps for a single murine adipocyte treated with chromium propionate showing a punctate localization of Cr and Fe.



limited so far by the resolution achievable at current facilities. The improved resolution of the nanoprobe beamline would reveal new information about localization and associations of heavy elements in mitochondria or lysosymes for example. Prior work has indicated that these localizations do occur (Figure 3), but are often evident as single intense spots when imaged with micrometer resolution. This capability would have wide application for projects in the following areas:

- fundamental biochemical processes involved in oxidative damage in cardiac myocytes and brain cells undergoing hypoxic stress, as a model of the ischemia reperfusion injury of myocardial infarction, strokes, neurodegenerative processes and prevention of such damage;
- the efficacy and toxicity of potential metal-based anti-cancer and anti-diabetic drugs; and
- heme proteins in cells, specifically: changes in neuroglobin (Nb), myoglobin (Mb) and indolamine 2,3-dioxygenase (IDO) in responses to diseases.

B2.1.4 Neurodegenerative diseases

J Camakaris, G Ciccotosto (University of Melbourne), S James, S Mao (CSIRO)

As the Australian population ages neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease and Motor Neuron disease will become an increasingly serious socio-economic problem. The current lack of effective treatments for this group of disorders requires an intensive effort directed at unraveling the biochemical basis of pathology, aiding in the generation of novel disease modifying therapeutics. The formation of insoluble protein aggregates and distortions of cellular



Figure 4: Elemental maps of primary cortical neurons. The minimum and maximum pixel range was equally set across the various mouse knockout tissue. The image shows changes in metal

architecture are believed to be fundamental to the disease processes. The inclusion of cryogenic sample mounting is a tremendous asset as this will minimize the introduction of preparative artifacts and preserve delicate cell structures while providing protection against radiation damage and allowing imaging of hydrated systems. The combination of diffractive imaging and SXM at high resolution (sub 100 nm) along with the ability to topographically reconstruct samples will allow

detailed, subcellular, images of neurons and tissues that will greatly enhance previous work that has measured transition metal levels in primary cortical neurons from AD knockout mouse models (Figure 4). Combing these studies and traditional optical microscopy will provide information on the specific changes in the metabolism of metals and biomolecules which underlie the pathogenesis of neurodegeneration. Furthermore this system will facilitate the study of how drug candidates interact with these systems to restore proper homeostasis.

B2.1.5 Biotechnology - Metal distribution in single bacterial cells

F. Reith, J. Brugger, B. Etschmann (University of Adelaide) Bacteria control metal turnover in surface environments and the metallophilic bacterium *Cupriavidus metallidurans* has been shown to selectively take up



Figure 5: Quantitative XRF-maps showing the distribution of Au, Ca, Cu, Fe, S, and Zn in an individual cell after 1 min exposure to Au(III) at pH 7.0; the quantified area is marked in the image, and concentrations (calculated errors) are given.



gold complexes⁵ (Figure 5). Because bacterial cells are small (~1 μ m in size), very high resolution approaches are required to obtain comprehensive element maps of individual cells. Beam-sizes of 150 nm can be achieved at state-of-the-art facilities in the US and France. This allows the collection of more than 30 full element spectra per cell, yet more than 100 full spectra would be required to comprehensively map these cells in order to make accurate predictions about uptake mechanisms. The proposed high-coherence nanoprobe facility will enable us to conduct these measurements in Australia, which ultimately will lead to the development of biosensor and bio-processing tools for the Australian mining industry.

B2.1.6 The role of metals in pathogenic bacteria

HH Harris, SP Kidd (University of Adelaide)

Pioneering work by the group of Kemner at the APS (2-ID-D, 150 nm beam spot) has demonstrated XRF imaging of single hydrated bacterial cells, which are commonly less than 1 μ m in two out of three dimensions⁶. More recent work by the same group⁷ has shown intracellular localizations of metals that promise the possibility of imaging what structures are present in prokaryotic cells. Operation of the nanoprobe in SXM mode at 25 nm resolution would allow imaging of heavier elements in single cells of pathogenic bacteria such as *staph. aureus* or *heamophilus influenzae*, which are very significant human pathogens and whose pathogenesis has been linked with metals such as nickel. Cells could then be imaged using CDI providing information about morphology under different environmental conditions.

