Medium-Energy XAS Beamline Scoping Group (MEX-BSG) Final Report

Executive Summary

This document outlines the rationale for construction and key features of an XAS bending-magnetic beamline that will strongly support cutting-edge research at the Australian Synchrotron in major societal areas in biology/medicine, the environment, materials, minerals, and art/archeology, as well as fundamental aspects of chemical bonding. The capability offered by this beamline will be strongly aligned with the National Research Priorities and it will be complementary to existing infrastructure at the Australian Synchrotron, foremost the XAS, XFM and Soft X-ray beamlines. The beamline will support a very large, diverse and internationally highly competitive user group that continues to grow in Australasia.

The beamline will cover the energy range from the K-edges of Si through to Se, which encompasses most of the elements of interest in, e.g., biological and environmental systems. This beamline will also allow access to a large range of L and M edges of the heavier elements, thus permitting a number of structural studies to be carried out that are otherwise impossible at their respective K edges. Access to the L and M edges will also enable projects where ultra high vacuum (Soft X-ray Beamline) is detrimental to obtaining outcomes. Thus, XAS data may be obtained from at least one edge of most elements of the Periodic Table using the MEX beamline. This beamline will furthermore feature a low-resolution microprobe capability to support or enable high-quality research outcomes and to complement existing capabilities offered by the XFM beamline.

The conceptual layout of the beamline emphasises the incorporation of the desired functionality with a simplicity that will enable users to be able to perform certain changes in modality in order to study more than one element and, thus, provide comprehensive solutions to certain scientific problems. The use of a low-cost light source (bending magnet), and the implementation of a simple and modular design based on standard components, will assist with budget considerations in the next stages of the Australian Synchrotron Development Plan.

The key technical parameters of this beamline are:

Light source	bending magnet
Energy range	1.7-13 keV (Si-K – Se-K edges; L and M edges of most elements of the periodic table)
Monochromator	DCM - Si(111) for 2-13 keV - YB_{66} or InSb(111) for low energies
Mirrors	- 1 horizontal collimating mirror (Rh or Cr coated) - 2 harmonic rejection mirrors (Rh or Cr coated) - 1 horizontal focusing mirror (toroidal)
Brilliance	3-4 $\times$ 10^{14} photon/s/0.1%bw/mm^2/mr^2
Beam size	Hutch A: ~ 2 $\times$ 10 mm (collimated)
	Huthc B ~ 0.2 $\times$ 7 mm (focused) < 5 μm (KB mirrors)
Detectors	Station A: 3 ion chambers fluorescence (Si drift; 4-element Vortex) electron yield Station B: 2 ion chambers fluorescence (Si drift; 4-element Vortex) BioMAIA for fluorescence

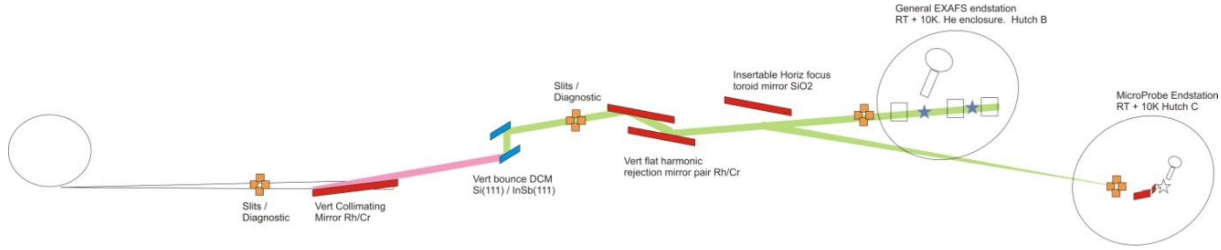

Figure 1. Schematic of the MEX Beamline

Scientific Case

1. World-class experimental capabilities and science.

The XAS experiments that will become available with the new beamline include cutting-edge scientific problems in: advanced materials; arts and archeology; catalysis; clean energy technology; biology; earth sciences (mineral and agricultural); environmental sciences; forensic science; medicine; pharmaceutical research; and many other areas of fundamental and applied sciences and engineering. Unlike many insertion-device beamlines that strive for the highest performance in photon flux per unit area for specific applications, including the current XAS beamline, this bending magnetic beamline will be driven by different cutting-edge science:

- in which high beamline stability is required with unfocussed beams (such as transmission experiments);
- where minimization of beam damage to the sample is essential for high quality data to be achieved by optimizing detection; and/or
- where an extended range of energies for elements with lower K-edges (some of which are very sensitive to photodamage under environmentally relevant conditions) are the driving scientific imperatives.
- The need for such a beamline is very high in order to produce the best possible science outcomes for a large and internationally competitive Australasia XAS user community.

The plan is to draw on the best features of the relatively few state-of-the-art beamlines of this type (which are in high demand) at other synchrotrons, and incorporate local breakthrough technologies, such as the drift Maia detection systems, to design and commission a beamline that places it at the forefront of technical and scientific achievements that a possible with such as beamline.

There is a wide range of cutting-edge science that this beamline will support and in which the very strong Australasian XAS community has already established an international reputation that includes, for example: three-dimensional local structural information on photosensitive metalloproteins that is crucial in understanding their biological activities; characterization of unstable complexes that are too reactive to crystallize and very susceptible to photodamage by X-rays; speciation of complex mixtures of species for a given element in biological, environmental, geological, materials, pharmaceutical, and other hard/soft materials (coals, biomass, combustion-driven particles) samples; distribution of local environments in amorphous materials; fundamentals of chemical bonding; changes in the structures, distribution and concentrations of elements in normal physiological processes, diseases, or drugs at target sites; identification of pigments in art, archeology and forensic science; distribution and speciation of elements in minerals and composite materials; and specialist phase-contrast imaging, amongst a range of other experiments. Below is a summary of examples of the types of experiments that will be performed on this beamline, but is by no means comprehensive.

(a) Biological and medical sciences.

Determination of protein structures and their active sites is of fundamental importance in understanding physiological functions, disease processes, and development of new drugs and treatment. Synchrotron techniques have been of paramount importance in these developments, including local structural information on absorbing atoms in solutions and membranes using XAS. Australia's outstanding record in the field of structure-based drug design is founded on the ability to solve the structures of these molecules, yet it is well-recognized that these projects rarely produce crystals of sufficient size and diffraction quality for use on conventional synchrotron beamlines. The AS XAS beamline is usually highly oversubscribed and is not yet suitable for certain protein structures due to photodamage, and the ANBF lacks sufficient sensitivity for XAS of dilute proteins. This has resulted in XAS studies on the roles of heme proteins being conducted at SSRL (Lay, Harris),[1] APS, and other facilities. The new MEX beamline will enable such experiments to be conducted at the AS.

Studies on the biotransformations and biodistributions of drugs rely heavily on XAS and X-ray microprobes.[2] For example, high profile research is being conducted into understanding the mechanisms and drug development in the area of Pt anti-cancer drugs (Hambley),[3] Ru anti-cancer drugs (Harris, Lay),[4] As anti-leukemia drugs (Dillon, Harris),[5] Se anti-cancer drugs and other methods for the treatment of cardiovascular disease (Harris, Lay),[6] Cr, V and Mo anti-diabetic drugs and supplements (Harris, Lay),[7] Gd-Pt neutron capture conjugates for the treatment of cancers (Harris, Rendina),[8] Ga anti-cancer drugs and radiopharmaceuticals (Lay) and many others. Much of this high-profile research, some of which is published in premier journals such as *J. Am. Chem. Soc.* and *Angew Chem., Int Ed.*, has been conducted at overseas synchrotrons. With the very high level of oversubscription at the AS X-ray microprobe and the AS and ANBF XAS beamlines, this research would be crippled without continuation of ANBF and, at the end of the ANBF agreement, with the proposed new MEX beamline. In addition, neither the AS nor the ANBF covers the entire energy range of ~1.8-14 keV (K-edges Si-Se) for XAS, *i.e.*, most of the elements of interest to biology and medicine (except for H, C, N, O, Na and Mg). The distribution of the lighter elements (S, P, Cl, Ca, K) and their chemical forms are crucial to understanding many biological processes, including diseases and their treatment. For example: the redox status of cells, which is defined by the RSH/RSSR ratio and their distributions, and those of other S-containing biomolecules, are crucial in many biological processes;[9] thiolates are also used in cellular resistance responses to anti-cancer drugs; the degree of protein phosphorylation and the ratio of free phosphate compared to organic phosphate are important in many physiological functions; and the release of Cl^{-} ligands from metal-containing anti-cancer drugs can also be monitored as a function of time, space and biological environment, which is very important in understanding their biological activities. Finally, the Si K-edge is important in certain biological samples, since Si is commonly incorporated into biominerals. Thus, this beamline will greatly enhance the strength of Australian research that uses XAS to improve drug design, understand fundamental processes involved in diseases at the molecular level, and determine normal physiological processes in biology and medicine.

