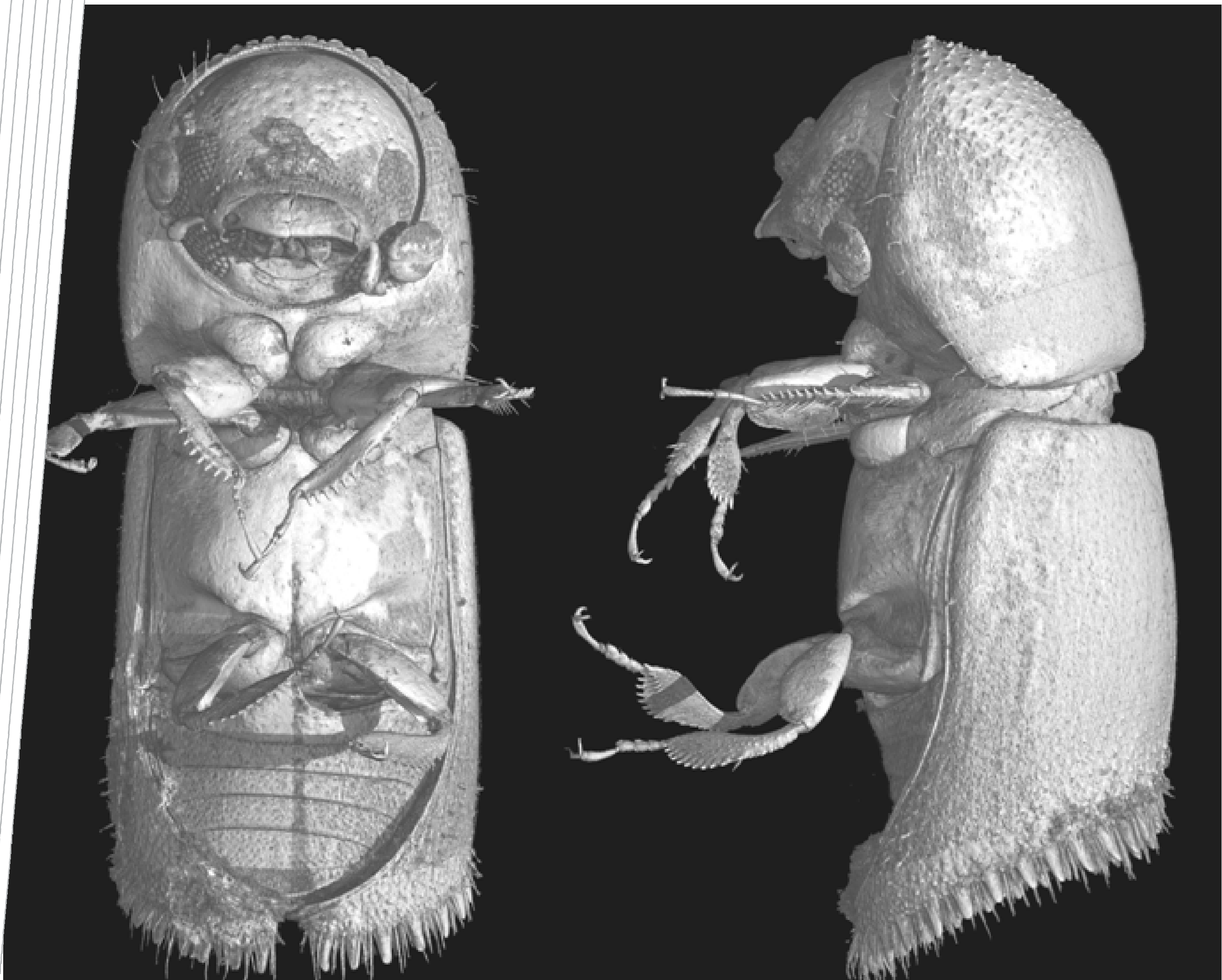

Miocene insect fossilised in opaque amber from Cape York (Paul Tafforeau, ESRF, Susan Hand, UNSW)

Micro-CT Beamline Scoping Group Final Report

Sheridan Mayo, Karen Siu, Florian Fusseis, Anton Maksimenko, Dean Morris

August 2011-07-11

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1. EXECUTIVE SUMMARY

Three-dimensional and time-resolved characterisation at the sub-millimetre and sub-micron scale is essential to current research in biological, medical, geological and materials sciences. Micro-Computed Tomography (MCT) has opened up the 3rd dimension, and modern synchrotron sources have made time-resolved investigations feasible. Over the last decade, Australian scientists have embraced microtomography as part of their research repertoire, and are active innovators in microtomography methods and applications. Current requests to ISAP for travel funding demonstrate that MCT is amongst the highest demanded techniques for overseas synchrotron access. The proposed MCT beamline will ensure that the benefits of these exciting research endeavours are available to all of the Australian community.

The dedicated micro-tomography beamline for the Australian Synchrotron will be a versatile beamline, both scientifically and technically. It will operate at an energy range of 8-40keV, permitting high speed acquisition in both phase and absorption-contrast imaging and tomography. Spatial resolutions will approach submicron in standard parallel-beam mode and 100nm in focussing-based imaging mode.

The proposed beamline will be world-class, building on carefully selected, successful instrument assemblies in Europe, the US and Japan. High-speed acquisition will utilise the increased flux available from broad-band monochromators or pink beam. New super-fast detectors will enable data collection rates of up to several thousand frames per second. High-throughput operation will be enabled by beamline automation and robotic sample exchange, supported by remote access.

The beamline will outperform other similar beamlines in:

- World leading local expertise in algorithm development for phase contrast modes and tomographic reconstruction
- Prioritisation of dynamic process imaging by provision of a suite of sample environments
- High performance computing support for real time reconstruction and quantitative analysis of very large and time-resolved data sets

We anticipate that the impact of at least some of these innovations will be multiplied by their adoption by the wider micro-CT community within Australia and overseas.

A critical capability of the beamline will be enhanced visibility when examining low contrast specimens. This will be achieved by taking advantage of tunable radiation or via phase contrast imaging modes, including both inline and grating-based phase contrast. An additional focussing-based high-resolution imaging mode will enable resolutions approaching 100nm in imaging and 200nm in tomography to be achieved.

Multi-scale characterisation from the centimetre to the nanometre scale is critical for understanding hierarchical systems. Within the Australian Synchrotron, the MCT beamline forms an essential link in the available chain of size scales between the Imaging and Medical Beamline (IMBL), SAXS/WAXS and crystallographic methods that are already in high demand. Investment in this area is extremely timely and will return high impact outputs in the near future.

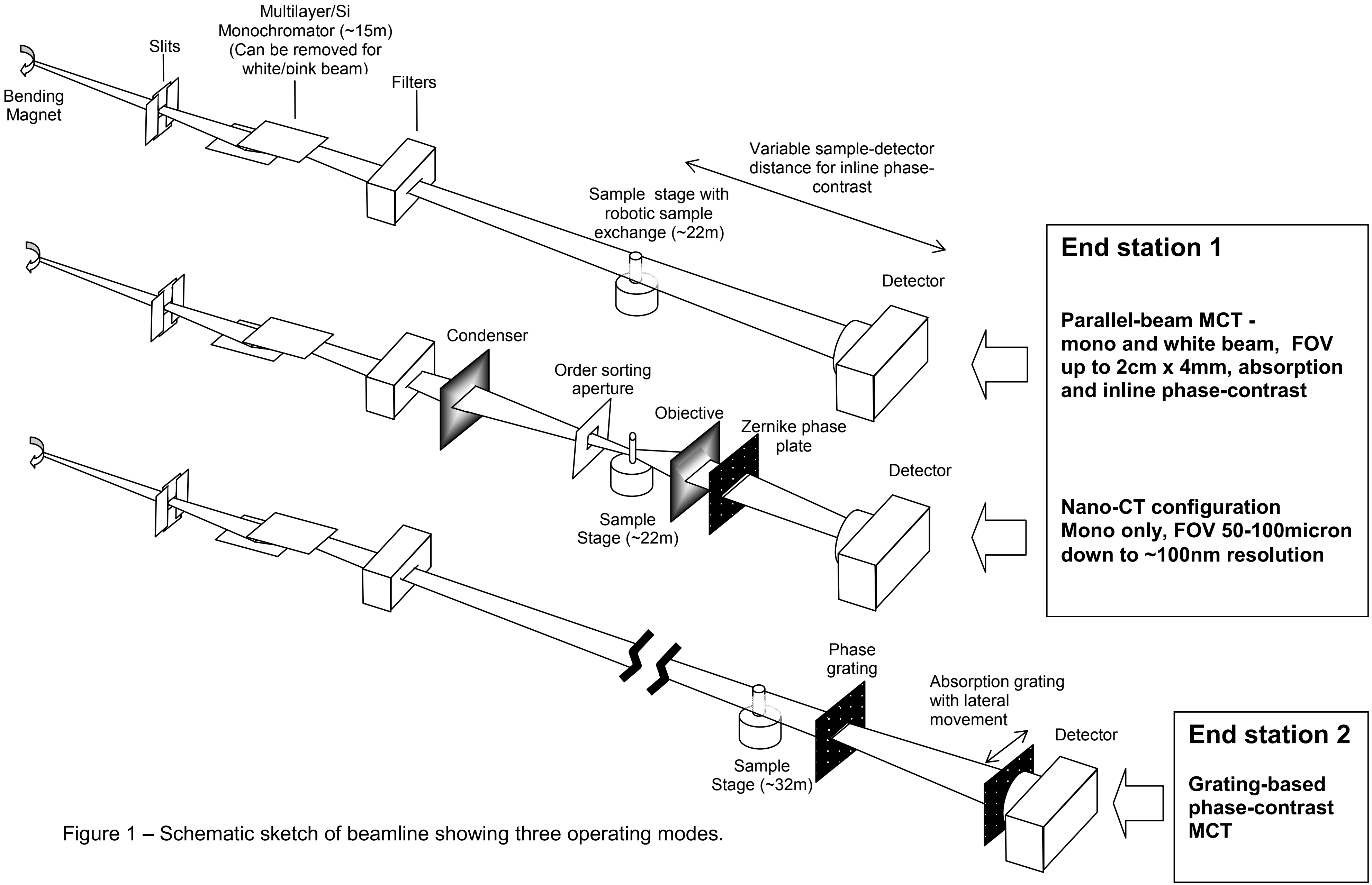

Figure 1 – Schematic sketch of beamline showing three operating modes.

2. SCIENCE CASE

Micro-Computed x-ray tomography (MCT) has proven itself to be a versatile workhorse for 3-dimensional characterisation of samples ranging from the geological to the biological, with many commercial devices now available in research and industry laboratories. This robust instrumentation forms a platform from which many advances in tomographic methods and application have been made by Australian researchers.