B2.1.7 Human toxicology of nanoparticles

T Turney (Monash University), P Wright (RMIT)

Nanoparticles are increasingly used in a range of human topical applications, including ZnO in sunscreens and silver in antibacterial treatments. However the toxicology of these nanoparticles is not clearly understood. The SXM/XANES capability of the nanoprobe would allow study of the generation and quenching of reactive oxygen species in cells by nanoparticles containing REDOX centres (eg ZnO, CeO₂, Fe₂O₃) and the ability to correlate that information with biological structure available from CDI.

B2.1.8 Subcellular location of trace metals in human neutrophils

Stuart Ramsay (Mater Hospital Townsville, James Cook University), Natkunam Ketheesan (James Cook University) The ability to superimpose spectroscopic information onto a coherent diffraction image using biological samples exposed to minimal processing (eg frozen hydrated samples) would allow new understanding of (for example): how TcSn colloid labels phagocytic leukocytes in nuclear medicine; and the function of Complement Receptor 3, an integrin which is expressed on the surface of cells (such as neutrophils) involved in innate immunity and which acts as both a phagocytic receptor and a cell adhesion molecule.

B2.1.9 Nano-scale structure in teeth and bone

N Cochrane, J Clement, E Reynolds, D Thomas D Vine (University of Melbourne), N Voelcker (Flinders University) Both teeth and bone have a hierarchical structure of organic and inorganic material. Tooth decay is a widespread worldwide public health problem that ideally would be managed with non-invasive treatments that biochemically reverse the disease process. In bone understanding structure and aging as well as treating osteoporosis are significant research goals. It has, for example, been shown that bone becomes more brittle as the individual ages and this is probably related to changes in both crystal habit and in the cross-linking of the collagen and complex interactions between these two phenomena. Atoms and ions in the structure of hydroxyapatite are fairly readily substituted by other elements (e.g. fluoride and carbonate in the crystals of dental enamel) with sometimes dramatic changes in their material properties and susceptibility to dissolution and/or remineralisation. The behaviour of the inorganic crystals at nanometer resolution are of critical importance in understanding the processes of demineralisation (progression of tooth decay) and remineralisation



(the chemical process of non-invasively reversing tooth decay). The nanoprobe beamline will provide imaging and spectroscopic information that will allow us to properly investigate these issues for the first time at the nano-scale.

B2.1.10 Cellular tomography

MD de Jonge, DL Howard, D Paterson (Australian Synchrotron), A Micelli, I McNulty, S Vogt (Advanced Photon Source), C Holzner, C Jacobsen, SB Baines (Stony Brook, NY), BS Twining (Bigelow Laboratory for Ocean Sciences, ME), K Ignatyev (King's College, London), J Diaz (Georgia Institute of Technology, GA) With 18 to 20 billion metric tons of organic carbon produced by diatoms through photosynthesis each year, their effect on global carbon cycling is predicted to be of similar magnitude as all rain forests combined. Based on large scale iron fertilization experiments, iron



Figure 6: Quantitative Fluorescence tomography of *C*. *Meninghiania* with an estimated spatial resolution of 300 nm.

has been found to be a key element regulating primary productivity in major regions of the global ocean. Diatoms frequently dominate marine phytoplankton blooms initiated by iron fertilization, and their success is therefore predicted to be highly dependent on their iron uptake and storage mechanisms. Figure 6 shows a reconstruction of high-resolution scanning x-ray fluorescence tomography of the diatom *C. Meninghiania*, captured in the process of cell division⁸. The iron in this diatom is clearly localised within bands that run around the circumference of the shell. What has not been so clear before this image is that these bands lie buried just underneath the inside surface of the silicon shell.