(b) Environmental and Earth Sciences.

These areas require the same XAS and X-ray microprobe techniques described above and have the same limitations with regard to AS access. Many crucial aspects of these sciences have not been able to be addressed previously using the AS XAS or ANBF beamlines because of the energy range limitations and much of the research on transition metals in the environment has been conducted at the ANBF, which the current beamline will replace. The new experiments that will become available include studies on: redox status and speciation from S-K-edge,[10] distributions and speciation of inorganic and organophosphate pollutants and their breakdown; speciation of organochlorine pollutants and their breakdown to inorganic Cl^{-}, etc. An example is the use of Cl K-edge XAS to study the fate of NaCl in coal

(Monash U.), where Cl K-edge XAS will be used to study the fate of NaCl in coal in order to determine temperature thresholds for the formation of organochlorine species. Along similar lines, coal is a heterogeneous mixture with nearly all of the elements in the periodic table embedded in its organic matrix. Heavy metals, e.g., As, Se, Cr, Ni and Zn (ppm level), vaporise and coagulate into inhalable fine/ultra-fine particulates during coal combustion. The toxicity of resulting particulates is essentially dependent on the oxidation states of the trace heavy metals, which are, however, very difficult to be determined/quantified using conventional instruments. Determination of the oxidation states of heavy metals in coal fly ashes, particularly the ash samples collected during carbon pollution reduction coal conversion processes, is one major research target in the R&D of the clean coal technology strategy at Monash (Zhang).

In soils and minerals, silicates, phosphates, sulfur anions, (S_2^{-}, S_2^{2-}, SO_4^{2-}, etc.), chloride, etc. are found in many minerals and the XANES from these anions are sensitive to the nature of the metal to which they are bound and the unit cell (environment). When combined with the metal XANES on the same samples, superior speciation and spatial distributions will be possible, than simply relying on a metal K-edge alone. With controlled environmental cells, information can also be obtained on the speciation of complexes under hydrothermal conditions, the precipitation of certain minerals, and crystallization processes. An example of a project that requires such access is the use of S Kedge XAS to characterize acid sulfate soils (Burton, Sullivan). The S K-edge XAS will be used to identify reactive intermediates in reduced S sediments in order to characterize biotic versus abiotic reaction chemistry, as well as key chemical differences between different acid sulfate soil environments. It is also important that research with soils and other environmental samples can be conducted at the AS, since it is increasingly difficult to send such samples overseas due to customs restrictions.

Research conducted by Berry and O'Neill and coworkers have used XANES at the ANBF and other XAS beamlines extensively to study the oxidation states of metals and S in hydrothermal solutions and minerals under conditions of high temperatures, pressures, etc. that mimic geological conditions. These have been instrumental in determining information of mineralization processes and geochemistry under extreme conditions and have provided many new insights into this important area of research for Australia. The new MEX beamline will be instrumental in furthering these studies.

The loss of the ANBF facility would also have a devastating effect on many projects currently spread between the AS and ANBF beamlines, unless the new beamline is built. It is widely recognised that the toxicity of metals to aquatic organisms depends on both the metals' chemical speciation, which in turn is dependent on water quality characteristics such as pH and dissolved organic carbon concentration, and also on the competitive binding of the metal to the critical receptor site on the organism. Because of their key position as primary producers in aquatic ecosystems, microalgae are an important test species for regulatory assessments of metals. Consequently, XAS is being pursued to study the Cu intracellular oxidation state and structural chemistry (Dillon). Research by Collins and Waite[11] is aimed at gaining mechanistic insights into (mainly) natural biogeochemical processes. These applications range from determining: (1) how plants detoxify metals, including the peculiar metal-hyperaccumlating plant species that can accumulate metals to concentrations many orders of magnitude higher than 'normal' physiological concentrations; (2) the transformations of iron in acid sulfate environments and so identify mechanisms with which these can be manipulated to reduce iron transport to Australian estuaries (and the associated problems with estuary acidification, deoxygenation (resulting in massive fish kills) and eutrophication (leading to toxic algal blooms); and (3) how toxic metallic elements interact with mineral surfaces to either promote the removal of these metals from wastewater streams or natural processes that can immobilize these metals in polluted groundwaters. The Lombi group is also performing extensive research on metal accumulating plants, including new developments that enable experiments in hydrated plant samples. The ANBF is also being used extensively for studies of speciation of As pollution from various sources (Burton, Bush, Harris, Johnston, Noller, Sullivan), which is very important in understanding it potential toxicity and the best method for remediation.[12] The Applied Centre for Structural and Synchrotron Studies and Ian Wark Institute (Harmer-Bassell, Gerson and others, U South Australia) have accessed ANBF for over 10 years and many other synchrotrons (encompassing XPS, K- and L-edge XANES, and photoemission spectroscopies: SPEM, PEEM and SPLEEM) for diverse studies of relevance to Australian mining industries.[13,14] These include: the adsorption of Cu ions from solution onto metal sulfide minerals for enhanced separation by flotation; and the study of the mineralogy of Ni in nickel laterite ores and leach products; crucial for optimisation of industrial Ni leaching processes. The above techniques are also used for studies on minerals including: species formed at fracture sites, adsorption of metal ions, leaching, oxidation, galvanic interactions and spatial distribution of reaction products resulting from these processes, e.g., surface oxidation process that occurs on the sulfide mineral pyrite, the primary contributor to the environmentally challenging issue of acid mine drainage. RMIT University (Tardio, Bhargava) conducts research in minerals and materials science and catalysis. The ANBF is used to characterise nano-structured catalysts and minerals/inorganic compounds encountered in hydrometallurgical processes including: characterisation of natural and synthetic forms of complex uranium minerals (brannerite and coffinite) to understand fundamental aspects of U leaching from U-bearing ores; characterisation of nano-structured mixed metal catalysts for carbon dioxide reforming of methane; and characterisation of nano-catalysts for catalyzing the oxidation of elemental Hg vapour in gaseous effluents emitted from coal fired power plants. Clearly, while the AS provides a growing collection of outstanding facilities, many experiments of this type can only be accessed currently through ISAP travel and the ANBF for experiments that play a considerable role in enabling science, such as those directly related to sustainability and wellbeing in the Australian environmental and earth sciences and it is essential that the new beamline is built to meet this demand.

(c) Materials.