There is continued high demand from Australian researchers to access overseas synchrotrons offering distinct capabilities due to the unique source characteristics, such as:

- *Three-dimensional characterisation of a large number of samples with submicron resolution in a very short time,*
- *Easy access to hierarchical length scales from the submicron to the centimetre scale,*
- *Tunable monochromatic radiation for elemental sensitivity and for avoiding artefacts such as beam-hardening,*
- *Enhanced contrast using various modes of phase contrast imaging, particularly useful for low density samples, and*
- *Tracking of time-dependent changes in three-dimensional structures in a variety of environments.*

In recent years, not only has MCT data acquisition matured to very high standards but increasingly sophisticated data analysis and visualisation routines have became available to the non-expert. MCT usage has gained momentum across a large range of research disciplines, in both basic and applied science and is now used to study materials and processes as diverse as bread dough, meteorites, water migration in plant tissue and mouse airways, muscles in fossils, and geopolymers. To acquire tomographic data, Australian researchers have shown themselves willing to travel to synchrotron facilities in Europe, Japan and the USA.

The MCT beamline will provide fluxes, energies and resolutions that are unrivalled by popular lab-based tomography systems and add the 4th dimension of time to 3-dimensional imaging. The end stations will enable acquisition of datasets in less than a second using pink beam, enabling dynamic studies. It will satisfy increasing demand for rapid processing of a large number of specimens using robotic sample handling.

Phase contrast techniques will reveal three-dimensional features even in soft tissue, while absorption edge data acquisition tracks the concentrations of chemical elements in materials in three dimensions. Access to the MASSIVE cluster provides computational power and software to not only produce stunning visualisations, but more importantly, to extract quantitative data.

These novel capabilities impact on scientific endeavour in a wide variety of research fields, and there is a rapidly increasing demand for access to suitable facilities. In communication with the user community we identified the following key areas in which the beamline is likely to produce high impact: Material Sciences, economic geology (including petroleum geology), sustainable energy, biomedical sciences, palaeontology and X-ray optics.

The MCT beam line complements and extends the tomography capabilities of the existing Imaging and Medical Beamline (IMBL) at the Australian Synchrotron, permitting users to access multi-scale information over 6 orders of magnitude. It also bridges a gap between the macro scale and the length scales accessed by small and wide angle scattering techniques. In addition MCT provides an invaluable 3D framework, or context in which to better understand data from other methods such as XFM, electron-microscopy, EDX and FIBs.

As well as supporting a wide range of applications, the beamline will also support research into the fundamentals of phase-contrast techniques, phase-retrieval and tomographic algorithms. Australia is home to some of the pioneering scientists in the field of phase contrast imaging and tomographic methods. Further developments in these areas will enable the beamline to stay at the forefront of these areas and increase impact by developing methods that can be adopted by both the Australian MCT community and also synchrotrons overseas.

2.1 Capabilities & example applications

The table below lists the capabilities for the beamline together with a selection of representative applications driving those requirements. The four key areas identified by the scoping group and the user community as essential are Dynamic/high speed, Ultra-high resolution, Phase-contrast and High throughput. The provision of custom sample environments is also seen as critical to the beamline's success. Local tomography and element specific capabilities are highly desirable attributes that are by-products of the essential capabilities and will not require additional hardware. Overlapping requirements emphasize the benefits that the various applications will enjoy from the versatile technical capabilities.

Table 1 – Key beamline capabilities and representative applications

	Dynamic imaging	High throughput	Phase Contrast	Micron Resolution	Nanometre resolution	Custom sample Environments	Local tomography	Element specificity
Particle aggregation	x			x		x		
Fracture propagation	x		x	x				
Breadmaking	x		x			x		
Bubble-particle interactions	x		x	x			x	
Pore formation and thermal damage to rocks and minerals	x		x	x		x		
Micro-paleontology		x	x	x	x		x	

Phenotyping in biology		x	x	x		x		
Metal corrosion	x	x		x		x	x	x
Bone/Paleo-histology		x	x	x	x		x	
Nanoporosity (coal, rocks, fuel cells)					x			
Fluids in porous materials	x		x	x		x		
Vascular and neural networks		x	x		x		x	x

2.2 Alignment with community & industrial research interests and National Research Priorities

Sub-micron structures are often key to understanding the properties of macroscopic materials, whether these materials are inorganic in nature (geological, metallurgical) or living organisms such as plants or animals. Consequently, the need for three-and four-dimensional data generates ubiquitous demand for MCT across the entire range of scientific disciplines, and from end users engaged in pure research through to those in industrial applications.

The following list provides only a sampling of known **current** research effort utilising MCT, aligned with Australia's National Research Priorities, drawn from the existing MCT user community.

2.2.1 An Environmentally Sustainable Australia

Transforming existing industries - Observation of nanoporosity and fluid inclusions in coal and rocks (Clennell, CSIRO); thermal expansion and fluid-rock interactions (Fusseis, UWA)
Overcoming soil loss, salinity and acidity – In situ root response to environmental change (Aylmore, UWA)
Reducing and capturing emissions in transport and energy generation - Dynamic studies of fluids and fluid boundaries in porous rocks relevant to petroleum extraction, geothermal applications and geo-sequestration. (Clennell, CSIRO Petroleum, WA, ANU/UNSW XCT)
Sustainable use of Australia's biodiversity – high throughput data for virtual entomology database (La Salle, CSIRO); Morphology of teeth in modern and Pleistocene Australian mammals (Evans, Monash Uni)
Developing deep earth resources – Fluid inclusions in minerals (Liu, CSIRO), 3D morphology of magmatic sulphides (Barnes, CSIRO), mineral mapping in 3D (ANU/UNSW XCT); dynamic studies of hydration in geosynthetic clay liners (Gates, Monash Uni)
Responding to climate change and variability

2.2.2 Promoting and Maintaining Good Health

A healthy start to life – understanding muscular dystrophies by phenotyping developmental models (Bryson-Richardson, Monash Uni)
Ageing well, ageing productively – Hierarchical studies of bone structure to combat osteoporotic fractures (Clement, Uni Melb)

Preventive healthcare – Effects of medication on bone health (Myers, Uni Melb), factors leading to arterial plaque rupture (Siu, Monash Uni), understanding mechanisms of tooth decay (Cochrane, Uni Melb)
Strengthening Australia's social and economic fabric

2.2.3 Frontier Technologies for Building and Transforming Australian Industries

Breakthrough science –Frontier technologies - Imaging stem cells in mammalian tissues (Jenkin, Monash Institute Medical Research).
Advanced materials - High throughput MCT for metal corrosion studies (Knight, DSTO).
Smart information use – Numerical simulation of rock microstructures (Pervukhina, CSIRO); data constrained modellings (Yang, CSIRO); fundamental studies of CT methods (Svalbe, Monash Uni)
Promoting an innovation culture and economy - ANU/UNSW spinoff company DigitalCore P/L which services the oil and gas industry is a significant potential commercial user of this beamline
Creation of the beamline itself is an innovative achievement of a high order which will significantly advance local capability in areas such as nanofabrication and tomographic algorithms, which may well have spin-off benefits.

2.2.4 Safeguarding Australia

Critical infrastructure - High throughput MCT for metal corrosion studies (Knight, DSTO).
Understanding our region and the world
Protecting Australia from invasive diseases and pests
Protecting Australia from terrorism and crime – Identification of unknown deceased from teeth microstrucutre (Clement, Uni Melb)
Transformational defence technologies

2.3 Complementarity & interaction with existing beamlines & facilities

2.3.1 IMBL

The beamline is envisaged to provide a complementary set of capabilities to the IMBL which is the only other beamline capable of full-field MCT at the synchrotron. It will focus on applications requiring higher resolution and lower x-ray energies and will be particularly targeted at applications where collecting many datasets in a short time-frame is required, whether for statistical analysis of many samples or observations of a single system that is changing over time or subject to a controlled environment.

When considered as a pair of beamlines, the IMBL and the proposed MCT beamline are particularly attractive for applications where a hierarchical approach is required to fully understand the system under study; that is, characterisation over many orders of magnitude in size ranging from submicron constituents to millimetre or centimetre sized subunits, through to gross morphology and structure up to tens of centimetres across. This requirement is common to many systems both in biology and materials science.

The IMBL is anticipated to be in great demand for radiotherapy and a wide range of clinical and other imaging applications requiring its high-energy, high-coherence and large-size beam. The dedicated MCT beamline will enable the IMBL to be reserved for those MCT projects where its specific properties are required and will provide a more suitable beamline for the significant demand for MCT at lower energies, but which cannot be satisfied with lab-based systems. It is also possible that the micro CT beamline could share some equipment used for MCT on the IMBL such as grating phase-contrast and grating-based phase-contrast assemblies, environmental cells, strain stages and so forth.

2.3.2 Existing Computational hardware and software

The MCT beamline will be able to capitalise on high speed CT reconstruction software being developed for the synchrotron's MASSIVE cluster under the NeAT project to develop a Remote CT Reconstruction Service. This will be particularly valuable for high-throughput work in providing real time feedback to users on how their data collection is progressing, thus enabling a more efficient use of beam time.

There is a possibility of a second NECTAR proposal to further develop the Remote CT Reconstruction capability and we will aim to ensure that any additional requirements specific to the MCT beamline are taken into account. This could include, for instance, improved support for grating-imaging and tomography, or region-of-interest tomography.

2.3.3 Melbourne Centre for Nanofabrication (MCN)

The MCN is adjacent to the synchrotron site and has capacity to fabricate gratings and other optical elements such as multi-layers and zone plates now that the new e-beam facility has been commissioned. Taking advantage of these facilities is highly desirable for sourcing some of the beamline components and for building capabilities for future improvements. This may include new types of multi-layer mirrors, new types of gratings for grating-based phase contrast, and improved hard x-ray zone plates.

2.3.4 Local X-ray imaging/detector community

There is a strong scientific community around Melbourne in the areas of x-ray imaging techniques – especially phase-contrast methods, and detector development. This user community will contribute to the enhancement of the beamline, as well as benefitting from it. Engagement with collaborators in the area of phase-retrieval algorithms, for example, would ensure that the beamline has access to the best and newest available algorithms for image analysis.

2.3.5 Existing lab-based MCT facilities

One reason for the increasing interest in MCT in recent years is the much wider availability of 'off-the-shelf' lab-based MCT systems. Many of these have been installed in university departments and research institutes in recent years, most operating as multi-user characterisation facilities. It is likely that in addition to users who are already making use of synchrotron MCT, a growing proportion of future users will emerge from users of these lab-based facilities who find they need the additional capabilities a synchrotron offers to take their research to the next level.

The managers of these lab facilities will therefore be extremely valuable allies in making sure that appropriate applications are directed to the synchrotron after preliminary lab-based studies have been carried out, resulting hopefully in a better prepared and informed user-base and therefore more effective use of beamtime. Maintaining good lines of communication with the scientists running these lab-based MCT facilities will be of great importance to the success of the beamline. It is also desirable that, where possible, innovations such as algorithms developed for the MCT beamline are made available to be adopted by the MCT community around Australia.

2.4 Potential demand & user survey

The user community for the MCT beamline includes both scientists already using synchrotron MCT at overseas facilities and the growing number of researchers using MCT in the laboratory, many of whom have expressed interest in the MCT beamline proposal (over 100 people have joined the MCT mailing list).