B2.1.11 Microfibril organisation

E Hanssen (La Trobe University)

Fibrils and microfibrils are a major component of the extracellular matrix. They act either as a reserve of growth factors, mechanical stress protection or transfer of signal between cells amongst multiple other roles. In the aorta, the major artery of the human body, the fibrils and the microfibrils give resilience and elasticity, properties necessary to maintain the homeostasis of the circulatory system. The mechanism of deposition of the elastic protein (elastin) on the microfibrils scaffold is poorly understood. Microfibrils seems to embed themselves in a matrix of elastin (Figure 7). No imaging technique has so far been able to capture the interaction of these microfibrils within the elastin matrix. The SXM capability of the nanoprobe will provide a way of imaging within the elastic layer therefore increasing our knowledge of the real architecture of a medically significant tissue.



Figure 7: Fetal mouse aorta showing showing the elastic layer of the aorta (Black sections, surrounded by cells in the middle) and collagen fibers on the left.

B2.2 Environmental Sciences

W Gates (Monash University), D Paterson, M de Jonge(AS), I Porter, C Schefe (DPI, Victoria)

The absolutely referenced positioning offered by the CDI/SXM instrument will guarantee proper focal tracking and therefore the ability to perform single point XANES scans without loss of resolution or positional accuracy and large rapid changes in incident energy, a capability critical to many environmental studies. The advances in fluorescence detection (e.g. Maia) and the brightness of the nanoprobe will enable fast XANES imaging to create high definition chemical state maps. Marine and soil scientists have begun to capitalise on the unique possibilities for *in situ* studies⁹. The addition of "wet cell" capabilities will provide an opportunity to study *in situ*:

• subcellular imaging of key trace elements in bio-medical studies;



- transfer of contaminants (e.g. heavy metals) from the inorganic to the organic (living or otherwise) phases;
- breakdown mechanisms of contaminants (e.g. pesticides or solvents) by engineered materials; and
- mechanisms of infection of plant roots by microbial (fungi, bacterial or nematodes) pathogens.

These examples are not exclusive, and it is expected that the capabilities and applications will continue to grow with the SXM and micro-spectroscopy communities.

B2.2.1 Soil chemistry, mineralogy and ecotoxicology

B Singh (The University of Sydney), M Grafe (CSIRO), D Paterson(AS), I Porter, C Schefe (DPI)

The development of a dedicated nanoprobe beamline is a significant step forward from the existing beamlines at the Australian Synchrotron, especially where it is not possible to take biological and/or contaminated samples to overseas facilities. The nanoprobe beamline will provide novel insights into the composition of (i) nano-particulate soil and residue minerals, (ii) various components of plant and soil invertebrate tissues, and (iii) the interface between soil and root, and the rhizosphere. 3D spectropscopic techniques will enhance understanding of soil structural and compositional changes due to soil-microbe, -root, and organic matter interactions. Compositional variations in nano-sized minerals will enhance our understanding of the mechanisms (e.g. structural incorporation or adsorption reactions) of heavy metal sequestration in soil as well as illuminating those mineral-solution interfaces at which nucleation and dissolution reactions occur (e.g., ferrihydrite surface). Sub-micron resolution will be essential to complement other techniques to assess the ecotoxicological behavior of manufactured nanoparticles in the environment.

B2.2.2 Plant nutrition and food quality

E. Lombi (University of South Australia)

The distribution and speciation of nutrients and contaminants in plants play a key role in terms of plant physiology processes that ultimately control food quality. For instance, the quality of cereal grains, which represent the major class of staple foods worldwide, in terms of micronutrients and pollutants has become a central issue of in plant nutrition, animal and human health. The high intensity of synchrotron radiation is essential to probe trace elements in plants. However, current synchrotron approaches are usually conducted at tissue level with little information available at the subcellular level. The development of a nanoprobe able to accept frozen hydrated tissues is essential in order to progress this field of research.

B2.2.3 Fate and ecotoxicology of nanomaterials

M.J.McLaughlin (University of Adelaide/CSIRO Land and Water), G. Cornelis (University of Adelaide), D. Chittleborough (University of Adelaide) .