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XAS is used for many important scientific and technical problems; e.g., understanding amorphous Si phases (including structurally relaxed) and Si oxides of importance to mass produced solar cells. Since the information required for understanding these types of materials is often associated with small changes in XAS spectral information, this beamline will be an important addition to studies on high technology materials. Specialist powder XRD and XAS facilities at overseas synchrotrons have been used to investigate temperature-dependent and/or host-dependent changes in the properties of advanced microporous materials. Such studies on these advanced materials is essential to further their development in many high technology processes such as switches, zero thermal expansion materials, molecular sieves and gas separations, hydrogen storage, and will become available with the new beamline (Kepert).[15]

Research on Zr and Ru materials that have a variety of potential applications require the use of experiments at the Zr L-edges (~ 2.1 keV) and the Ru L-edges at 2.5 keV, which are currently being conducted at beamline 16A at the NSRRC with very simple optics (vertically collimating pre-mirror, fixed-exit double crystal Si(111) monochromator, toroidal focusing mirror; Kennedy, USyd). While the Zr L-edge research can theoretically be performed on the existing AS soft X-ray beamline, the need to explore a large number of samples (20-50) in order to establish the systematic trends, such as a transition from a ZrO_6 to ZrO_8 coordination environment, requires the simple and time-efficient sample changeover that will be available at the new MEX beamline without the need for ultra high vacuum conditions to be preserved. The research is being conducted at the L-edge because it is very sensitive to subtle changes in the coordination environment, thus enabling the scientific goals to be achieved, whereas data acquired at the K-edge (AS XAS or ANBF) are not sensitive enough to detect these changes. There are similar issues involved in the Ru L-edges, which are not accessible at either the AS soft-X-ray beamline or the current XAS beamline.

(d) Fundamental Synchrotron Science Studies.

Research by Chantler[16] has focused on measurements of roughness, inelastic mean free paths, beamline diagnostics, absolute XAS measurements, the characterization of diffraction standards, and development of XANES and XAFS theory and analysis that impinge on many areas of XAS and XRD.

(e) Surfaces, Electrochemical Sensors and Photocells.

Calibration-free coulometric electrochemical sensors are being developed (De Marco) for a range of applications including the analysis of important nutrients (nitrate, ammonium, phosphate, etc.). The rationale design and development of these sensors requires a diverse synchrotron techniques (XPS, surface-enhanced XAFS, grazing-incidence SAXS and X-ray reflectometry).[17] This beamline will be able to be used in such XAS experiments.

XANES and other techniques are being used to study mimics of the Mn photocentre for oxidation of water in Nafion supports under different conditions for their potential as industrial catalysts[18] (Spiccia and Hocking). Synchrotron X-ray reflectometry and polarized total reflection XAS are also being used to study the two-dimensional structures of species, such as porphyrins, adsorbed on surfaces and complexes that involve multi-component monolayers (Gentle),[19] and this beamline will be capable of performing grazing angle XAFS experiments.

(f) Art and Archeology.

Many pigments found in art and archaeology contain metals, as well as, S, Cl^-, and/or phosphate anions. In previous research, access to the ANBF and other overseas beamlines for XAS, SAXS, microdiffraction and other techniques has enabled their definitive identification (Creagh).[20] Such studies, when related to historical records of the use of pigments, are important to identify forgeries, aging and weathering processes (for restoration purposes), dating of samples, and trade associated with the use of pigments (using spectroscopic signatures of the same mineral from different sites). As such, these investigations are important in understanding many aspects of the development of civilization. For example, XANES and microfocus XRF of iron-gall inks on parchment that are presently studied at the ERSF will be able to be studied using the new MEX beamline.

(g) Bonding.

The S, P and Cl XANES and L-edge metal XANES[21] are very sensitive to the degree of covalency in bonding of a whole range of ligands with these donors bound to metal ions. A combination of such XANES spectroscopy, together with complementary information from Density Functional Theory calculations, is revolutionizing our understanding of covalency in bonding in metal complexes and no other technique provides such detailed experimental information to compare with theory (Hocking). Such studies not only answer fundamental questions of the nature of chemical bonds, but they are also important in understanding the reactivity of metal complexes in biological, medical, environmental, earth and material sciences. These experiments require energy ranges that are not currently available at the AS XAS beamline.

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2. Existing research strengths, National benefit, the National Research Priorities and Potential for industrial impact.

It is clear from the publication list above, which is only a small representative example, that the XAS community produces research that is published in the highest quality journals and this demonstrates that international research strength of this community. The XAS community in Australasia is also a very large community that has developed rapidly over the last two decades through the Australian Synchrotron Research Program and the Access to Major Facilities Program, even before the Australian Synchrotron was built. The number of users that were producing quality science that enabled them to obtain beamtine at many of the most sought-after XAS beamlines around the world was such that the demand at the time the Australian Synchrotron was built was sufficient to fill two beamlines in order to maintain the current level of activity. This has necessitated the continuation of the ANBF and both the AS beamline and the ANBF have been oversubscribed and, in addition, Australasians continue to use overseas facilities for experiments that cannot be performed at the AS or ANBF. The fact that well over two beamlines are used currently to produce high quality research clearly demonstrates our research strength in this area. The same is true the XFM community, which will also be served to a lesser extent by this beamline.

In terms of National Benefit, the research outlined above is a clear indication of the potential impact on a range of important Australian industries and to the health of the Australian community. In addition to the direct impact on Australian industry and reductions in environmental impacts of industry that this research will bring, there are many other impacts on health and society, as outlined in the subsequent sections. In addition, research conducted at the beamline will provide high quality research training for Honours and postgraduate students and other researchers, which will benefit both research institutions and industry.

In particular, the studies to be conducted on the beamline incorporate research that covers all of the National Research Priorities and the great majority of the sub-themes and will have the capacity to greatly expand the range of quality research.

With regard to the National Priority ***An Environmentally Sustainable Australia***: the research to be conducted has important consequences for meeting the objectives of all seven themes. For example, on how toxic metallic elements interact with mineral surfaces to either promote the removal of these metals from wastewater streams or natural processes that can immobilize these metals in polluted groundwaters is important with regard to the category: *Water – a critical resource*. Many researchers will be involved in the projects outlined (as well as many others users) to reach the aim of: *Transforming existing industries*. New technologies will be developed for resource-based industries to deliver substantial increases in national wealth, while minimising environmental impacts on land, atmospheric and aquatic environments. These rely on an understanding of the mineralogy and chemical processes required to develop more environmentally sound minerals processes that require less energy and are less polluting. The research on solar energy based devices, whether they be based on Si photovoltaic technology or in catalysts for the oxidation of water for use in H_2/O_2 fuel cells, is of paramount importance in developing new and improved technologies that can help transform Australia from reliance on fossil fuels. The theme of: *Overcoming soil loss, salinity and acidity* is also well-represented in the research outlined above. This includes identifying the mechanisms of producing and the potential remediation of the environmentally damaging increases in Fe concentration and acidity of the oxidation of pyrite. Similarly, studies on the use of plants that are metal hyperaccumulators of toxic metals that are introduced into the environment through industrial processes and agriculture, or are in high natural abundance are important in meeting this goal. The research to be conducted also impinges on the theme of *Reducing and capturing emissions in transport and energy generation* in research aimed at understanding the generation of organochlorines from NaCl in the combustion of coal, or the release of toxic metals in fly ash. By understanding the chemistry associated with the generation of such species, ways can be developed for reducing their release into the environment. The theme of *Sustainable use of Australia's biodiversity* is also covered in the research that is aimed at understanding and mechanisms of acidification and heavy metal pollution of estuarine environments, which is essential for managing and protecting these hotspots for terrestrial and marine biodiversity in Australia. *Developing deep earth resources* is a theme that it also covered under the research to be conducted, as the high pressure capabilities enables the study of a range of research that includes the study of bioleaching and associated hydrometallurgy of metals from deep deposits using ore-metabolising microbes that enable low-energy mining of otherwise uneconomical deep deposits while minimising negative ecological and social impacts. Finally, with regard to the theme *Responding to climate change and variability*, examples of research that impinge on this theme is research associated with new technologies for solar energy devices, and cleaner and greener catalysts, and carbon storage. The beamline can also be used to study certain aspects on how plant biochemistry alters to cope with climate change, which will be important in understanding and adapting crops for climate change.