Laboratory use of MCT techniques has grown considerably in recent years with the growing availability of turnkey MCT systems from companies such as Skyscan, GE/Phoenix and Xradia a number of which have been installed as multi-user facilities in many Australian universities and research institutes in the last few years. The MCT community will be holding its third national meeting later this year, and a number of regional workshops have been held in recent times, reflecting the growing interest in MCT methods.

Using the measure of publication rate, the use of MCT for both laboratory machines and synchrotron-radiation, can be seen to have boomed in the last decade; in bone microstructure the publication rate has been particularly impressive (see Figure 2).

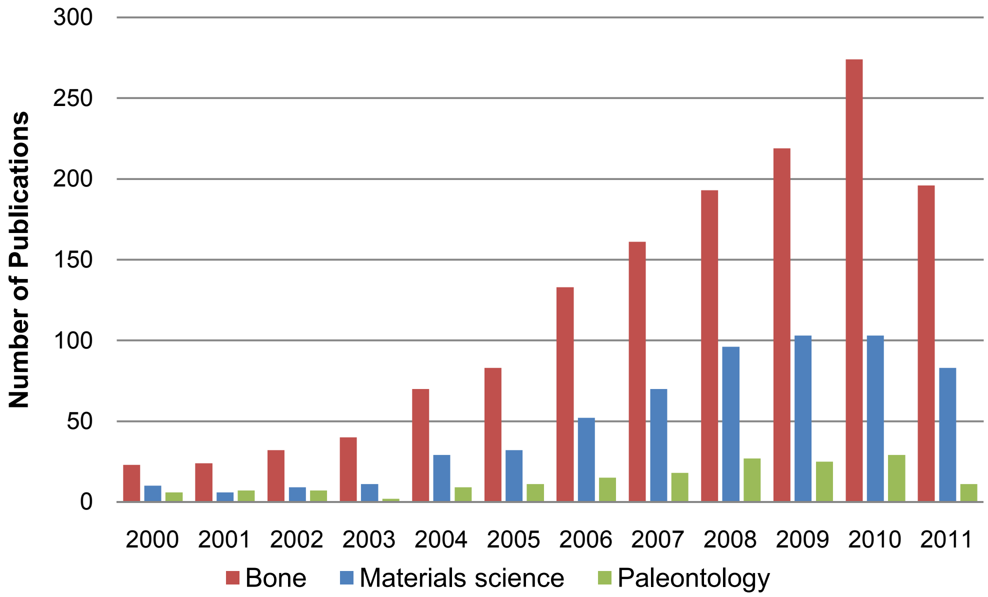

Figure 2 – Web of Science Publication rates for micro-computed tomography use in several disciplines (as at mid-August 2011). Note that engineering-related fields including the geological and materials areas are not well captured by Web of science and are likely to be underestimated.

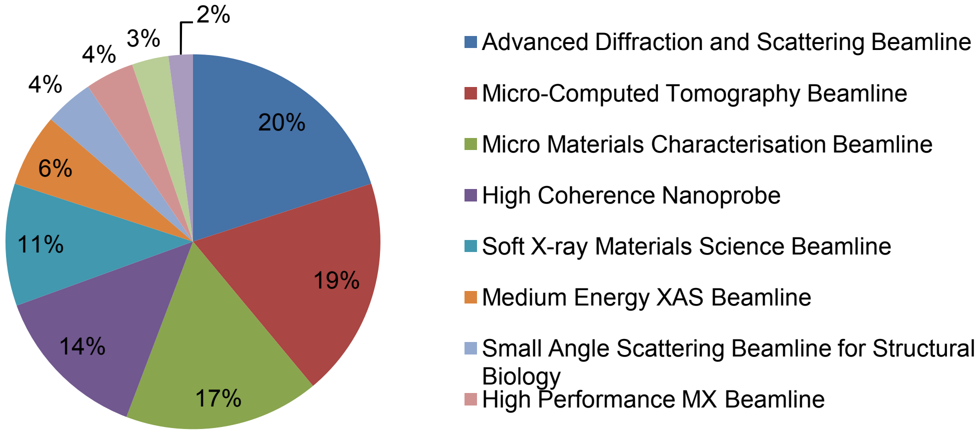

Figure 3 – ISAP demand for the ten SC2 beamlines

Data from the International Synchrotron Access Program (ISAP), 2009-11[1], indicates that MCT is arguably amongst the top 3 techniques sought by Australian researchers at overseas facilities (see Figure 3). Demand for travel funding support for synchrotron MCT is already comparable to that requested for large scale imaging that is likely to move to IMBL when it opens to general users (expected late 2012).

The MCT BSG has sought input from the existing and potential users of the beamline to assist in defining the beamline's key performance criteria (full details of the survey are included in Appendix D). It is noteworthy that the respondents are conducting both fundamental and applied research, and are drawn from the broadest possible range of disciplines. The predominant discipline areas using MCT are materials science (23% of responses), physics (23%) and medical/health/biological sciences (32%), with significant activity also in geosciences, environmental sciences and engineering (note that many respondents have self-identified themselves as working in more than one discipline area). It is also noteworthy that approximately 30% of the survey respondents have (or at least have access to) a laboratory CT device, but 75% of the respondents had also accessed an overseas synchrotron facility (on average, each survey respondent had used 1.25 overseas facilities). The most highly accessed overseas facilities for MCT were SPring-8 (20B2, 20XU), APS (2-BM-2) and ESRF (ID19, ID 22).

There is a significant community of x-ray imaging specialists within Australia with strong interest in x-ray phase-contrast and synchrotron techniques. This is reflected in the (somewhat anomalously) high participation rate from physicists in the user survey. This community will enable the MCT beamline to benefit from cutting edge software methods in phase-retrieval and tomographic reconstruction which will considerably enhance its performance.

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[1] Data provided by ISAP covers Quarter 4 2009 – Quarter 2 2011

3. TECHNICAL OUTLINE

3.1 Beamline outline

The primary parameters of the beamline are listed in Table 2 below. The layout relative to the IMBL hutches on the experimental floor is sketched in Figure 4, and the three operating modes are sketched in Figure 1. The specific questions raised in the BSG Guidance Notes are directly addressed in Appendix A.

Energy Range	8-40keV	
Source type	Bending magnet	
Monochromation type	White beam, Pink beam, Multilayer broadband monochromator (bandwidth 2%), Si monochromators (bandwidth 0.02%), possible option of extra broadband multi-layer (bandwidth 8-10%)	
End stations	Station 1 (upstream)	a) parallel-beam imaging and MCT with option of inline phase contrast. Including high-speed with automated sample exchange. b) Focussing-based high-resolution imaging/MCT mode.
	Station 2 (downstream)	Grating-based phase-contrast imaging/tomography
Field of view	Station1	4mm V x up to 2cm H (standard) 50-100microns (focussing mode) (can cover larger areas by stitching)
	Station 2	6 mm V x up to 3cm H (can cover larger areas by stitching)
Pixel size range & max resolution	Inline phase-contrast/absorption contrast	Pixels: 0.2 - 10um Max resolution: ~0.7um
	Grating-based phase-contrast	Pixels: 1- 10um Max res: ~4um
	Focussing-based high-resolution mode	Pixels:20nm Max res: (~100nm imaging, ~200nm tomography)
Minimum tomographic data collection speed	Inline phase-contrast/absorption-contrast	Subsecond in high-speed mode, 5-10min at maximum resolution
	Grating-based phase-contrast	15-45 min
	Focussing-based high-resolution mode	15-30min

Table 2 - beamline parameters

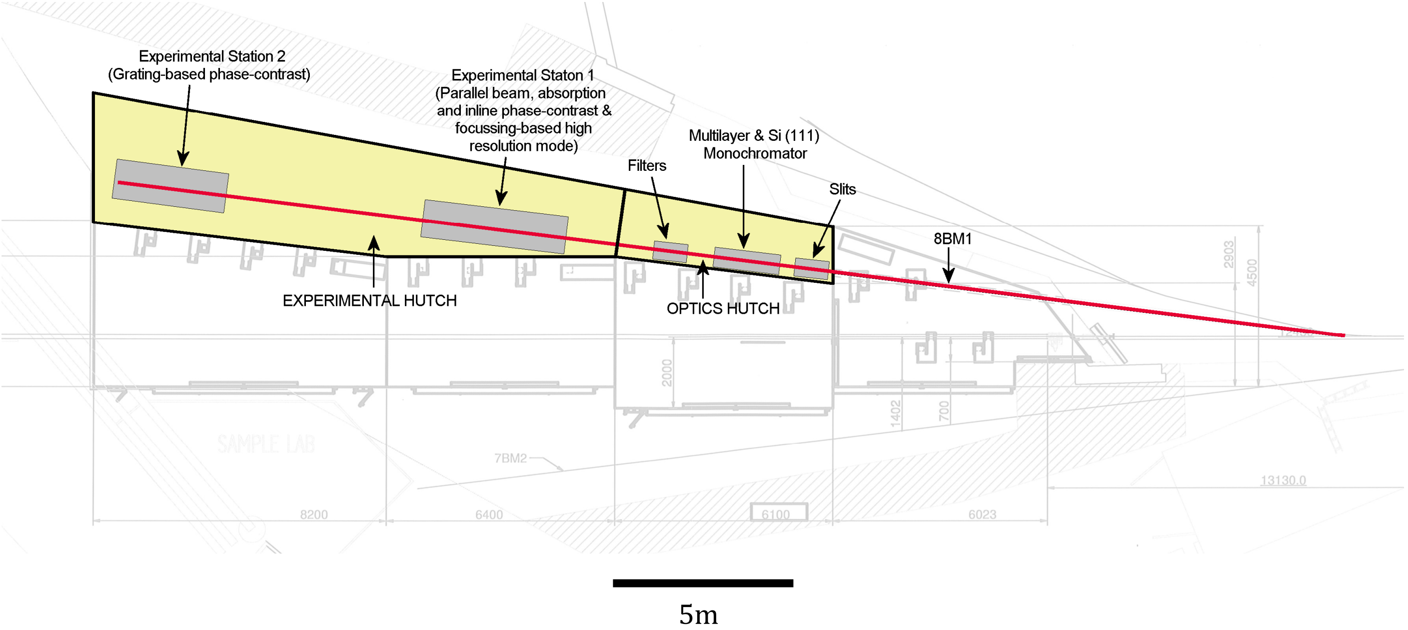

Figure 4 - Sketch of beamline location and major components relative to existing IMBL hutches

3.2 Comparable beamlines around the world

3.2.1 General survey of beamlines

Tables 3-5 give details of the basic parameters of a number of hard x-ray MCT beamlines at synchrotrons around the world operating in absorption, phase-contrast and focussing optics-based modes. In many cases a single beamline will operate in at least two of these modes. These tables have been adapted from Borbely et al in Fabrication and Characterization in the Micro-Nano Range, Advanced Structured Materials, 10. The equivalent parameters for the proposed beamline have been included for comparison at the top of each table (NB the tables don't include data for maximum possible data collection speeds or grating).