Nanomaterial behaviour in soils and sediments in relation to dissolution, diffusion and transformation is poorly characterized, and the uptake and ecotoxicology of these materials depends on an accurate understanding of this behaviour. Sub-micron resolution is essential to permit information at the nano-scale to be gathered. Initial work is focused on behaviour of Ag, ZnO and CeO_2 nanoparticles in soils and interactions with plants and soil invertebrates. There is a need to map and speciate these metals in both soils and biota, and to understand the behaviour of nanomaterials at interfaces between the organism and the environment (e.g. rhizosphere).

B2.3 Nanotechnology

B2.3.1 Nanoelectronics

GJ Williams, KA Nugent(University of Melbourne), AG Peele (La Trobe University), I. McNulty (APS) The integrated circuit industry is already able to create devices with features beyond the imaging ability of current x-ray (zone plate) focusing technology and beyond the capability of SEM, TEM or AFM techniques, as these devices are often 3D in nature. CDI can close this gap in capability and



become an important diagnostic tool. An example, showing sub-30 nm resolution using CDI and coupled with SXM spectroscopic imaging^{4,10} is shown in Figure 8.

B2.3.2 Nano-MEMS

P. Pigram (La Trobe University), A. Khan (Monash), S. McArthur (Swinburne), M. Altissimo (CSIRO/MCN), M. Austin(RMIT), B. Sexton (CSIRO)

The Melbourne Centre for Nanofabrication is located on the same site as the Australian Synchrotron and, with \$45 M initial funding from NCRIS, Victorian State Government and partner institutions, is set to become a National leader in nano-scale applications. The facility is well set up for fabrication and SEM-type characterization. However, the 3D and high resolution capabilities of a synchrotron facility – especially when coupled the ability of SXM to provide chemical information – means that a nanoprobe beamline could become a key characterization tool for MCN.



Figure 8: (a & c) Scanning Transmission x-ray microscopy showing high resolution spectroscopic information on a fuse section of an integrated circuit¹⁰. (b) Fresnel coherent diffractive imaging showing a full field image at sub-30 nm resolution of the same sample. The colour scheme represents the phase of the sample and material differences are readily identified⁴.

B2.3.3 Dynamics in self-assembled nano-arrays

C. Pakes, AG Peele (La Trobe University), P. Moriarty (Nottingham)

Self-assembled arrays of gold (and other) nanoparticles will form patterns, features of which will change in response to environmental inputs. Modeling the dynamics of these changes is a key requirement for understanding and manipulating nano-systems. Using the imaging and spectroscopic capability of the nanoprobe will allow the evolution of such systems to be tracked, possibly *in situ*.

B2.3.4 Nanocomposites, polymer blends and morphology

P. Dastoor (U. Newcastle), W. Skinner (U. South Australia), W Gates (Monash)

For semi-conductor polymer blends used in electronic device applications, it is possible to correlate local composition with electronic/optical device characteristics, which paves the way to characterizing a whole new class of materials with SXM — multicomponent organic electronic devices that have intrinsically nanoscale dimensions. Understanding where charge transport and recombination occur in these materials helps explain the efficient performance of polymer-based light-emitting diodes (LEDs) and will lead to a new avenue of research on organic electronic devices, supporting emerging technologies such as molecular computing and promoting increased efficiencies in existing organic technologies (organic LEDs and solar cells).). Other areas of intense industrial interest are ultra-structural arrangements of sol-gels and detailing oxidative coupling reactions in clay-based catalysts and ion-transfer in clay-based electrodes.

