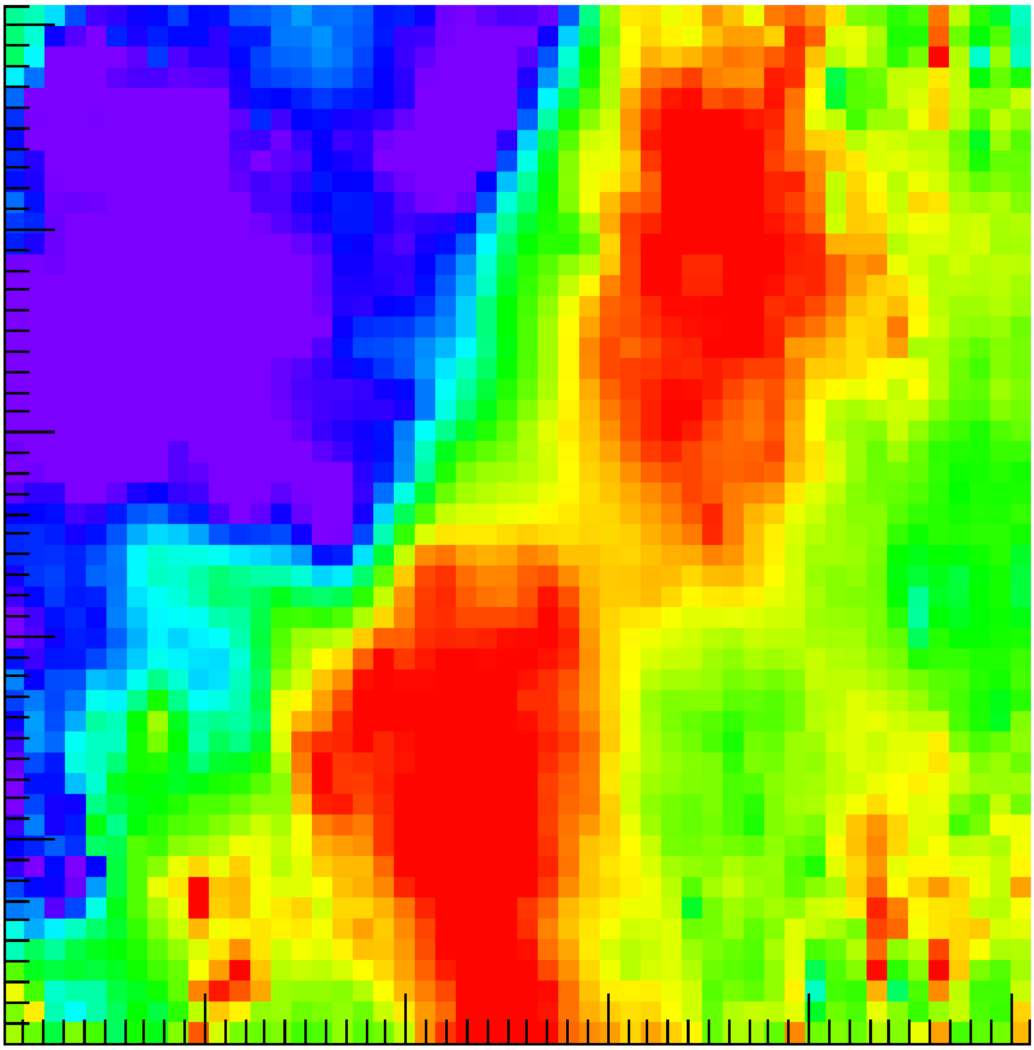
Micro Materials Characterisation Beamline:

Scientific Case and Design Discussion

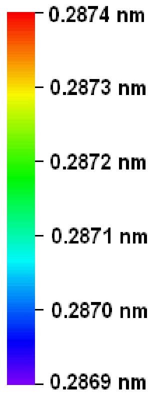
August 2011



Prepared by: Beamline Scoping Group

Prof. Andrea Gerson (UniSA);
Dr. Steve Wilkins (CSIRO);
Dr. Brian Abbey (Uni. Melb.);
Dr. Peter Lynch (Deakin Uni.);
Prof. Tim White (ANU);
Mr. Ian Madsen (CSIRO);
Dr. Justin Kimpton (AS)
Dr. Kia Wallwork (AS)
Dr. David Paterson (AS)

Figure on title page: 50 × 50 μm *a*-parameter map calculated from the {211} martensitic diffraction peak for an high performance hot work H13 tool steel sample slow cooled for 3 hours to liquid N_2 temperature and then held for one hour. Neither this spatial resolution nor sensitivity to structural variability would be possible using a laboratory X-ray source or large incident X-ray spot sized synchrotron diffraction.