The majority of these beamlines have been built on the high GeV synchrotrons, ESRF, APS and Spring 8, and have access to the high-flux and harder energy range available on those sources. In addition to the beamlines tabulated below, other hard x-ray MCT capable beamlines exist or are in development at ALS, SSRL, SSRF, PETRA III (IBL), ANKA (IMAGE) and Diamond.

Some of the beamlines are on synchrotrons more comparable to the Australian synchrotron, based on bending magnets and targeting an energy range comparable to what is envisaged for the MCT beamline. These are ANKA TopoTomo, ALS Beamline 8.3.2, SLS TOMCAT and NSLS X2B (little information is available about this last beamline). The ANKA, ALS and TOMCAT beamlines can all operate in white-beam mode for high flux, and ALS 8.3.2 and TOMCAT have multilayer monochromators for high-flux monochromatic applications, whereas ANKA TopoTomo is planning a Multilayer upgrade in the near future.

Of these beamlines SLS TOMCAT provides a very attractive model in terms of user-experience and scientific impact. There is also considerable technical information available about this beamline both in papers and also from the very open and helpful beamline team led by Marco Stampanoni.

Facility/Beamline		Source type	Beam types (WB, BBMono, SiMono)	Energy range (keV)	Min voxel size/ Max resolution (µm)	Min scan time at highest resolution
AS MCT (proposed)		**Bending magnet**	**SiMono, BBMono, WB**	**8-40**	**$(0.2)^2$ / ~1**	**~10-20min**
ESRF 6GeV	ID19	2 Undulators/wiggler	SiMono, BBMono, WB	7–60	$(0.3)^3$/~1	~15 min
	ID15	Undulator/wiggler	SiMono, WB	30–250WB	$(1.1)^3$/~2	100 ms
	ID22	2 undulators	Undulator monochromatic	7–65	$(0.3)^3$/~1	~30 min
APS 7GeV	2-BM-B	Bending magnet	SiMono, BBMono	5–30	$(0.67)^3$/~1	~6 s
	5-BM-C	Bending magnet	Ge(220) Mono	10–45	$(2.4)^3$/~4	~6 h
	13-BM	Bending magnet	SiMono	6–70	$(1.0)^3$/~2	~30 min
	32-ID	Undulator (APS A)	WB, SiMono	8–35	$(0.3)^3$/~1	~250 ms
SPring-8 8GeV	BL20B2	Bending magnet	SiMono	8–113	$(2.74)^3$/~1	~100 min
	BL20XU	Undulator	SiMono	8–113	$(0.2)^3$/~1	~25 min
	BL47XU	Undulator	SiMono	6–37.7	$(0.2)^3$/~1	~25 min
DESY (4.45 GeV)/HARWI-II		Wiggler	SiMono, SiGe gradient mono	16–150	n.a./n.a	. n.a.
BESSY-II (1.7GeV)/BAMline		WLS	WB, SiMono, BBMono	6–80	$(1.4)^3$/~4	2–3 h
ANKA (2.5GeV)/TopoTomo		Bending magnet	WB	6–35\40WB	$(0.9)^3$/~2.5	~2.5 h
SLS (2.4GeV)/TOMCAT		Superbend	WB, BBMono, SiMono	8–45	$(0.37)^3$/~1	~10–15 min

Table 3 – Details of hard x-ray MCT beamlines operating in absorption contrast mode (WB=white beam, BBMono = broadband monochromation, SiMono = narrowband monochromation)

Facility/Beamline	Energy range(keV)	Min voxel size (µm)/Max resolution (µm)	Min scan time at highest resolution
AS MCT (proposed) in-line [grating]	**8-40 [12-20]**	**(0.3)^2 / ~1 [(1.0)^2/4.0]**	**~15-25 min [~15-60min]**
ESRF (FR) ID19	7–60	(0.28)^3/~1	~15 min
ESRF ID15 (white beam)	20–250	(1.1)^3/~2	100 ms
ESRF ID22 (propagation technique)	7–65	(0.3)^3/~1	~30 min
APS (USA) 2-BM-B	5–30	(0.67)^3/1	~6 s
APS 13-BM (propagation technique)	6–70	(1.0)^3/~2	~30 min
APS 32-ID	8–35	(0.3)^3/~1	~10 s
SPring-8 (JP) BL20B2 (Bonse-Hart interferometer)	15–25	(11.7)^3/~30	~120 min
BL20B2 (Talbot interferometer)	8–15	(5.5)^3/~12	~90 min
BL20B2 (propagationtechnique)	8–113	(2.74)^3/~10	~100 min
BL20XU (Bonse-Hart interferometer)	10–25	(2.74)^3/~10	~180 min
BL20XU (propagation technique)	8–37.7	(0.2)^3/~1	~25 min
BL47XU (propagation technique)	6–37.7	(0.2)^3/~1	~25 min
BESSY II (DE)/BAMline	6–80	(1.4)^3/~4	2–3 h
ANKA (DE)/TopoTomo (WB)	<40	(0.9)^3/~2.5	~2.5 h
SLS (CH) TOMCAT (propagation technique)	10–40	(0.37)^3/~1	~10–15 min
SLS TOMCAT (differential phase contrast)	14–35	(3.5)^3/~5	~10–45 min
ESRF (FR) ID19 (holotomography)	7–60	(0.3)^3/~1	~15 min per distance
BESSY II/BAMline (holotomography)	6–80	(1.4)^3/~4	2–3 h per distance

Table 4 – Details of hard x-ray MCT beamlines operating in phase-contrast modes

Facility/Beamline	Type of contrast	Energy range(keV)	Max sample diam. (μm)	Min voxel size/Max resolution	Min scan time(min)
Magnified synchrotron tomography using FZP					
AS MCT (proposed)	**Absorption/zernike**	**10keV**	**50-100um**	**(<30nm)^2 / ~(150nm)^2**	**~20-45**
SPring-8 (JP) BL47XU	Absorption	6–12	~70	(40 nm)^3/~(200 nm)^3 at 8 keV	~25
	Zernike Phase plate	~8	~70	40 nm)^3/~(200 nm)^3 at 8 keV	~25
	Differential phase contrast by Talbot interferometer	8–10	~70	(40 nm)^3/~(200 nm)^3 at 8 keV	~90
APS (USA) 26-ID (multilayer Laue lens)	Absorption/phase	8–10	~10	(30 nm)^3/n.a.	120
APS 32-ID	Absorption/phase	7–17	~25	(11 nm)^3/(40 nm)^3 at 8 keV	~20
SLS (CH)/TOMCAT	Absorption	8–12	~50	(16 nm)^3/(144 nm)^3	~15–40
	Zernike phase contrast	10	~50	(16 nm)^3/(144 nm)^3	~20
Magnified synchrotron tomography using Kirkpatrick-Baez mirrors					
ESRF/ID22	Holotomography (e- density map)	17–29	~400	(50 nm)^3/~(180 nm)^3	~80
Magnified synchrotron tomography using Compound Refractive Lenses					
ESRF/ID15A	Absorption	30–50	~100	(100 nm)^3/~(200 nm) 3	~5
Magnified synchrotron tomography using Bragg crystals					
BESSY II/BAMline	Absorption/phase	10–40	~100	(150 nm)^3/~1 μm3	n.a.

Table 5 – Details of hard x-ray MCT beamlines operating in additional imaging modes with focussing optics

3.2.2 SLS TOMCAT as a guide to design, specifications & performance

As noted above SLS TOMCAT provides an attractive template for a MCT beamline at the Australian synchrotron in a number of respects:

- Sufficiently similar parameters to a BM beamline at the Australian Synchrotron to be useful as a guide to expected performance
- Using multi-layer mirrors to get the most benefit from a bending magnet source,
- 3 phase-contrast modes (phase-contrast is a major interest of the Australian scientific community)
- Focus on high-speed and high-throughput applications
- Well integrated beamline components giving a good user experience and supporting high-impact science outcomes.

In addition the TOMCAT team have been very helpful and open with information about the design and operation of this beamline.

In using SLS TOMCAT as a template and starting point for the design of a MCT beamline at the Australian Synchrotron it is important to be mindful of some differences which will impact performance at the Australian Synchrotron relative to SLS TOMCAT. These are the lower critical energy of an AS bend (7.8keV) relative to an SLS superbend (11.1keV), and the somewhat larger electron beam-size (effectively the x-ray source size) at the AS (σ_x = 87 vs 47μm).

The difference in critical energy will reduce the flux at the upper end of the energy range, so that the AS flux density at 40keV will be approximately 20% of that at SLS. At lower energies the effect will be less marked with 40% of the SLS flux density at 20keV and 70% at 8keV (see Figure 5). In the light of this, additional steps in optical and monochromators design to give higher-flux for the 20-40keV range should be considered. A greater focus on pink-beam operation at higher energies may also be warranted with close attention paid to the most efficient possible detector scintillators. This would be particularly valuable for geological, paleontological and bone/tooth specimens each of which represent significant areas of user interest.

The difference in horizontal source size between AS and SLS BMs will mean that in phase-contrast modes, such as in-line or grating-based, penumbral blurring may start to affect the phase-contrast signal at shorter propagation distances than at TOMCAT. However, given the high resolution focus of the beamline this will not be apparent under experimental conditions used for most experiments. Only at the lowest resolutions and highest energies will this have an effect.

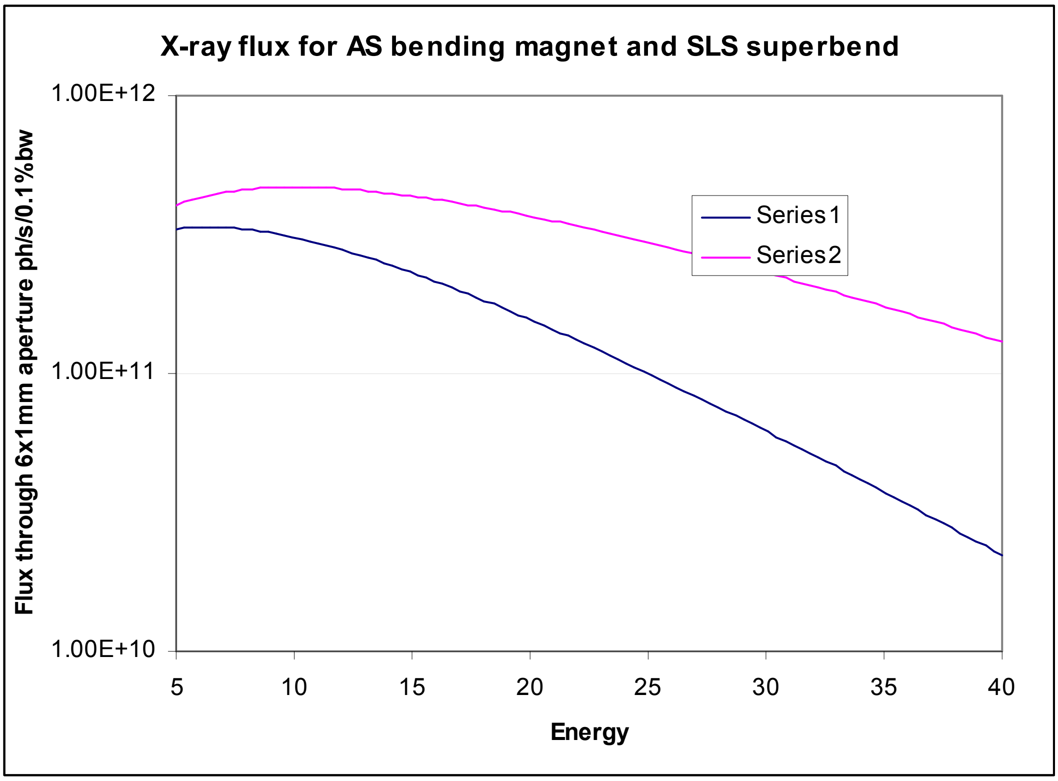

Figure 5 – Plot showing comparison of flux through aperture at 25m from SLS TOMCAT (pink) superbend vs Australian bend (blue).