B2.4 Geology, Mineralogy & Geochemistry

C.G. Ryan (CSIRO)

The development of the Maia detector system for fluorescence imaging provides a view of the complex textural and chemical detail in geological samples spanning 4 orders of magnitude of spatial scale. Used with the XFM and proposed μ XRD/XFM beamlines this spans spatial scales from sub-micron to cm. The proposed High-coherence nanoprobe beamline provides the opportunity to push this range below 30 nm (e.g. 20 nm to 200 μ m) and potentially to ~10 nm with emerging diffractive focusing technologies, such as the Laue multilayer lenses demonstrated at the



APS and central to NSLS-II nano-probe ambitions. This pushes ever closer to fine-scale surface and grain boundary deposits important to advancing understanding of ore formation, environmental science and mineral processing, thus providing a bridge between micron scale chemical imaging and in-vacuum surface science techniques.

B2.4.1Nanoparticulate inclusions

C. Ryan, R. Hough, J. Cleverley (CSIRO)

Signatures of fluid histories in the formation of high and low temperature ore deposits are recorded in complex minerals at the sub-micron scales and vary in 3D. Recent research has shown that microstructural domains and small (sometimes nanoparticulate) inclusions require element mapping by XRF at very high spatial resolution and in 3D in order to reveal the true nature of trace element residence. A high coherence nanoprobe, together with fast mapping detectors and a tomography capability will provide the tool to reveal unprecedented levels of detail in ore system minerals and lead to far more robust interpretations of ore fluid chemistry, pathways and controls on deposition for key elements such as Gold.

B2.4.2 Magma chamber growth history

H. Wright (Monash University)

Micron scale concentration zonations in trace elements in silicate crystals in magmatic rocks tell us about the magma chamber growth history of crystals (and thus act as time capsules for the evolution of magma chambers). To understand this structure the throughput and imaging capability of a high-coherence nanoprobe will be required.

B2.4.3 Evolution of life

D. Wacey (University of Western Australia), C Marshall (University of Kansas)

The ability to identify and study functional groups in organic material is crucial in distinguishing biological material and reactions from non-biological equivalents on the early Earth - with the overall goal of elucidating when life arose on Earth, what metabolisms came first, and how these data can be used in the search for life on other planets. The nanoprobe will provide the throughput and resolution in STXM mapping and STXM based XANES that will provide this capability.

B2.4.4Functionality of near earth surface materials

W. Gates (Monash)

The focal tracking of the nanoprobe beamline over rapid and large changes in incident energy, enabling single point XANES scans without loss of resolution or positional accuracy, will provide unprecedented capability for improved accuracy in determining speciation, distribution, reactivity, transformations, mobility and potential bio-availability of near earth surface materials and the chemical processes occurring at their surfaces.

B2.5 Condensed matter and materials

B2.5.1 Crystal defects and strain

J. Thornton (DSTO), GJ Williams (University of Melbourne)

Understanding the structure of crystal defects and their relationship to crystal properties is a longstanding problem that may be uniquely addressed by CDI¹¹. Rare defects in epitaxially aligned and patterned nanocrystalline GaAs materials are one such example. Strain within crystals due to surface effects, anomalous thermal expansion and lattice mismatch is another. The ultimate challenge in this area would be to image a single buried defect such as a dislocation or to image the atomic displacements (strain fields) induced by the defect inside a crystalline nanoparticle. This powerful capability would open up unique opportunities to understand and control crystal defects and strain in semiconductor nanostructures.



B2.5.2 Opal

J. Webb, R. Glaisher, P. Pigram, A. Fink (La Trobe University), GJ Williams(University of Melbourne) Opals consist of a matrix of spheres with a characteristic scale of about 100nm, well suited to the resolution limits and capabilities of coherent diffractive imaging. CDI approaches will allow the direct imaging of their three-dimensional structure for the first time, which couples with SXM spectroscopic information will provide valuable insight into their structure and organisation. Another interesting goal is the nanometer-scale imaging of three-dimensional quantum dot arrays, which exhibit a wide range of optical and electronic properties. This goal is made possible by the ability of CDI to image arbitrary sub-regions on large complicated samples.

B2.5.3 Condensed matter physics

GJ Williams (University of Melbourne), I Vartaniants (HASYLAB).