There is a large amount of research that can and will be conducted using the MEX beamline that will be important in achieving certain aspects of the National Priority of ***Promoting and Maintaining Good Health***. While the introduction of all new practices that promote and maintain good health requires years of evidence-based research, they all rely on high quality fundamental and applied science at all stages, and particular the early stages, of their development. The use of synchrotron science that incorporates protein crystallography and increasingly, XAS and XFM elemental mapping of tissues and cells is having an ever growing impact on the understanding of disease processes at a molecular and cellular level and to improved treatments. This research impacts significantly on three of the four themes of this National Priority.

With regard to the theme _A healthy start to life_, the research includes studies on the use of nutritional supplements, with regard to their efficacy and safety (which also impacts on pregnant women) who often take supplements, e.g., the potential cancer risk of widely consumed Cr supplements, which have been shown to greatly increase the risk of cancers in the progeny of rodents that have been fed the supplements. In addition, much of the research that is being conducted is aimed at reducing the environmental impacts of pollutants derived from human activities, which often impact most heavily on fetal development and many aspects of the healthy development of young children. Finally, research to be conducted with the beamline also examines trace nutrients in foodstuffs such as grains (Lombi), including understanding the chemistry that is important in their bioavailability. This is important in reducing malnutrition through delivery of essential trace elements in the staple diet of mothers and children in developing countries and also, to a lesser extent, in developed countries. The theme _Ageing well, ageing productively_ is well-covered in the research to be conducted with the beamline. As indicated in the examples in the previous section, a large amount of the research to be conducted is directly related to the key areas that are important to improve the mental and physical capacities of ageing people, through understanding and improved treatments of neurodegenerative diseases, cancer, cardiovascular diseases, diabetes, etc.

Understanding and improving the efficacy and safety of nutritional supplements is important in _Preventive healthcare_. The research conducted with the MEX beamline will include fundamental research on the effects of anti-diabetic supplements in terms of improved uptake and efficacy and reduced side-effects. In addition, the use of Se supplementation is known to be important in the reduction of cardiovascular diseases, cancer and neurodegenerative disease but not enough is known about the fundamental chemistry involved in the uptake and metabolism of this essential trace element. The research on extra- and intracellular Se biochemistry will provide the scientific basis for preventative healthcare based on improved efficacy and reduced toxicity of appropriate supplementation.

A large amount of the research to be conducted also falls under the National Priority Area of ***Frontier Technologies for Building and Transforming Australian Industries*** in terms of its ability to stimulate the growth of world-class Australian industries using innovative technologies developed from cutting-edge research. There are many examples in the area of _Breakthrough science_ that are covered by the research outlined in the previous sections that range from fundamental aspects of chemical bonding to the development of multi-modal bio-spectroscopic and bio-imaging technologies for a range of biomedical, environmental and materials research that will form the basis of research for a range of applications to industry.

Many of the projects to which the MEX beamline will be applied fall under the _Frontier technologies_ with the ability to enhance Australia's capacity in frontier technologies to power world-class industries of the future that build on Australia's research strengths in nanotechnology, biotechnology, photonics, and complex systems. As outlined in the previous sections, these include: nanotechnology (using XAFS to examine the variability of chemical bonds in amorphous materials for a range of high technology applications, chemical bonding and structure in nanoporous materials, etc.); biotechnology (including drug design and electrochemical sensors; photonics (silica materials for photons applications); and complex systems (single cells and tissues).

With regard to _Advanced materials_ the extended edge range provides new opportunities to study new ceramics and biomaterials that were not previously available at the Australian

Synchrotron and the microprobe capability is invaluable for studying the spectroscopy/local structure within composite materials, especially containing lighter elements not normally accessible on XAS beamlines.

Finally, in term of *Promoting an innovation culture and economy* this beamline will expand the cutting-edge capabilities of the Australian Synchrotron, which will drive new areas of science that were previously not available to Australian and New Zealand scientists except at overseas facilities. By having access to these facilities, and appropriate expertise that they will generate, it will be easier to demonstrate the value of this technological capability to gain local industry acceptance of the innovative opportunities that the MEX beamline will provide for a range of Australasian industries.

Although the research to be conducted on beamline will have a lesser impact on the National Priority of ***Safeguarding Australia*** than in the other National Priority areas, it still has a major role in safeguarding Australia from terrorism, and crime. Synchrotron techniques, including XAS and XFM can be used in forensic science to indentify materials that may be crucial evidence in solving the source of materials that can be used to solve crimes. One of the features of these techniques is the ability to provide spectroscopic signatures of pure compounds, mixtures, and composite materials from very small samples. This can be used to identify the source of even very small fragments of materials that a linked to a crime scene and, hence, falls under the category of *Protecting Australia from terrorism and crime*. The theme of *Transformational defence technologies* is also covered by XAS experiments that can provide information on new materials that can be used in a variety of technologies that apply to both civil and defence problems. Grazing-angle XAS experiments can also provide information of a range of different surface coatings that can be used to reduce corrosion (important for many military applications) and other coatings for specific applications.

In summary, the research to be conducted on the new MEX beamline will not only be of fundamental importance to a range of cutting-edge scientific programs, but will also have a range of applications with direct and indirect value-add for industry. For instance, the ANBF already attracts proprietary research involved with environmental aspects of the mining industry and there is the potential to expand this at the Australian Synchrotron. However, by far the greatest industry impact will be associated with research conducted by university, CSIRO, and ANSTO researchers involved in collaborations with the mining, pharmaceutical, photonics, and high technology industries that involve advanced materials.

3. Demand for the techniques offered by the beamline so that there is a good possibility that the beamline will be oversubscribed for many years.

The Australian XAS and XFM community is very large and already has resulted in oversubscription of two XAS beamlines at the AS and ANBF, as well as other specialist XAS beamlines for which access has been provided by ISAP or other sources. In addition, the new beamline will provide new XFM capabilities, which is also heavily oversubscribed at the AS. With the loss of the ANBF beamline over the next few years, the XAS community will still have access to only two beamlines after this XAS beamline is commissioned. With the continued growth of the XAS community and the extra capabilities that the new beamline will deliver, the level of XAS oversubscription will be even higher than it is currently when the new beamline is commissioned and will require the planning of a third XAS beamline within the next decade in order for Australia to maintain its standing in the area.

4. Complementary capabilities to the other existing and proposed beamlines at the AS.

The new XAS beamline will be entirely complementary to the existing XAS beamline at the AS. It will provide a new energy range that covers the K edges of the elements from Si to Ca that is important for many applications and will be superior for obtaining transmission XAS data. The lower brightness and larger beamsize associated with this beamline will make it superior for obtaining fluorescence XAS from many materials, proteins and solutions that are susceptible to photodamage. On the other hand, the existing XAS beamline can be devoted to very dilute samples, fast XAS and specialist XAS techniques for which it is designed.

Similarly, the XFM module of the MEX beamline will be complementary to that at the current XFM beamline, since it will enable XFM followed by XANES/XAFS studies on the lighter elements specified above. This module will also not suffer from the photodamage issues associated with the new proposed nano-XFM beamline for elements that are sensitive to photoreduction.

5. The beamline does not unnecessarily overlap with the capabilities of the other existing or proposed beamlines at the AS;

As indicated above, the beamline is designed to provide complementary capabilities rather than overlap with existing capabilities. Its characteristics have been carefully designed to fill niches that will provide a greatly expanded capability to provide new types of experiments or optimize the measurement conditions that are currently performed sub-optimally at other beamlines, for the reasons discussed above.

Technical and Commercial Issues

General Considerations

This beamline is designed to have specialist capabilities not presently available on the current wiggler beamline in the medium energy range (Si-Sc K edges), as well as being a ‘workhorse’ XAS beamline over an energy range that overlaps with part of the wiggler beamline range (Ti-Se K edges). Both of these requirements have been identified as important by the User Community and various stages of the review and ranking processes of the beamlines. The BSG felt that it was very important that the specifications be optimized for the capabilities not presently available, and that the beamline not be made too complex in order to minimize set-up time for optimal performance and to give users some control on changes to edge energies, etc., as is the case with the ANBF for experienced users. There are a range of overseas beamlines that work in this energy range and it is the intention that we incorporate the best components of all beamlines and use appropriate expertise from beamlines scientists involved in the design, development and running of these beamlines to come up with an optimal design for our requirements.