Executive Summary

This document provides the scientific case for construction of the Micro Materials Characterisation (MMC) beamline on the Australian Synchrotron as well as a preliminary technical design discussion.

The MMC beamline is designed to provide simultaneous measurement of chemical composition in 2D, and extended crystalline structural form in 2D or 3D, with a spatial resolution less than 1 micron. This beamline will combine these capabilities to provide these two types of information simultaneously and on essentially the same volume of sample. These capacities will be further extended by the capability to also probe local environment via X-ray absorption spectroscopy. While there are many synchrotron microprobes that provide a 2D structural capability the provision of 3D structural information that is obtained in a non-destructive manner, will be truly world leading and will facilitate cutting edge research.

The scientific potential for the MMC beamline is virtually unlimited across broad areas of materials science. The ability to study chemical composition, oxidation state/chemistry, crystal structures and defects with micron scale resolution creates completely new scientific opportunities with implications for everything from fundamental studies of materials behaviour and evolution, to characterisation of specific systems with key mechanisms that can now be addressed. For example, the MMC beamline can address critical issues with respect to solar, high-temperature and nuclear energy materials, can enable novel studies of pollutants in the environment, can help understand mining and mineral recovery processes and can even provide new information on biological materials. The reality is that the world is heterogeneous and that micron scale is an important length scale where heterogeneities start to resolve themselves into homogeneous crystals and structures. Such intrinsic variability in samples can be used to advantage, *e.g.* as a means for carrying out combinatorial materials science on a single bulk sample. The ability to non-destructively study samples with micron scale 3D resolution has the potential to fundamentally change the way we understand a wide range of minerals and materials!

The MMC beamline will provide capabilities that will not be available from either the initial nine beamlines at the Australian Synchrotron or the other phase two beamlines planned for development and construction. The wide range of applications proposed by Australian researchers demonstrates:

- The potential value-addition to be created by the MMC beamline to the fundamental, strategic and applied sciences in Australia;
- The direct application of the MMC beamline to core and growing export areas central to Australia's continued economic health;
- The broad fields of application of the MMC beamline promoting multidisciplinary world leading research including the training and longevity of internationally competitive post-graduate students and researchers.

Evidence of the very high level of demand for the MMC beamline is demonstrated from a survey of a *limited* number of organisations and only those that specifically require micro-diffraction. It should be noted that the number of organisations who have voiced support of this develop far exceeds those specifically surveyed. It is clear that the MMC beamline will be fully utilised from the day of commissioning with demand far exceeding available instrument time and resultant world class science.

Contents

1. A description of the desired experimental capabilities

Crystalline phase determination, polycrystallinity, strain, grain orientation as well as defect structure, migration and organisation are fundamental to the understanding of materials' properties. The Micro Materials Characterisation (MMC) beamline is the only facility proposed for the Australian Synchrotron that will enable these properties to be measured, in 2 or 3 dimensions and at the micron scale. This beamline will combine micro-diffraction and micro-fluorescence capability in a single experimental station and will be capable of providing these two types of information simultaneously and on essentially the same volume of sample. These capabilities will be further extended by the capacity to also probe local environment, via X-ray absorption spectroscopy, at selected regions of interest.

Synchrotron X-ray microprobes have commonly used a monochromatic X-ray beam. When the crystallite size is smaller than the incident beam size, monochromatic diffraction measurements yield either complete or fragmented Debye-Scherrer diffraction rings. These rings can provide considerable information, including phase identification, preferred orientation from intensity variations and strain information from the distortion and broadening of the ring. However, monochromatic radiation has the important disadvantage that where the crystallite size is of the order of, or larger than, the beam size, few or no diffraction peaks may be observed for a given sample and detector geometry, and hence vital information may be simply overlooked. With improved focussing optics, enabling smaller and smaller incident X-ray beam sizes this occurrence is becoming more frequent. However, these problems may be overcome by using a broad band pass incident X-ray beam, *i.e.* Laue ("polychromatic") diffraction (Fig. 1). The important difference of Laue diffraction as compared to monochromatic diffraction is that, because the incident beam is composed of a continuous spread of wavelengths, there is a greatly increased likelihood that Bragg's law ($\lambda=2d\sin\vartheta$) will be satisfied thus enabling observation of diffraction peaks.