Some additional specific issues that may warrant significant differences between a design for the AS versus SLS are as follows:

The multilayers will need to be further from the source than at SLS where they are inside the shield wall (~14m compared to 7m). This will have implications for multilayer length required to capture a similar vertical extent of the beam. In addition the TOMCAT experience suggests a greater vertical spacing between white and monochromatic beam would be desirable (and this is a likely consequence of longer multilayers in any case).

Since the focussing-based imaging mode is being recommended to be built in from the start, this may offer options that enable improvements to be made over the TOMCAT design. Options to improve the proportion of the beam captured by the condenser should be investigated. A more speculative possibility is that of an achromatic objective which would make better use of the broadband monochromatic beam and significantly speed up data collection.

3.3 Source considerations

The source for this beamline will be a bending magnet and the beamline will operate in the 8-40keV energy range. As such the beamline will be more tightly focussed on the small scale applications with lower x-ray energy requirements but a need for higher resolution and high speed or high-throughput. This will make the beamline complementary to the capabilities of IMBL which is the obvious beamline for larger scale imaging/tomography at higher energies.

During the BSG deliberations higher energy sources were initially considered in the light of reviewer & SAC comments. It was found that use of an insertion device for a beamline operating inside the experimental hall would result in significant reduction of phase-contrast performance relative to a bending magnet due to the larger electron beam size in the straight sections (σ_x=300um vs σ_x=80um in the bends – see Figure 6). The second option of a superbend is attractive in theory but impractical at the Australian Synchrotron on account of the lattice design. It was decided that remaining with a bending magnet targetted more specifically at smaller-scale, higher-resolution applications would produce a better focussed beamline that is complementary to rather than overlapping with IMBL.

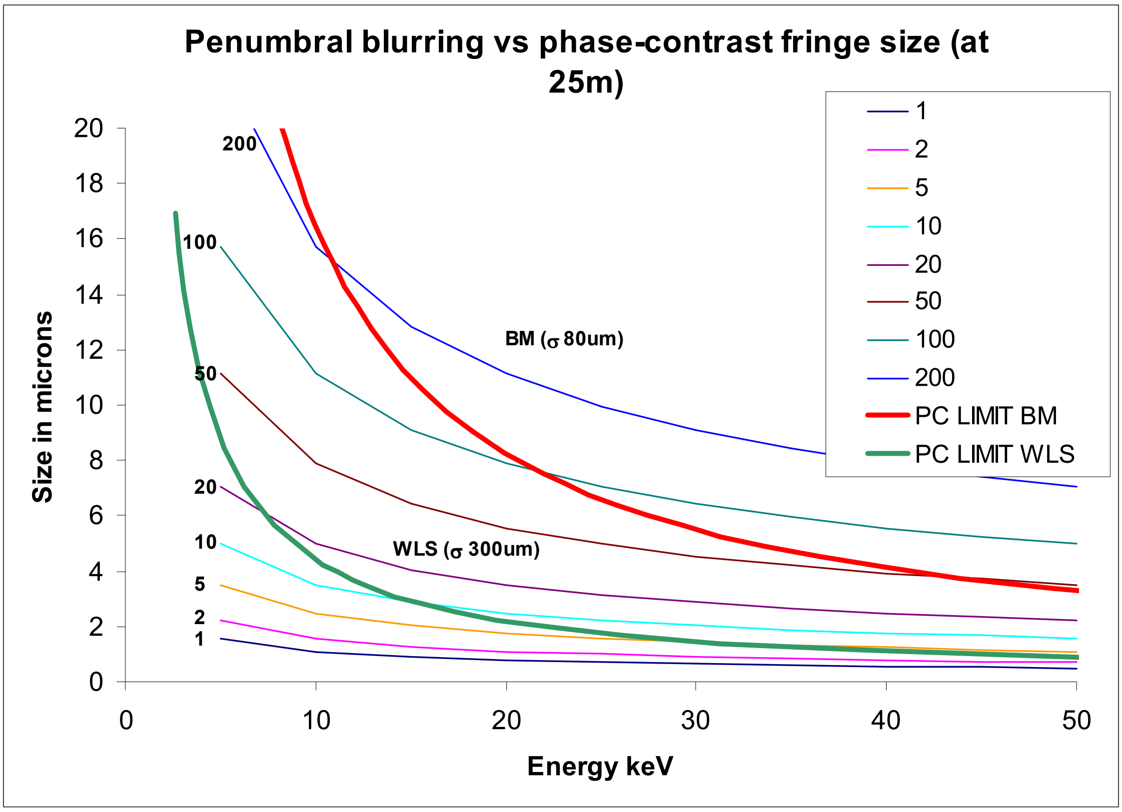

Figure 6 – The thin curves show approximate size in microns of phase-contrast fringes for a point source (estimated from $\sqrt{(\lambda R)}$ where λ is wavelength and R is propagation distance) for various propagation distances (cm) versus energy in keV. The thicker curves indicate the point at which penumbral blurring due to source size is equal to the point-source Fresnel fringe size for a bending magnet (red) and a wavelength shifter in a straight-section (green). Above these curves phase-contrast will be significantly affected by penumbral blurring. This effect is much worse for a wavelength shifter in a straight section than for a bending magnet.

3.4 Operating modes

3.4.1 Parallel-beam absorption-contrast and in-line phase-contrast MCT/imaging

Parallel-beam absorption-contrast and in-line phase-contrast imaging/tomography will be the most straightforward imaging modes of the beamline. In these modes it will be possible to use a white or pink beam as well as with a broad-band monochromatic beam from a multilayer and a narrowband monochromatic beam from a Si monochromator. Changing to in-line phase-contrast only involves moving the detector further from the sample.

Good quality sample stages (especially the rotation stage) and good high resolution detectors will be needed to get the most out of these imaging modes.

3.4.2 Grating-based phase-contrast

This mode of operation enables a phase-contrast mode which is similar to that of analyser-based imaging (sometimes known as 'DEI') but which works effectively with the broad-band monochromatic radiation produced by the multi-layer monochromators. This will be situated at the second experimental station at the downstream end of the hutch. Here there will be a somewhat larger field of view available which will suit the slightly larger scale and the resolution of a few microns available in this mode. It will be ideal for getting good contrast from biological specimens.

This mode requires a pair of gratings and associated translation/rotation stages between the sample stages and the detector. This will remain set-up at the second experimental station to minimise changeover time between this and other modes.

3.4.3 Secondary focussing-based high-resolution imaging mode

While parallel beam imaging can achieve slightly better than 1 micron resolution, this leaves a resolution gap between that and the 100nm scale which is the upper end of the length-scale for SAXS analysis. A secondary imaging mode based on focussing optics aiming for a resolution of 100-200nm would bridge this gap. Given the increased focus on the smaller-scale, high resolution applications for this beamline, the BSG has come to the conclusion that this capability should be built into the beamline from the start.

A system of this type has been operating successfully at the SLS TOMCAT beamline via a reasonably straightforward adaptation of the primary experimental station to accommodate a condenser and objective optic, both of which are diffractive optics. Interestingly this system is run using the broadband monochromatic beam and achieves 144nm resolution in imaging and 200nm in tomography with a 50 micron field of view. The regular rotation stage, carefully characterised, has been found to be sufficient at this resolution.

By designing this mode in from the start it may be possible to improve on the TOMCAT design in some respects as there is greater flexibility in, for instance, the location (and therefore design) of the condenser to potentially capture more flux, or perhaps an improved objective design.

3.4.4 High-speed/High throughput operation

High-speed operation is a central focus of this beamline. High-speed enables dynamic MCT where changes over time can be observed in 3D via fast tomography. Alternatively high-speed enables high-throughput operation where many similar samples can be imaged relatively quickly with automated sample exchange.

Retaining the ability to use the white beam from the source is particularly valuable in terms of high-speed operation for observation of dynamic processes, which will require the maximum flux we can supply, particularly since we are using a bending magnet source. A pink beam modified with filters to remove low energy radiation and reduce beam-hardening would be most suited to this. This type of operation is available at a number of MCT beamlines.

The requirements of high-speed operation include high-speed detectors with good sensitivity, high-speed rotation stages and suitable robotics together with kinematic sample mounts for sample exchange.

3.5 Critical components & specifications

3.5.1 Hutch layout & location

The proposed location for the beamline is as suggested on the original proposal, namely the bending magnet immediately adjacent to IMBL. One potential issue for the beamline is that access to the beamline is restricted by IMBL which passes through the synchrotron's outer wall on one side, and by the proposed high-coherence beamline which will also pass through the outer wall on the other. Access to the rest of the synchrotron will therefore be rather difficult and this issue will need to be addressed. The existing hutch layout of IMBL also places some restrictions on the hutch shapes and sizes for the MCT beamline, however, a satisfactory layout should be achievable.

The beamport for 8BM1 Emerges in the optics hutch of IMBL (1a). Space constraints mean that few components for the MCT beamline's optics can be accommodated in the IMBL hutch. Beyond the IMBL optics hutch the BM beam runs parallel to the outside of IMBL 1b initially. The space would be tight as the beam path is only 50cm from the wall at this point, however, it would be desirable to make used of this section as the optics hutch for the monochromators and filters in order to preserve more space for the experimental hutch.

The experimental hutch should be as long as possible so as to be able to get higher flux at the upstream end and better phase contrast (especially for gratings) at the downstream end. Ease of moving components along the length of the hutch, possibly using some kinds of track or rail would also be very valuable. There would be two main experimental stations in the hutch.

Experimental station 1: This would be close to the upstream end and would include the components for parallel beam micro CT with absorption-contrast and in-line phase-contrast. It would also accommodate the components for the secondary imaging mode with focussing optics. A long table (4m at least) with well thought out and flexible layout should reduce time to switch between these modes. An important requirement is a rail for moving the detector to increase the sample-detector distance up to 2m, and the ability to fix a condenser around 1m or so upstream of the sample. The components of the first station should be capable of being moved laterally out of the beam-path, with sufficient margin to enable a He-filled beam-transport pipe to be moved into place to reduce scattering when experiments are being carried out at experimental station 2. This station will need to accommodate a robot for automated sample exchange.