With these considerations in mind, the BSG believes that the appropriate energy range was that which covered the K edges from Si-Se (1.8-14 keV compared with 5-45 and 5-30 keV at the AS insertion-device beamline and ANBF bending-magnet beamline, respectively).

The brilliance of this bending magnetic beamline will be fairly constant over the entire energy range going from about 3×10^{14} photon/s/0.1%bw/mm^2/mr^2 at the lower energies to 6×10^{14} photon/s/0.1%bw/mm^2/mr^2 at the higher energies. This is very appropriate for the energy range of operation. While the brilliance is 1-5 orders of magnitude less than for a range of possible insertion devices, this is not an issue for transmission experiments where a larger beam spot and increased beamline stability of the BM beamline will provide superior data than that available on an insertion device beamline. With regard to fluorescence detection, which will be used for the majority of experiments, the important parameter is the total number of photons on the sample and the sensitivity of the detection rather than the number of photons per unit area. Thus the lower brilliance is compensated by the larger beamsize, such that the performance of a BM beamline is much better than would be expected by just considering the brilliance. Since this beamline is designed to deal with photosensitive samples and samples that are not at the lower extreme of concentration, its capabilities are in many ways superior for producing the best data, and thus the best possible science outcomes, for a range of specific scientific problems for which it has been designed compared to what can be achieved with an insertion-device beamline.

The following is a description of the desirable design features of the beamline and our assessment of the requirements for such a beamline, but some of these features may need to be modified in order that the technical requirements are able to be met without making too many compromises for the critical lower energies of the beamline. The general design is given below in Figure 1 (page 2).

Hutches and Experimental Stations.

The beamline layout includes two hutches. The first hutch will be optimised for normal XAFS experiments in both transmission and fluorescence modes. The second hutch will include KB mirrors for X-ray microscopy, which could also moved aside to make room for other specialist experiments as described in the subsequent sections.

In order to minimize experimental set-up times and to enable as much user-control of beamtime as possible, we envisage three experimental stations in two experimental hutches to cover the scientific needs of the community. We plan to meet this goal by placing emphasis on standard large modular components, as opposed to the Lego-type approach.

Station A: This Station will be the first priority station and will be a standard routine XAS setup in the first experimental hutch and will not generally be modified. It will be used for bulk samples and will have a relatively broad spot that is typical of bending magnetic beamlines, such as the ANBF (very desirable for transmission mode and increased signals from dilute biological samples, with minimal photoreduction). It will allow for fluorescence and transmission XAS in the energy range 1.7-12 keV at room temperature and at ~10-20 K. The configuration of components will need to be optimized to maximize beamline intensity on the sample and to maximize the detected signals. This will involve the use of low-vacuum or He atmospheres only in all of the flight tubes and sample environments including the space between the sample and detector. Even though these environments will not be required for the higher energy range, it is our intention that all these components will remain in place in this station, although the sample chamber may not require He for some experiments.

For both the cryostat and the room-temperature sampling, multi-sample capability with fast sample exchange will be an essential design feature in order to maximize use of the beamline for experiments and to enable batch sampling. Sample holders will be compatible with those used in the other XAS beamline and/or XFM/Station B.

For fast sample changes at low temperature and maximized signals, it is desired that the cryostat is windowless in order to ensure measurements at low energies as well as the higher energies. This will result in increased beam intensity at the sample and an additional increase in signal due to elimination of absorption of the signal by cryostat windows compared wit the ANBF. This could be achieved by a cryostat set-up that is similar to that at BM29 at the ESRF, for example.

Most probably gate-valves with windows in them around ion chambers will be required to allow for either He or other gases. The chamber could be made out of Al LF type fittings (eg, like that at HASYLAB).

Detectors included in this arrangement, and built into the chamber, will be three ion chamber detectors, a four-element Si drift fluorescence detector on a translation stage that will be windowless or fitted with a thin window, and a simple electron yield detector (in He). An allowance will also be needed to upgrade to a BioMAIA detector once available.

The beam within this chamber will be vertically collimated only, be non-focused, and defined in beamsize by slits to be $< 2 \times 10$ mm.

This Station will be the first priority endstation for construction and commissioning with the aim of commencing 'standard' XAS experiments as soon as possible while the second hutch continues to be developed.

Station B will be the second priority endstation for the beamline for construction and commissioning. This station will be a standard routine KB microprobe station, aimed at a micrometer (< 5 μm) beamsize; higher spatial resolution than that will not be required. Thus this Station will have complementary capabilities to both the current XFM beamline and the new nano-XFM beamline. It will have an extended energy range compared to the current XFM beamline and the use of both KB mirrors and a bending magnet source will make it superior to both for XAS spectroscopic measurements. The relatively large beamsize together with KB focusing will still enable imaging directly comparable to PIXE, but with a much greater sensitivity (due to the lower fluorescence background at lower energies for XRF compared to PIXE). Critically for spectroscopic measurements, the flux on the sample will be much less than at the current XFM and XAS beamlines, which will be important in reducing photodamage at the S edge, for example. This will probably require a secondary source point, which will be located in the second hutch, and the beam will pass through Station A (with the chamber filled with He and/or low vacuum environment).

The KB setup will be fixed so that it can be moved in or out of the beam (e.g. on rails) with a precise location that will enable fast transition to and from Station A or Station C. The sample environment will be He and all sample-holder geometries and sample exchanges will be standardized and compatible with the other XFM as well as IR beamlines. Cryo-cooling sample stages will need to be investigated that are compatible and interchangeable with the XFM and the HC nanoprobe beamlines.

Detectors will consist of two ion chambers, and a four-element vortex detector, with a plan to upgrade to BioMAIA once it is available. There will also be a phase contrast detector as a standard item. Cameras will be used to visualize both the front and back of the sample for positioning.

Station C will be the third priority endstation for construction and commissioning. Any experiments that require specialist cells or set-ups (apart from a normal cryostat) will be performed at this station and this will enable a range of non-standard experiments to be performed. In terms of maximizing the output from the beamline, it will enable experiments that require specialist components or extended set-up to be put in place while experiments are being conducted in Station A. This will maximize the versatility of the beamline to conduct specialist experiments that are currently being conducted at the ANBF and various new types of experiments to enable the beamline to continually evolve to meet the requirements of challenging new scientific investigations. This hutch should be of sufficient size to enable setup of these specialist experiments downstream from the KB mirror set-up. The space will need to be at least ~ 2.5×2.5 m^2 in order to incorporate these specialist experiments. It must be possible to wheel in user supplied apparatus, or to wheel in a beamline-supplied table and apparatus.

The beam size will be vertically collimated only (2×10 mm^2) or pre-focussed provided by Station B as a virtual focus to perhaps ~ 0.2×0.7 mm^2. Thus a table that will be able to provide a reasonably large range of motion will be required.

The following will be provided by the Australian Synchrotron for these specialist experiments:

- an experimental table (1.2×2.4 m^2).
- ion chambers, fluorescence detector (four-element Si drift), Lytle detectors.
- sample stages (two translation, two vertical and one rotational).
- large 'glove box' with electrical feedthrough and gas feedthroughs to house specialist equipment
- He/low-vacuum flight tubes
- Gas lines and exhaust for specialist gasses.

While beamline scientists can assist in providing some appropriate technical information, detailed construction, planning and implementation of equipment for specialist experiments will be the responsibility of users. Conditions for the introduction of new experimental set-ups are described in the next section.

Optical Design.