Several transition metal oxides, notably the half-doped perovskite manganites, exhibit fascinatingly complex phase diagrams driven by the many charge, spin, and lattice degrees of freedom in the ground state. The interplay of these degrees of freedom gives rise to dramatic changes in electrical and magnetic behavior, such as colossal magnetoresistance. A coherent diffractive imaging microscope with a resolution of 10 nm or better, resonantly tuned to 3d transitions in rare-earth elements, could enable imaging of buried orbitally ordered domains in these materials. Orbital domains are suspected to exist on the 30-100 nm scale based on conventional diffraction measurements but have never been imaged in bulk samples. The question as to whether these domains are static or can fluctuate is currently a topic of intense debate; coherent diffractive imaging with *in-situ* temperature control may help to answer this question.

B2.6 Infrastructure and Method Development

KA Nugent, GJ Williams (University of Melbourne), AG Peele (La Trobe University), I. McNulty (Advanced Photon Source), D Paterson, M de Jonge (Australian Synchrotron), C Hall (Monash)

Coherent diffractive imaging is driving the development of new beamlines at several facilities worldwide. The goal of such work is to develop capability in the types of projects described above but also to develop techniques suitable for application at the next generation of x-ray sources – Free Electron Lasers. Ultimately such applications may lead to structure determination methods in protein molecules that are resistant to crystallization. A goal of the ARC Centre of Excellence for Coherent X-ray Science is to develop such methods and, as a pathway to this, to demonstrate CDI structure determination for a membrane protein. Such proteins play a major role in drug treatments as they are the gateway between the extra and intra cellular environment.

B3: Match to Selection Criteria

Much of the case here is implicitly made out in the user project descriptions given in section B2. We have added some short additional comments below.

B3.1 Demand for New Techniques

The bulk of the applications listed in section B.2 require capability that is not currently available at the Australian Synchrotron. This includes:

- Full-field nano-scale imaging;
- Sample cryogenics;
- High-throughput nano-scale SXM with differential phase contrast and/or CDI-enabled super-resolution enhancement;
- Fluorescence tomography;
- Complementary (with some overlapping) energy range to tender x-ray regime; and
- High coherence imaging.



B3.2 Take Advantage of the AS 3rd Generation Source

To deliver the requirements of CDI and high-throughput SXM improved transverse spatial coherence will be required. In order to achieve this, the beam must have a high degree of transverse spatial coherence in the sample or optics plane, which will only be achieved for the AS by using a long beamline. Fortunately, the emittance properties of the AS are such that this can be achieved while still delivering high flux.

B3.3 Will Position Australian Scientists at the Leading-edge of their Field.

The high coherence nanoprobe provides the capability to perform cutting-edge science across a range of disciplines. This is demonstrated in section B2 above where a broad range of applications are cited. Importantly, it should be noted that the feasibility and demonstration work referenced in section B2, typically in high impact factor journals, is overwhelmingly dominated by the Australian scientists listed in this proposal. In particular, the Australian community already boasts leading imaging and spectromicroscopy groups. The new capability provided by the high-coherence nanoprobe beamline will be a valuable new discovery tool for these groups that already have a proven track record in the field.

B3.3 Can be Demonstrated to be Feasibly Constructed Within a Three Year Timeframe

While the concept and capability of the proposed beamline will be unique at the AS, and nearly worldwide, there are precedents for all aspects of its construction at other facilities. The integration of the entire beamline design poses no unsolved design or engineering problems. Similarly, based on previous cases we believe that specification, design and construction within three years is feasible.

B4: Potential Users

As demonstrated by the diversity of applicants and institutions listed as proponents, this project clearly addresses a need within the Australian Scientific community. We have listed as proponents in section A only those who have explicitly indicated their support (in the time available) for the beamline concept. The projects in section B2 also list the names of additional collaborators of the proponents. There are also more than 20 additional names in the project mailing list who have not (yet) explicitly signed on as proponents. We have also included a number of overseas collaborators where these have strong connections with Australian researchers and the development of the research will strengthen the Australian community. Accordingly, we feel that the proposed beamline will meet an immediate need as well as displaying great potential for growth.

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