Experimental station 2: This would be at the downstream end of the hutch. It would be another long table accommodating a second sample stage (including rotations/translations) and the stages, gratings and detector for the grating-based phase-contrast mode. It would be useful if the grating unit could also be moved out the way to enable this station to also be used for absorption or in-line phase-contrast MCT (like station 1) in cases where the somewhat larger field-of-view is required. It my be necessary to have a small separate table for the gratings enabling them to be decoupled from sample stage vibrations.

3.5.2 Monochromator

The beamline will use multi-layer mirror monochromators. These have a broader bandpass (~1%) than conventional monochromators thus giving a flux increase of around a factor of 100. Developments of MCT beamlines around the world confirm that this is a good choice as new beamlines are being built with MLM monos and older ones are being upgraded to use them. The high flux is essential for our high-speed and high-throughput modes of operation, and will enable us to get the most out of our bending magnet source. Stability of the monochromators set-up is essential to ideally minimise the movement of any flat-field features on the detector to sub-pixel during a typical data collection run. This will require particular attention to vibration, including up to high frequencies of a few kHz as very high speed data collections of 1000’s of frames a second are envisaged.

It is also valuable to have the option of narrowband monochromation for certain quantitative applications. SLS TOMCAT have solved this by having their multilayers (two stripes to cover the whole energy range) on a Si 111 substrate so that both narrow-band and broadband monochromation are available using a single assembly. This has worked well at SLS and is an attractive design option for our beamline, particularly given the space constraints. The mirrors are mounted on two towers, one of which can move up to 80cm with respect to the other to enable the switch between Si and MLM modes.

Multilayers for both SLS TOMCAT and the upgrade to APS 2BM were both supplied by Incoatec. The rest of the monochromator assembly at SLS was designed and manufactured by Cinel, whereas the systems at APS was of in-house design & manufacture. Our colleagues at SLS did indicate that they would prefer a slightly larger gap between the white and mono beam than they have with their current setup. MLMs at the AS would have to be longer to accommodate the greater distance from the source.

As noted previously the AS bending magnet source has lower flux at the upper end of the desired energy range than SLS TOMCAT. For this reason it is worth investigating the option of an additional multilayer stripe for the higher energy range which is depth-graded to give a wider energy band than the typical 1%. Rigaku have produced this type of high-bandpass depth-graded multilayer for CLS (Vespers). Another approach to boosting flux density (at the expense of vertical field of view) is to have bending for vertical collimation on the second multilayer as implemented at BESSY BAMline and ANKA Topotomo.

Either of these options would have to be weighed against any potential consequences for performance with respect to system stability /susceptibility to vibration and beam coherence, which are ultimately of higher priority.

3.5.3 Windows & filters

As the beamline will frequently be used in phase-contrast mode it is essential that the beam is delivered as cleanly as possible with the minimum of phase-artefacts introduced by the windows and filters. The final window should be CVD diamond rather than Be which cannot be polished sufficiently well to eliminate phase artefacts. Filters will be essential for pink-beam operation but likewise will need to be high quality and highly polished.

3.5.4 Tables and stages

Long stable optical tables will be required for each of the experimental stations so that all components for a given experimental mode are on a common stable surface. Excellent stability and damping of vibration will be essential.

Two tables will be required, one for each experimental station. The first table will accommodate the focussing based imaging mode hardware as well as the standard parallel beam with absorption/phase contrast. This table will need to be at least 4m long. The second table will accommodate the grating-based imaging setup and a somewhat shorter table of 2-3m should be sufficient.

It may be useful to have a smaller third table that can move between the two to give flexibility for experiments requiring unusual distances between components eg testing optics or novel techniques. A further consideration is the provision of a table dedicated to the gratings to decouple them from any vibrations arising from the sample stage.

A sample stage is required for each of the two experimental stations. Each sample stage will require a stable goniometer base and XYZ movement and 2 tilt stages. The rotary stage for the first experimental station should be an air-bearing stage to give the precision required for the secondary focussing based imaging mode. X-Y movement on top of the rotary stage is required for sample alignment, and additional tilt stages are also desirable

Detectors will need a stable base with tilts for alignment.

The grating-based phase contrast systems will require stages for alignment of the gratings with respect to one another (tilt, rotate, separation translation movement) and nanometre precision movement of the second grating laterally with respect to the first. SLS have developed a high precision flexure-based stage for this lateral movement task. At SLS the grating assembly is mounted independently of the sample and detector stage to prevent transmission of vibration. This option should be considered.

The secondary focussing-based imaging mode will require stages for the condenser, objective, phase plate and order sorting aperture. These are required to align and position the components but are not required to move during an experiment. These require micron level precision and need to be very stable when not moving.

3.5.5 Grating-based phase-contrast components

The grating-based phase-contrast imaging set-up requires two gratings, a phase grating and an absorption grating at half the pitch of the phase grating. These will be mounted in stages to allow the distance between them to be varied (as required for different wavelengths, to tilt the phase grating about the Y axis (again to match a 2pi phase shift for the selected wavelength), and to align the two gratings precisely. A high precision lateral movement of one grating with respect to the other will also be required as noted above.

Working with MCN to produce suitable gratings would be desirable.

3.5.6 Secondary focussing-based imaging mode components

The primary components required for the focussing based imaging mode are condenser and objective lenses plus a Zernike phase plate. The condenser and objective, if following the SLS model, would both be diffractive optics. The condenser would be a large scale diffractive optic of 1mm x 1mm at least and the objective smaller scale but higher resolution optic of about 100nm in diameter.

The components together with the phase-plate could be manufactured by MCN as the new e-beam writer has sufficient resolution and speed for this task. Working with MCN to build these components would also build the capacity of MCN to make similar useful components for the synchrotron, and offers the possibility of research into improved optics. Matteo Altissimo, who runs the e-beam facility, has considerable previous experience in manufacturing novel Fresnel optics for synchrotrons and it would be of benefit to the synchrotron to capitalise on this.

3.5.7 Detectors

High-speed detectors are essential to meet the requirements for dynamic MCT and high-throughput MCT. High-speed CMOS cameras optically coupled to scintillators are the best option currently. Such high-speed cameras are available from PCO and are in operation at APS, SLS and IMBL. Optical couplings are available from Optique Peter or

Hamamatsu. It may be that more conventional CCD cameras, possibly with different optical coupling, will also be required for specific applications.

IMBL has recently purchased high-speed cameras from PCO (the PCO Edge) together with Optique Peter and custom-designed front-ends. These cameras offer an opportunity to gain experience with the types of detectors required for the MCT beamline. For very high-speed work PCO offers even faster models than the Edge (PCO Dimax) which are being used at other high-speed MCT beamlines.

The detectors will need a range of types and thicknesses of scintillators to cover energy and spatial resolution ranges required.

3.5.8 High-speed shutters

High-speed shutters coordinated with the detectors will be essential for reducing the dose during data collection by ensuring there is only beam on the sample when the detector is actively acquiring. This will be particularly important for grating operation when multiple images are collected for each tomographic rotation angle with grating stage movements between each image. In additional to the amount of time spent on stage movements in this mode, the samples which are more likely to require gratingphase contrast are typically biological and more radiation sensitive.

3.5.9 Automated sample exchange

The SLS TOMCAT beamline makes use of a Staubli robot for automated sample exchange. This has been integrated with EPICS and has a Python-based GUI interface. This has been running smoothly at SLS TOMCAT for some time and frequently does high-throughput data collections of 300-400 samples over a weekend at a typical rate of 5-10min a sample. If possible it could save time and expense to use the same type of system and make use of this existing software if SLS are willing. A similar system is currently being developed on MX using an Epson robot which could be adapted to MCT requirements.

A second essential component for automated sample exchange is a kinematic sample mount which will locate a sample on the sample stage with close to a micron repeatability. Such mounts are in operation at SLS TOMCAT (their own design). An APS designed kinematic mount is also in successful operation at the XFM beamline at the Australian synchrotron.

3.5.10 Sample environments

Given that high-speed dynamic experiments are a major focus of this beamline, the availability of specialised sample environments is essential to the feasibility of many experiments . Even experiments that are not necessarily focussing on dynamic changes may make use of controlled sample environments to keep a sample in its optimum condition, for instance controlled humidity or cryo-environments.

It has been the experience at MCT beamlines at other synchrotrons that the use of sample environments is increasingly common. Marco Stampanoni at SLS TOMCAT estimates over 80% of user experiments use a sample environment of some kind and the beamline is moving to make a series of standard sample environmental cells available including a laser based furnace (up to 1600 degrees), a cryo stage, humidity chambers and a tensile stage. Advice from Kentaro Uesugi also confirms the importance of assisting users to build sample environments.

Surveying our own users has indicated significant interest in a number of sample environments. After robotic sample positioning (for high-throughput), the most popular environments requested were temperature control (including furnace and cryogenic capabilities), humidity and pressure control. In addition to environments provided by the beamline, there should be a common platform & assistance for users to build and bring their own specialised sample stages, such as custom tensile rigs or fluid flow environments.

3.6 Computational & networking requirements

The MCT beamline will require access to real-time tomographic reconstruction including phase-retrieval processing for the in-line and grating-based phase-contrast modes. Most of this capability is already available through the Remote CT project which was developed for the IMBL, and based around the MASSIVE cluster for high-speed computing.

The X-TRACT software is the basic platform underlying the remote-CT project and already incorporates most of the features that would be required for the MCT beamline. Some additional features that would be required or desirable for the MCT beamline include phase-retrieval methods for grating-based phase-contrast, region-of-interest tomography, spiral-scan tomography and limited view tomography. The X-TRACT team already have experience with algorithms of these types and they could be readily incorporated into X-TRACT. It is likely that some of these additional features would also be beneficial to IMBL.

3D image rendering and segmentation is also an important requirement for tomographic datasets. Image rendering is already a component of the Remote CT project, and a proposed extension to this project could enable these capabilities to be extended. To ensure rapid publication and dissemination of results, analysis tools that permit extraction of quantitative information from data sets are particularly important. This need is not currently adequately serviced by existing computational infrastructure and software.

High throughput operation will generate vast amounts of data very rapidly (several TB per day). Consideration must be given to internal transport and management of this data as well as availability to users after their beamtime has concluded.

3.7 Priority List/ Stages for Beamline Commissioning

The beamline is intended to operate in three main modes, however, early availability of end station components would enable operation at least in a limited number of modes before the whole beamline is completed. The following list outlines a possible staging of various operating modes and components being commissioned:

1) White/pink beam operation – This could be available from an early stage in the beamline's development. As soon as a filtered beam can be delivered safely to the hutch it would be possible to carry out white or pink-beam imaging and tomography in both absorption and in-line phase-contrast modes, provided white-beam capable detectors and the sample stages were available.

2) Monochromatic (DCMM & SiMM) operation including in-line phase-contrast would be possible on installation of the monochromators.

3) High-throughput mode will be available following commissioning and testing of the sample exchange robot (this could happen in parallel with other activities).