The optics need to be designed to meet these requirements:
energy Range ~ 1.7 – 13 keV
focus properties:
~ 2×10 mm^2 unfocussed in Hutch 1 (Station A)
~ 0.2×0.7 mm^2 focussed in Hutch 2 (Station B/C)
~ at least 5×5 μm^2 (preferably down to 2-3 μm) for microprobe in Hutch 2 (Station B).

The following is our current assessment on how this can be achieved:

One of the biggest challenges is the large energy range, which makes the aspect of harmonic rejection (1 in 10^5) difficult to achieve over the full energy range and this may require further detailed investigation. Also the Si edge means that we will need to rely on Si-free, coated mirrors only. As a large angle of incidence is envisaged, the mirrors do not need to be 1.4 m long and will thus be fairly low-cost.

Due to the low energies used at MEX, a Be window to separate the beamline from the storage ring vacuum is not suitable. This is the case in the HASYLAB Beamline A1 where the first window is the window of the first ion chamber. However, it may be appropriate to have a window before this that filters out visible light from discussions that Peter Kappen has had with the beamline scientists at HASYLAB. Depending on the beamline diagnostics installed (e.g., phosphorescence screens, etc), filtering out the optical component of the BM radiation may be critical for diagnostics operation.

1. *Monochromator*

This is the most crucial component of this beamline and it is essential that priority be placed on obtaining the best monochromator available for the task. This would be a fixed exit DCM with water cooling. We expect the beamsize on the crystals to be ~ 2×7 mm^2 (for Station A) or up to ~ 2×20 mm^2 (for focused operation).

Two Si(111) crystals will be required for the energy range ~ 2 – 13 keV with phi = 0º and 90º cuts to manage harmonic rejection for the different edges and to minimize glitches for a particular experiment. It will be preferably to mount both of these within the DCM but this will not be required. If both are mounted in the DCM, experienced users should be able to exchange them.

Two materials were considered for the Si K-edge, YB_{66} or InSb(111). There is conflicting comments from Bruce Cowie and Fred Mosselmans as to which of these materials are more stable, but issues with stability appear to be more of an issue with an insertion-device beamline than a bending magnet beamline. InSb(111) crystals are far superior in terms of the amount of transmitted light and ability to produce larger crystals that are appropriate for a BM beamline and will cover the energy range 1750 to 3750 keV, which includes the Si K edge. However, further discussions with suppliers and the beamline designers in order to ensure that long-term stability is not a problem. Only one crystal cut will be required due to the small energy range to be covered. It is expect that it will require a beamline scientist to change to the Si edge mode of operation.

We also considered extending the range to the Al K-edge as there was some user demand for this edge. This would require an additional crystal and such an arrangement has been included on a number of beamlines and, hence, it is technically feasible. However, on balance, the extra complexity added to the beamline with a more complicated monochromator and the fact that there would be other extra demands including greater emphasis on minimising absorption of the beam within the components and measuring environments was inconsistent with the aims of making this beamline relatively ease to use for beamline scientists and users alike.

The large Bragg angles of this DCM, will challenge the degree of crystal parallelism required, as the monochromator will operate “fully tuned” and should rely on feedback-based stabilisation. Since the DCM is at the heart of any XAS beamline; its quality will impact directly and critically on the quality of the data obtained. Hence as mentioned above, the

BSG advises the AS to procure this item separately from a wider tender for the beamline in order that we can focus on obtaining a monochromator with the best possible performance.

2. Mirrors. The following mirrors are envisaged:

A collimating mirror – probably two stripes at largish (4-5 mrad) fixed angle of incidence to collimate the beam. The cutoff of ~ 13 keV is requited for the high energy stripe. The coatings need to be carefully considered, but at this stage we would envisage Rh and Cr stripes.

Bruce Cowie has kindly provided information on the reflectivity of Rh at 4.5 mrad, which showed excellent to very good reflectivity over the entire energy range 1.8-15 keV albeit with interference over the 3-3.7 keV due to the Rh 2p and 2s absorption L edges (see Figure 2). Thus for most experiments the use of this stripe would be the standard set up.

A chromium stripe would be a suitable material for the mirror placing the angle on to the mirrors at 12 mrad (0.7 degrees) to produce a high energy cut off of around 4 keV (Figure 3).

A number of other beamlines use a Ni stripe over this energy range and further consideration should be given for the best stripe for the lower energy.

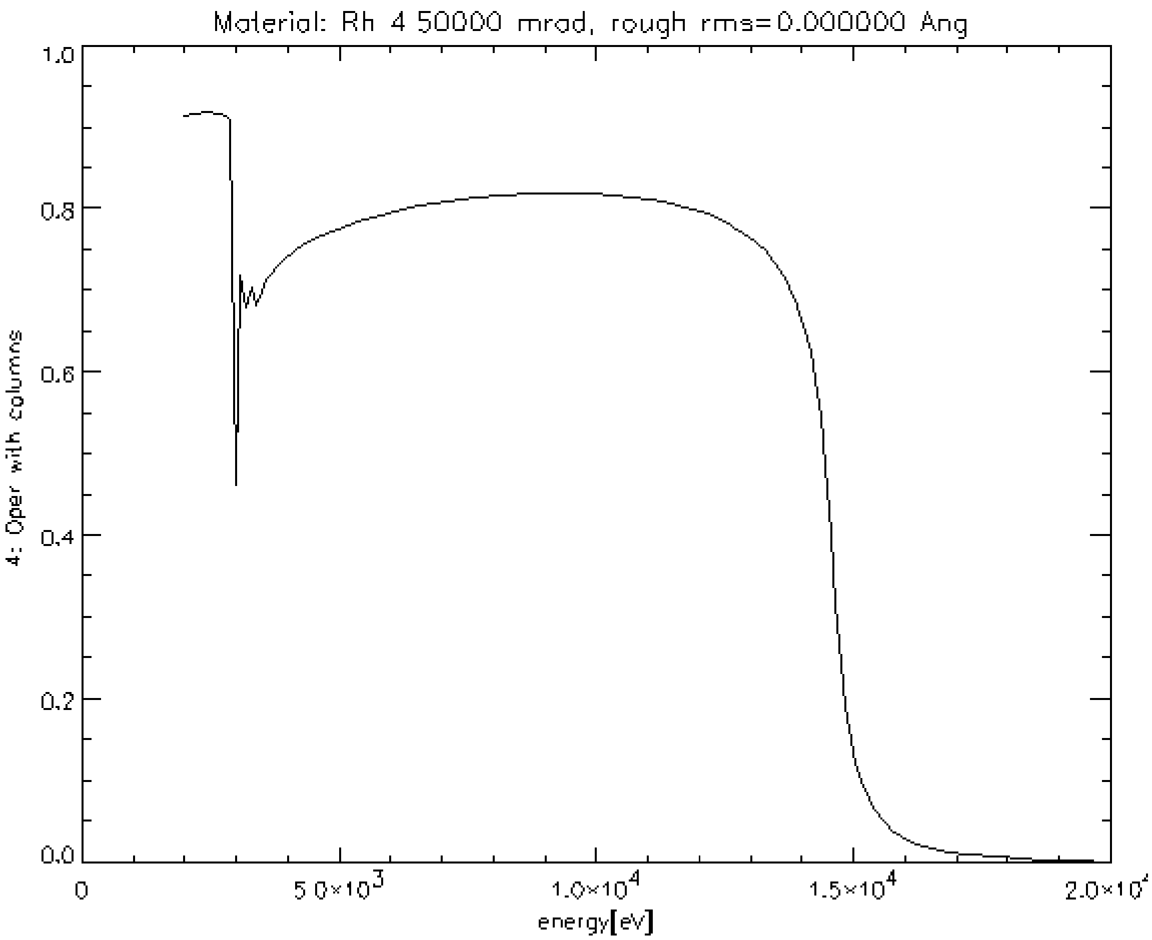

Figure 2. Reflectivity of a Rh stripe at 4.5 mrad.