4) Grating-based phase-contrast mode would be available following the commissioning and testing of the grating assembly

5) Focussing-based high-resolution mode would be available after commissioning and testing of the condenser and objective setup

3.8 Potential Technical Issues

3.8.1 Beamline location & difficulties with access

The proposed beamline location is bounded by the IMBL hutches in the 'anti-clockwise' direction relative to the ring, and by the proposed nanoprobe beamline on the other side. Both neighbouring beamlines pass through the outer wall of the synchrotron building, thus cutting the MCT beamline off from ready access to the rest of the experimental floor. The area just inside the outer wall is also occupied by the clean room which will become similarly inaccessible. The following issues should therefore be considered:

- Building the beamline may be made much harder if the nanoprobe beamline is built first and some direct access to outside is desirable (essential if nanoprobe is built first) for bringing larger pieces of equipment to the MCT beamline.

- There needs to be some form of internal access for users & staff to get to the rest of the experimental floor, or at least to the mezzanine. Will it be possible to go under the nanoprobe pipe? Also consider access requirements for special environments e.g. furnaces etc which may need forklift/crane (so also external door?)

- It is possible to pass under the beampipe of IMBL to access the proposed MCT area, however this is likely to be off limits during IMBL operation. Nonetheless this does provide a short-cut route for exchange of components between IMBL and MCT which may be useful on occasion

3.8.2 Optics location

The beamport for 8BM1 emerges in the optics hutch (1A) for IMBL and beyond this the beam runs within about 50cm of the external wall for the length of IMBL hutch 1B. IMBL hutch 1A is likely to have little room for optics components for the MCT beamline so the likely location for the MCT optics hutch is adjacent to IMBL hutch 1B as indicated in section 3.1. This means that space for the monochromator chamber and other optical components will be somewhat restricted by the proximity to the hutch 1B wall, which will have to be a consideration in the design of these components.

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APPENDIX A – RESPONSES TO QUESTIONS POSED IN THE BSG GUIDANCE NOTES

1. What is the required energy range of the beamline?
8-40keV (see section 3.1)

2. What is the required photon flux across that energy range?
Maximum accessible from an AS bend using either white/pink-beam, broad-band MLM monochromator or narrow-band silicon monochromators, making user of full vertical beam extent.

3. What spot size (or range of spot sizes) is required at the sample position?
The beam will not be focussed in most operating modes but used as a parallel-beam (see 3.4.1). In the high-resolution imaging mode the beam will be condensed to an area of 50-100 microns across (see 3.4.3).

4. Are there any special requirements for sample temperature or pressure?
Yes, provision of different sample environments is extremely important to meet users expectations. Basic environments requirements include high and low temperature stages, and variable pressure and humidity (see 3.5.10). Technical support for building specialised sample environments (furnaces etc) is critical to distinguish the beamline from others with otherwise similar capabilities worldwide, providing a key point of difference and attractiveness to users, and enhancing the beamline's ability to produce high impact outputs (at relatively low cost).

5. Are there any particular sample positioning, sample scanning or sample stability requirements?
See section 3.5 for further detail:

- Sample rotation with a high precision rotation stage (~100nm wobble -required for virtually all experiments)
- XYZ tilts below sample stage and XY (and perhaps tilts) on top of sample stage (positioning to a micron or better)
- High throughput robotic sample exchange with repeatability of sample positioning to a micron
- Ability to do vertical slot scanning of sample and detector simultaneously
- Ability to perform fine step scanning of grating for grating-based phase-contrast

6. Are there specific requirements for beam stability, ambient temperature stability or vibration suppression at the sample?
Yes, stability and vibration suppression are critical and require:

- Controlled temperature stability (+/- 0.5 degree) in hutch to prevent thermal drift
- Excellent vibration suppression on the monochromators for beam stability including up to high frequencies of a few kHz
- Excellent vibration suppression of the optical table holding the sample and detector - specifically relative movement between sample and detector need to be minimised to sub 100nm
- The sample, detector and grating motors should produce minimal vibration when in motion.

7. What are expected to be the main components in the beamline?
See section 3.5.

- Double Monochromators incorporating multilayers (broadband) and silicon monochromation with capacity to be moved out of beam for white/pink beam operation.
- Filters for removing low energy x-rays (including total external reflected x-rays from MLMs)
- At least 2 large optical tables in hutch
- High precision sample stage assembly including alignment stages and high-precision rotation stage.
- Grating-based phase-contrast assembly comprising gratings and stages, especially a high precision phase-scanning stage.
- Condenser and objective system for high-resolution imaging
- Robotic sample exchange for high-throughput

8. What types of detectors will be used?
Optically coupled CCDs for low noise) and CMOS (for high-speed) with optical couplings capable of a range of effective pixel sizes, and with exchangeable scintillators (see 3.5.7). It may also be useful to have a fibre optic coupled CCD for some purposes. High speed detectors especially need to be white beam capable.

9. Have we (or someone else) already developed the control software for the beamline, or control software that could easily be modified from another application?

- Tomographic control software for IMBL developed by Anton Maksimenko could be adapted for this beamline.
- Software for operation of filters at IMBL may also be capable of being adapted to this beamline.
- Control software for robotic sample exchange integrated with EPICS has been developed for TOMCAT SLS using a Staubli robot, and something similar is being developed for PX with an Epson robot (at an early stage).
- If the monochromators is produced by one of the manufacturers who have produced similar monochromators for other beamlines (eg Cinel for SLS or Axcell for ANKA) then it may be possible to adapt existing control software from one of these beamlines.

10. Are there any items which will require a specific development program, as they are not available commercially?
The Fresnel optics and gratings for the high-resolution mode and the grating-based mode are difficult to source commercially (see 3.4.3). Iit would be useful to investigate developing the skills to make these components at MCN (Matteo Altissimo at MCN already has experience in manufacturing these types of components).
The sample environments are not commercially available and some development program will be required. Fortunately there are a number of people who have developed sample environments for synchrotron and lab MCT systems including the ANU group, Florian Fusseis/APS, SLS TOMCAT beamline, Spring 8 MCT beamlines (user developed systems).

11. Are there specific suppliers that are preferred for certain components?
Yes, see appendix B.

12. Do we have price estimates already for some of the components?

Yes, see appendix B.

13. Are there specific software packages that will be required?
Reconstruction and visualisation software will be required – see section 3.6. Of the software requested by potential users X-TRACT and Drishti will already be available as part of the Remote CT project for IMBL on the MASSIVE cluster. Other visualisation software available on MASSIVE includes Amira/Avizo and ParaView. Freeware packages such as ImageJ are readily available.

14. What sample preparation or data analysis equipment will be required (that we don't have already in our support laboratories)?

- Light microscopes to support mounting of samples will be available in the IMBL laboratories but it would be beneficial if a microscope could be located closer to the hutch, particularly if access to the IMBL is restricted during mode 3 operation (i.e. x-rays being used in Hutch 3 in the Satellite Building).
- For high-throughput experiments (see 3.4.4), adequate kinematic mounts must be available to users in advance of their beamtime, with automated or semi-automated mounting and sample centring being highly desirable. This will need to be integrated into software for robotic sample handling.
- Data analysis is computationally intensive - see section 3.6. High-level user support for quantitative information extraction from tomographic data would be highly beneficial.

15. Are there any specific requirements for remote access to the beamline or automated sample handling and data capture?
Yes, for high throughput operation robotic sample exchange is required. Because of this it would be desirable to have remote access, at least to the extent of being able to check on the progress of high-throughput experiments running unattended. Remote access to data reconstruction and visualisation software on the MASSIVE cluster, as is already being developed for IMBL would be desirable (and presumably could be easily extended to include MCT as well).

16. If there are similar beamlines in operation at other facilities, explain any differences to our proposed beamline and why we are doing things differently.
See section 3.2

17. Who could help us with the detailed design of the beamline (we will consider paying specialist consultants)?
See Appendix C.

18. Do we have sufficient capabilities for the conceptual design with the AS or the BSG?
Yes, with adequate consultation with external expertise.

19. Are some of the identified experimental capabilities "desirable" but not "essential"?
Essential capabilities have been identified in section 2.1. Highly desirable capabilities include the provision of a variety of sample environments, and high level software support, particularly for quantitative data analysis.

APPENDIX B – SPECIFICATIONS, SOURCING OPTIONS & COST FOR CRITICAL COMPONENTS (PRELIMINARY LIST)

Note: In this table Z is vertical, Y is along the beam and X is horizontal, perpendicular to the beam

Main component	Sub-components	Specs	Potential Suppliers (and previous customers)	costs (where known)
Monochromator (DCMM)	Mirrors	• 2-3% bandwidth with 2 stripes to cover 8-40keV • Explore possibility of 3rd stripe duplicating high-energy range with higher bandwidth (8-10%) for improved flux , and/or bending on 2nd mirror for vertical collimation • slope errors figures in direction along and across the optic better than 0.5 *μ*rad RMS and 5 *μ*rad RMS respectively. • Surface roughness less than 0.3 nm RMS (Spec taken from SLS TOMCAT)	Incoatec (SLS/APS) Axo (BESSY & BAMline/ANKA Topotomo)	~EURO:80-85K (DO NOT SKIMP ON THIS COMPONENT) ?
	Mono assembly	• Must minimise vibration including at frequencies up to a few kHz (which would be visible for high-speed data collection). • Must minimise thermal (or other) drift over period of longest likely data-collections (hours).	CINEL Strumenti Scientifici, Padova, Italy (made the SLS DCMM) AXELL (ANKA and BESSY DCMMs) Oxford Danfysik (ESRF ID19) Rigaku (CLS VESPERS)	? (DO NOT SKIMP ON THIS COMPONENT)

Hutch		• Will require temperature stabilised aircon (+/- 0.5 °C) • Services: water, gases, gas extraction • Removeable beam-transport to far end		
Optical Tables	2 static tables, one at least 4m long (upstream end), second 3m (downstream end). Explore option of 3rd smaller moveable table between the two others.	• Highest possible specs for vibrations isolation (this is highest priority). • Some capacity for movement in X, Y and Z (manual OK) is desirable.	Kohzu (Spring 8) Newport	~$60K/ea. (manual) ~$120K/ea. (motorised)
Sample Stage & mount (motorised with suitable control software – probably beneficial to get the lot from one supplier)	Air-bearing rotation stage	• <+/-100nm eccentricity • Capable of high angular resolution and high speed continuous rotation (> 1 rev/s).	Aerotech Micos (Can either provide slip-ring connectivity for the substage?)	$20-30k
	XYZ & 2 tilts sub-stage	• 1 micron repeatability for sample relocation, • 0.1 micron for 1 axis perpendicular to beam (for moving sample to do flat-field) • travel +/- 25mm • perhaps also include larger coarse motions in both directions perpendicular to beam to move sample well out of the way – may depend on table movements		$10-12K +($5k for double coarse motion)

	XY & maybe 2 tilts sample alignment substage (on top of rotation stage)	• 0.1 micron repeatability for sample relocation, travel <10mm • Slip-ring connectivity so it doesn’t interfere with rotation stage		$4-7k (+$3-6k for double-tilt)
	Sample Stage controller	• Able to control all above axes and talk to computers/EPICS		$10K
	Kinematic sample exchange mounting system & sample stubs	• Mounting system must locate sample stub to 1 micron and at fixed angle about vertical axis. • Sample stubs must be numerous, cheap and able to make extras easily.	APS and SLS have designed their own systems – maybe we can copy one of these?	
Detector stage	XYZ & 2 tilt arcs	• 10 micron repeatability for XYZ, • travel +/- 100mm • Arcs need to be able to position within 1 pixel across whole detector (1:4000 or 250µrad for a 4K x 4K pixel detector)	Aerotech Micos Newport ...	
Sample exchange robot	Robot arm & controller	• Good programmable interface • 4 axis robot (at least)	Staubli (SLS have already integrated this model with EPICS & developed control s/w for MCT applications) Epson (Alan at MX is starting to intergrate one of these for PX applications)	~$55K (maybe less for 4 axis?) with controller ~$38K (for 6 axis) with controller
Detector	Optical Coupling (x2?)	• One system white-beam capable (no glass lenses in beam path) • Second system mono-beam (lenses in beam path with lead glass for protection for higher sensitivity)	Optique Peter Hamamatsu (examples of both have been purchase by AS/Monash recently)	~$60-80K each plus ~ $20K for a range of scintillators

	CMOS/CCD camera (x2?)	• CMOS for high speed • High dynamic range CCD also required • As low noise/dark current etc as possible	PCO Other?	~$30K each with control components
	Fibre optic bonded CCD detector	• Small pixel size, • structured scintillator	Princeton Photonic science Hamamatsu …	~$80-120K ~$60K
Window (s)		• Must be *very* smooth to avoid phase artefacts in beam • CVD diamond ideally, not Be • How many windows needed??What about extra beam transport tube??		$15k each Excluding front end modification
Filters & assembly (removeable filters to remove soft x-rays for pink-beam operation)		• Must have clean and smooth/polished surfaces to avoid introducing phase artefacts into beam. • Automated system for inserting/removing filters from beam path • Appropriate cooling		
Clean up slits & motors		• Motorised control for slit X,Y separation • Motorised XZ mounting stage		
Shutter		• Capable of high speed (speed? Would this really be used for high speed CT operation?)		

Grating assembly (Could we purchase a complete assembly from PSI?)	Gratings (specs taken from SLS version)	• 4μm pitch phase grating and 2μm pitch absorption grating • 10μm thick gold absorption grating (for 14.4keV) • 10mm	MCN Canon PSI	? US$80K (big ones!) Euro 20-30K
	Assembly	• Must be stable to 100nm (easier if using fine gratings like SLS so whole thing is only 10's of cm long) • Isolated from vibration/thermal effects due to other components	PSI	
	Phase-stepping stage	• Stepping resolution of at least 10nm (for a 2um final grating)	Kleindieke (concerned about wear over time with these) PSI/CSEM (these made a neat flexure stage for TOMCAT doesn't need piezos – design patented – can we get one?)	Piezo-based, with controller ~ $100K
	Alignment stages (Tilts, rotate and coarse translation for grating alignment)	• Tilts about beam axis need angular resolution to well below 1:2000. • Rotate (vertical axis) on first grating to 0.1° precision (this stage is optional – Spring 8 option) • Rotate (horizontal axis) on second grating to 0.1° precision (this stage is optional – Spring 8 option)	Micos Aerotech Newport ...	
	Long travel stand along beam axis to change grating separation	• Travel up to 400mm • Precision 10um (this is less critical)	Micos Aerotech Newport ...	

Beam transport tube when using experimental station 2	Pipe Windows	• Smooth windows • He filled • Easy to place in position (mounted from roof?)		
Additional stage controllers	For detector stage, clean-up slits motors, grating stage motors	• Able to control the stages motors and talk to computers/EPICS	Micos Aerotech Newport …	$10K for multiple axes $8.5K ea for 8 axis
Sample environments	Cryo-stage Furnace Fluid flow cell Humidity environment	• X-ray transparent • Compatible with rotation stage (in terms of weight and movement) • Protects stage from environment (eg high temps etc)	Cannot be purchased, will need to be designed and built. May be able to get sample designs from APS, SLS, Spring 8	

APPENDIX C – POTENTIAL CONSULTANTS FOR BEAMLINE DESIGN

Marco Stampanoni – SLS TOMCAT

Francesco de Carlo – APS 2BM

Naoto Yagi / Kentaro Uesugi – Spring 8 MCT beamlines

APPENDIX D – USER SURVEY RESULTS

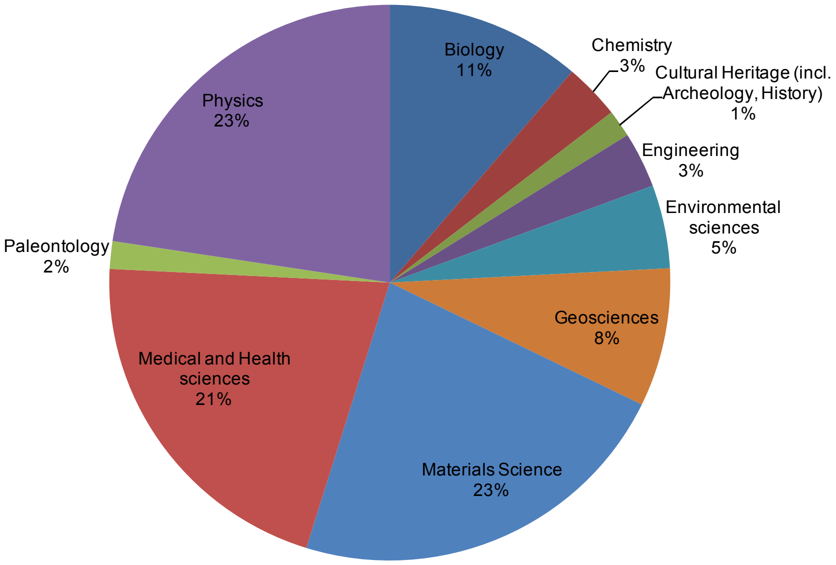
All those who were registered on the MCT email list were invited to participate on the online survey. All questions were optional.

The survey questions can be viewed at http://www.surveymonkey.com/s/H6PGN6X

Number of respondents:	24
Number completed all questions:	21 (87.5%)

C.1 MCT users by discipline

Users were asked to nominate their discipline area. More than one response was permitted.

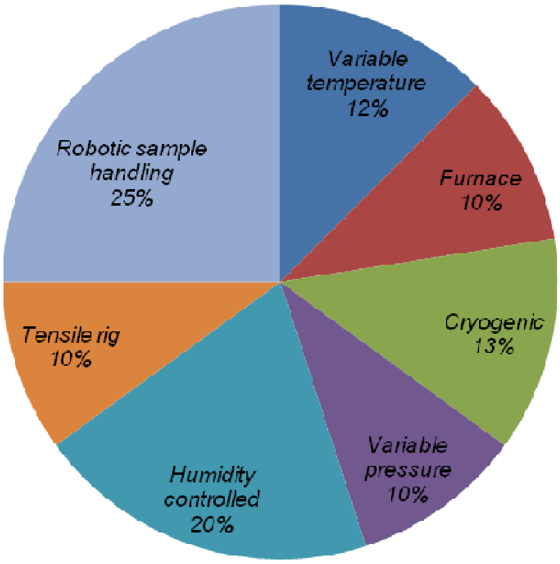


C.2 Technical requirements

	Mode	Max	Min	Mean	SD
Minimum essential energy (keV)	10	40	2	12	8.5
Minimum desirable energy (keV)	10	40	1	11	9.4
Maximum essential energy (keV)	40	150	10	48	39
Maximum desirable energy (keV)	60	150	13	71	38
Maximum Field of View (mm)	10	100	1	34	33
Minimum pixel size (micron)	1	20	0.1	2	4.4
Maximum pixel size (micron)	20	100	0.5	27	28

C.3 Sample environments

Users were asked to nominate sample environments they would like to have available from a predefined list, and nominate additional environments not on the list.



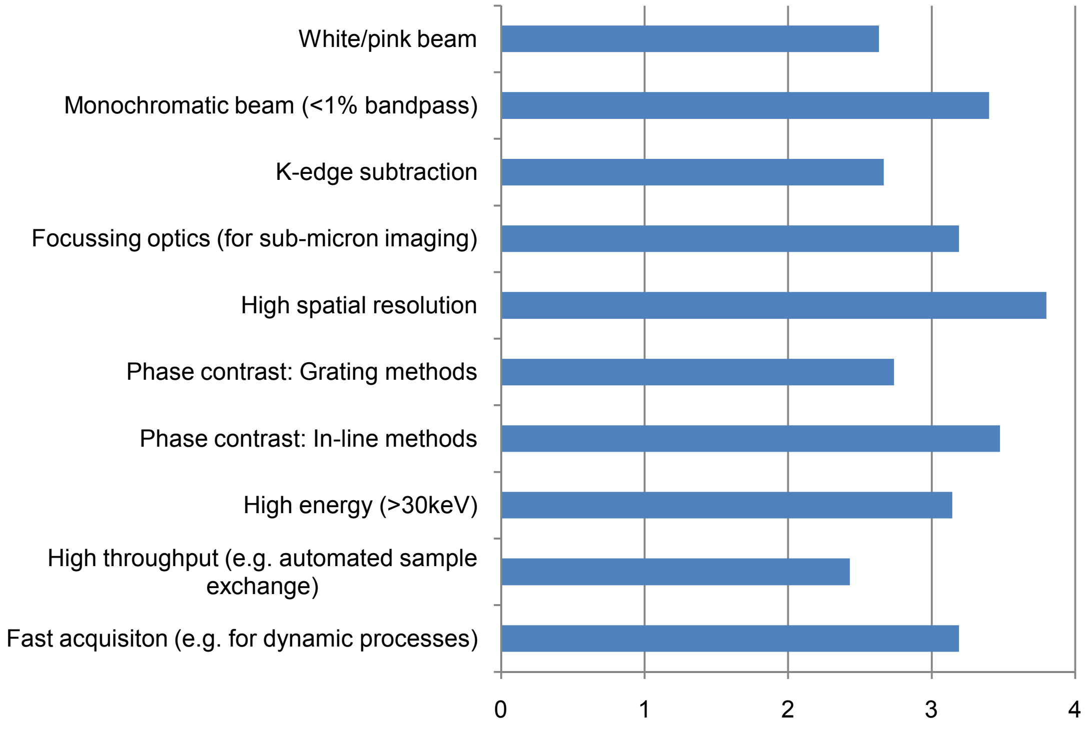
Additional suggested environments:

- Flow cells/controlled fluid flow
- Irrigation of samples
- Anaesthesia for live animal experiments
- Control of pH
- Acceptance of user designed cells

C.4 Performance priorities

Users were asked to rate the importance of capabilities on the following scale:

Very important	4
Somewhat important	3
Neutral	2
Unimportant	1
Don't know	0



C.5 Software requirements

Users were asked to nominate software that they would like to be available on the beamline (note that X-tract and Avizo will are already available via MASSIVE to IMBL).

Avizo/Amira (Visage)	6
X-tract/XLI	8
Drishti	3
Analyze	1
ImageJ	1

C.6 MCT use of laboratory and overseas synchrotrons.

Users were asked to specify if they had previously used MCT sources, both laboratory and synchrotron sources.