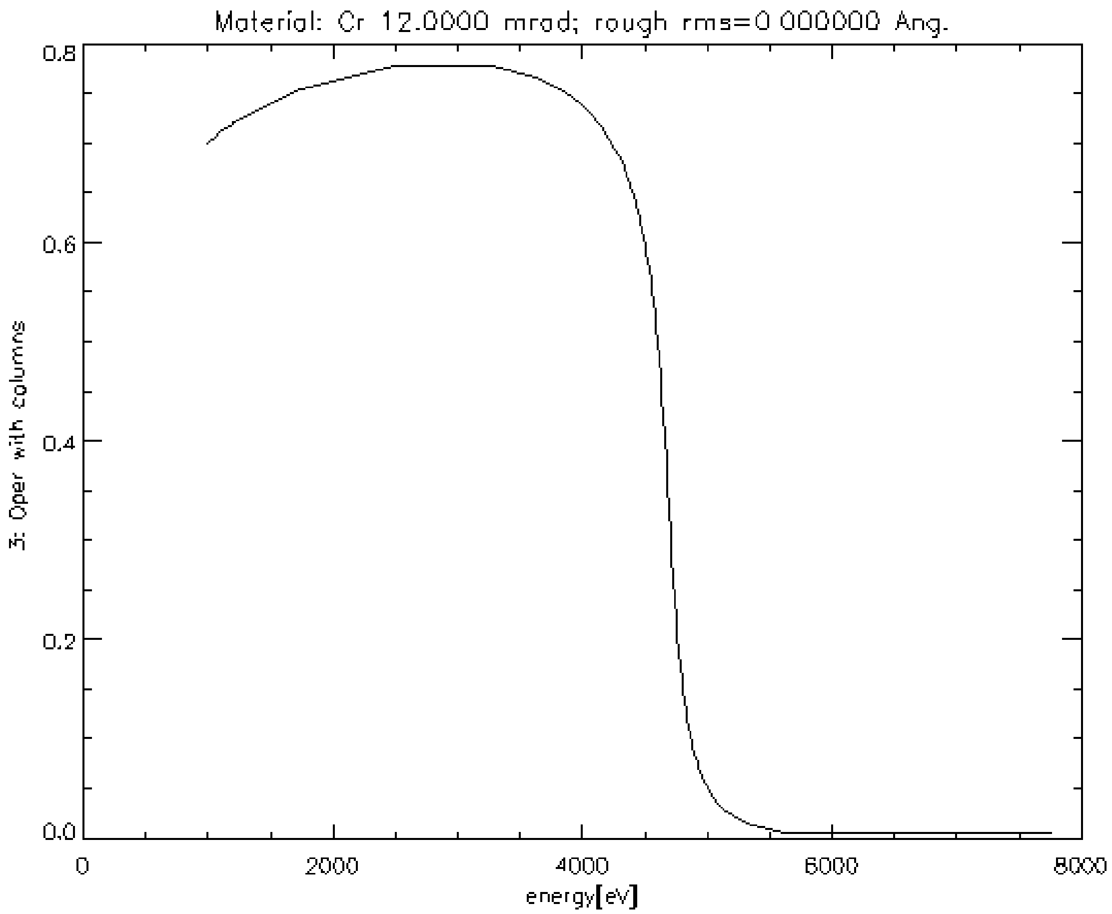

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Figure 3. Reflectivity of a Cr mirror at 12 mrad.

3. Harmonic rejection mirrors

There are two options. One would consist of a pair of mirrors with variable angle of incidence, such that there was no net change in the beam angle (but rather a change in beam height). These would be placed after the DCM in order that the user can change angle and thus an energy cut-off for harmonic rejection can be achieved without affecting the energy calibration.

The second option suggested by Fred Mosselmans at Diamond would have a number of mirrors at the correct angles that could simply be moved in and out of the beam path. This may be much easier for harmonic rejection, but the two options need to be considered further in terms of cost and ease of use.

4. Torodial refocusing mirror

This will take the beam after harmonic rejection mirror to focus it to a point in the second hutch and will be a virtual source for the microprobe, as well as being used for station C.

5. Dual K-B mirrors (smallish)

Considerable discussion was centred on the configuration to be used for KB mirror focusing. A low-resolution (few micron) resolution imaging capability was considered to be highly desirable by the XAS community. In terms of simplicity of operation, it was considered undesirable to have KB mirrors before the sample for normal XAS experiments. Hence, Station B will contain the KB mirrors, which could be moved out if necessary for other specialist experiments. The KB microprobe setup will be expected to be commercially obtained as a standard package.

Other Matters Associated with the Beamline Design and Implementation

Detectors. Requirements for each station are given in the above sections. Installation of the right detectors for the beamline will be essential for its success, as the bending magnetic beamline has been chosen to minimize photodamage for elemental environments that are very susceptible to such damage. The lower inherent signals produced will necessitate that the detectors are of the highest possible performance and the sampling arrangements are optimised to obtain high signal-to-noise performance.

Ion chambers will be available for transmission experiments (Station A) and for measurements of photon counts, and energy calibration from standards as a standard set-up in each station. Kapton windows have been used at HASYLAB Beamline A1, but there may be more appropriate materials to reduce absorption at the lowest energy and decrease He diffusion.

Multi-element Si-drift detectors (optimized for ~2-5 keV) will be the primary detector systems for the beamline. Two such detectors should be purchased, one for each hutch. In the first hutch, this should have a wide detector area that might be appropriate for more concentrated solutions of metals ions and various dilute solid samples for which transmission mode it not sensitive enough.

The second Si-drift detector will again be optimized in the lower energy range, but would have a much smaller detector area that would be appropriate for a very close approach to the sample that would be necessary for microprobe studies. This will minimize set-up times for both hutches and also be important for a back-up for the beamline (and other beamlines) should a Si drift detector be damaged.

These detectors are the best current option for these energy ranges and fit into the current program of the AS in optimization the software and electronic configurations of such detectors for rapid and sensitive detection for both mapping and spectroscopy.
An electron-yield vacuum cell will also be available for measurements conducted under moderate vacuum conditions in the second hutch.

A differential phase contrast detector will be available at the second hutch and should be of the type optimised at the APS.

Other detectors. A Si-drift Maia detector optimized for this energy range (*BioMaia*) is the next stage of development of this detector system and this is likely to be available during the construction stage. It is important than an allowance is made for such a detector in the budget, however, this needs to be considered together with other innovations in the rapidly developing detector field and an appropriate decision needs to be made on this detector at the time of building Station B in order that the best available option is procured within the available budget. It should be noted, however, that if such a detector is purchased, there will still be a need for a normal Si-drift detector system that would have the flexibility for all sample types.

Count rate considerations. The BioMaia detector is being developed for fast detection (high count rate capacity and virtually zero overheads), which is essential for fast mapping of large areas. Geometry considerations are also important as the annular geometry of the present 384 Maia would not be suitable for some samples. The back-end electronics as reported by Mark Rivers in which 4,000 spectra or 4,000,000 ROIs per second are obtained with: 650 EPICS support for high-speed digital X-ray spectroscopy with the 651 XIA xMap (10th Int Conf on X-ray Microscopy, Chicago, IL, 652 USA, 15–20 Aug 2010; see also http://cars9.uchicago.edu/ 653 software/epics/dxp.html for DXP 3.0 release; accessed 3 Dec 654 2010) may also provide fast acquisition times for the 'conventional' Si-drift detector. Allowances need to be made to have a complete package of detector hardware that includes state-of-the-art back-end electronics and compatible software, which will be of utmost importance in making this a world-class beamline that services this energy range.

Optical Detection. In the second hutch, optical detection systems need to be available to visualize the sample in both transmission mode and the front of the sample, for opaque samples.

Controlled Environments and Specialist Sampling. Given the energy range that is being used, the environments in the hutches need to be optimized in order to maximize both the photon count on to the sample and the fluorescence yield that reaches the detector from the sample. This will involve the use of He and/or vacuum flight tubes throughout the hutches, and the ability to perform all measurements in a He sampling environment or mild vacuum, if required. A cryostat capable of reaching about 10 K should be available in the first hutch for standard transmission and fluorescence measurements of the type currently being performed at the ANBF. A liquid-N_2-cooled stage (or some other cooling mechanism) should be available to enable a closer approach of detectors for both hutches. The low temperatures are required to minimize photodamage for sensitive samples but also to maximize the strength and energy resolution of XAS peaks. These should be standardized within the AS for use on the various microbeam beamlines.

Beyond these sampling parameters that will be available to all users, users would be invited to develop specialist sampling environments and include specialist equipment in the second hutch. However, the AS will not be responsible for the development and installation of the equipment, except for providing normal user support, unless they consider that it is in the interest of a broader synchrotron community and they have the resources and expertise to be involved in such developments. Similarly, there will not be any automatic right for users to introduce new sampling or equipment into the beamline. Such experiments will be vetted for approval in terms of the following principles:

(i) that it meets safety requirements of the facility;

(ii) it is consistent with management decisions on whether there are appropriate resources (including physical limitations of the hutch) to install and operate the specialist sampling/equipment; and

(iii) its installation does not compromise the performance of the beamline or constrain the hutch for future developments.

For any of these capabilities to be included within the initial budgeting and plans, users need to present a case to the BSG that would include:

(i) the nature of the experiments that would be performed, their scientific importance, and a demonstration of a significant user base; and

(ii) provide information on the three issues raised above (in consultation with current XAS beamline staff).

Offline Requirements

Apart from the requirements of chemical and biological labs and optical microscopes available for all samples, consideration should be given for having both Raman and FTIR-FPA microprobe instruments available for mapping/imaging the same samples for which X-ray microbe studies will be performed. Although an FTIR-FPA instrument is available offline at the IR beamline, this is often used by IR synchrotron users simultaneously and will be incorporated into a third IR beamline in the future.

For certain samples, polishing equipment needs to be available.

Spectroelectrochemical experiments are often performed both in situ and ex situ in conjunction with XAS. A suitable potentiostat and associated accessories need to be available that can be used either in the hutch or the chemistry laboratory.

File management. Data storage analysis for the mapping mode and access to software for analysis of large mapping files needs to be considered as an essential co-development of this and other mapping beamlines. Given the current trend in fast detection and full spectra acquisition, both on-line data storage and processing and off-line backup of files has to be integrated into the beamline from the outset. The advantage of a Bio-Maia option, over back-end electronics, is the interface with GeoPIXE, but software and hardware capabilities for dealing with a variety of large files needs to be considered. There is an issue of data storage and user ability to analyse the data. This problem would be more conveniently overcome by remote access to centralized computing and software at the AS rather than distributing software without back-up assistance to a large number of users, who may also not have access to appropriate computing facilities for very large files.

Staffing

It is essential that a principal beamline scientist be appointed as soon as practical to become involved in the detailed planning and specifications of the beamline and to interact with suppliers and AS staff to ensure that planning of the beamline, hutches and other considerations are in place and that this beamline scientist is familiar with all aspects of the beamline. This is important to ensure that the beamline becomes operational, as soon as possible. Recruitment of the additional beamline staff should start at least six months (and preferably a year) before the proposed delivery date of the beamline. This will enable these scientists to be present at the time of delivery in order to have a firm understanding of the beamline, as it is installed, and become involved in checking specifications and getting the beamline up and running in the shortest possible time.

Beamline controls and software development support will be required ahead of the beamline commissioning phase (e.g., half a year, alongside building the beamline team) in order to ensure efficient operation as soon as the beamline is made available to the user community. User-friendliness of the interface would be important to achieve. Given the overall aim for simplicity of the beamline, user-accessible features for experienced users should enable changes in edge energy and perhaps a user-accessible monochromator crystal change, thus achieving a high degree of flexibility in routine user operation on weekends and at other times when a beamline scientist is not present or is available to give instructions remotely.

Similar Beamlines

There is range a similar beamlines worldwide that incorporate some or all of the features. This is not a comprehensive list but is an indication of a range of beamlines from which information can be obtained to assist in the final specifications.

The HASYLAB Beamline A1 is a bending magnetic beamline that operates over the energy range 2.4-8.3 keV and has been open to users since Sept 2009. It uses the two Si(111) crystal pairs envisaged here for the same reasons discussed in the report. The main issues with this beamline were position instabilities due to floor instabilities and detuning of monochromators (neither of which are issues with our proposed beamline). Generally, there were no problems working over this energy range using a Ni stripe and SiO_2 on the mirrors (although our extended range will require Rh and Cr stripes instead of Ni. More details on this beamline can be found in a detailed report by Peter Kappen supplied previously.

Andrew Berry has used and discussed beanmline I18 at Diamond and discussed the MEX beamline with the principal beamline scientist, Fred Mosselmans and some of these comments have been included in the report. This beamline is an undulator microfocussed XAS beamline with an energy range 2-20 keV, KB focusing, Si-drift detector, so it contains many of the design features of our beamline (albeit with an undulator source instead of a BM source. They use a fast flushing He measurement chamber below 5 keV.

Beamline 06B1-1 is a BM beamline at the CLS with similar capabilities as the proposed beamline with an energy range of 1.7-10 keV (fixed-exit double crystal monochromator InSb(111) and Si (111)) and a similar scientific justification as in our science case. It also has microfocus and normal XAFS like the proposed beamline. The beamline scientists has had experience in optimising the InSb(III) crystals (see http://www.lightsource.ca/uso/pdf/06B1-1_SXRMB_Beamline_Characteristics.pdf).

Beamline 9A at the Photon Factory is a bending magnetic beamline that has operated over the energy range 2.1-15 keV for a decade. It uses Ni and Rh stripes to cover this energy range and has many similar design features, including the use of a He sample environment for measurements below 4 keV. It uses bent conical mirrors to increase the flux as well as produce high energy resolution. While this focusing could be considered it is probably not necessary or desirable in terms of the other parameters of the beamline. Further details can be found at http://pfwww.kek.jp/users_info/station_spec/xafsbl/9a/bl9a_e.html

Beamline 16A at NSRRC is used by a growing number of Australian researchers. It is a BM beamline (2 ~ 8 keV), which uses very simple optics and with a vertically collimating pre-mirror, fixed-exit double crystal Si(111) monochromator, and toroidal focusing mirror, i.e., many similar components as the requested beamline. It has a Ni stripe and users generally report no issues using it over this energy range. Further information can be found on http://140.110.203.42/EFD.php?num=251.

Beamline 6-2 at SSRL is a wiggler beamline, which is focused over 2.36-5 keV and unfocussed over 4-17 keV. It is Rh and Ni stripes. There was considerable issues with photodamage for samples at the S edge. Further information can be found at http://ssrl.slac.stanford.edu/beamlines/bl6-2/

Lucia beamline at Soleil (0.8-8 keV) incorporates InSb(111) and Si(111) monochromator crystals as well as three crystal sets on an undulator beamline with KB mirrors. Like many of the other beamlines it has Ni stripes. It has both solution cells and vacuum environments for sampling (see http://www.synchrotron-soleil.fr/Recherche/LignesLumiere/LUCIA).

Port 093 – Canadian DCM at the Synchrotron Radiation Center in Wisconsin covers the low-energy range of the new beamline 1.5-4.0 keV using InSb(111) and quartz (1010) crystals.

External Advice

Edmund Welter from HASYLAB and Fred Mosselmans from Diamond have offered to provide advice. Another suitable person who could be contracted to help design the beamline would be Thomas Rabedeau of SLAC. Given the similarity of the CLS beamline and experience in optimizing the InSb(111) it would be worthwhile to get Yongfeng Hu involved in the final beamline design.

MEX-BSG with helpful input from Bruce Cowie.
Revised 16/10/2011