Diffraction patterns, generated from high intensity broad band pass synchrotron radiation, may be produced from deep within a sample. Assignment of diffraction peaks to individual crystallites as a function of depth can be carried out by differential aperture X-ray microscopy (DAXM)[3] and/or detector triangulation for rapid 3D depth recovery. The 3D information that can be derived includes crystallite size, crystallite orientation, definition of grain boundaries and crystallite deviatoric strain *i.e.* distortion of the unit cell, or absolute strain, derived by scanning the monochromator across the energy of a single diffraction peak.[1] Moreover, the observed crystallographic spread (streaking) and splitting of individual Laue peaks provides a measure of the geometrically necessary dislocation (GND) and geometrically necessary boundary (GNB) content.[2]

1 G.E. Ice, B.C. Larson, J.Z. Tischler, W. Liu, W. Yang, X-ray microbeam measurements of subgrain stress distributions in polycrystalline materials, Materials Science and Engineering A, **399**, 43–48 (2005).
2 G.E. Ice,. J.W.L. Pang, R.I. Barabash, Y. Puzyrev, Characterization of three-dimensional crystallographic distributions using polychromatic X-ray microdiffraction. *Scripta Materialia*, **55**, 57–62 (2006)

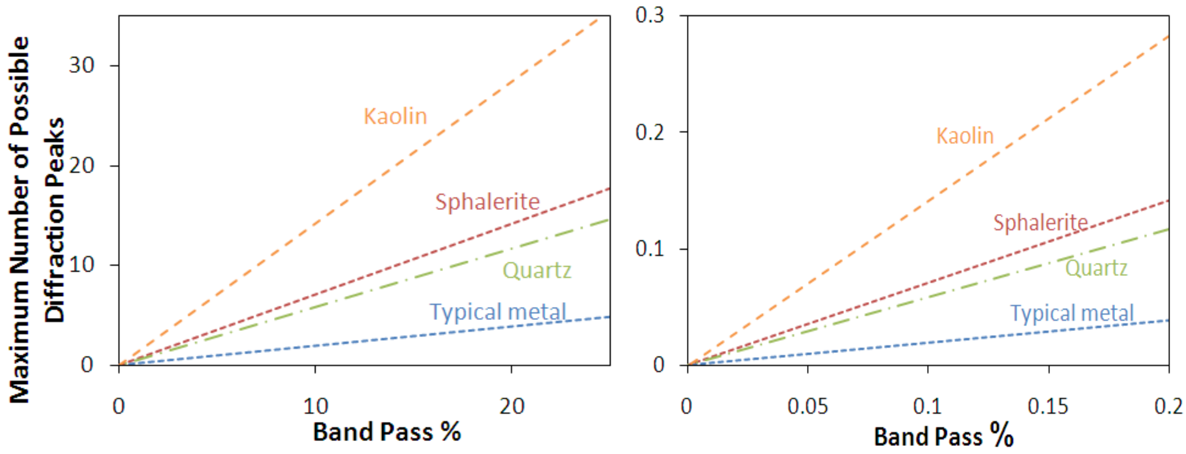


Figure 1: Maximum number of diffraction peaks possible (at 15 keV, 2 mrad divergence) for various band passes calculated for an area detector mapping out 1 steradian at diffraction angle 90 °2θ. The band pass arising from a Si(111) monochromator is approximately 0.1%. Left hand panel corresponds to multi-layer optics and right hand panel to perfect crystal optics.

It is the 3D structural mapping capability, coupled with corresponding X-ray fluorescence microscopy (XFM) mapping and X-ray absorption spectroscopy (XAS) that will ensure that the MMC beamline provides a world ranking facility located at one of the leading edge centres of materials science. Broad-band (high-speed) micro-diffraction is currently unavailable at the Australian Synchrotron and thus this beamline will fulfill a core need of the Australian materials science community. The MMC beamline will provide:

- Monochromatic and Laue micro-diffraction;
- Phase mapping, strain mapping, crystallite orientation mapping (either 2D or 3D via DAXM[3]) and composition (2D);
- Simultaneous, rapid and coincident X-ray fluorescence microscopy (XFM) and micro-X-ray diffraction (XRD) measurements not conceivable on laboratory-based equipment;
- Selected area X-ray absorption spectroscopy (XAS) for determination of local coordination and/or oxidation state;
- Spot size adjustable from below 1 µm and up to 5 µm.

3 B.C. Larson, W. Yang, G.E. Ice, J.D. Budai, J.Z. Tischler, Three-dimensional X-ray structural microscopy with submicrometre resolution, *Nature*, **415**, 887-890 (2002).

2. A digest of the science that would be enabled and perspectives on its importance

The scientific potential for the MMC beamline is virtually unlimited across broad areas of materials science. The ability to study chemical composition, oxidation state/chemistry, crystal structures and defects with micron scale resolution creates completely new scientific opportunities with implications for everything from fundamental studies of materials behaviour and evolution, to characterisation of specific systems with key mechanisms that can now be addressed. For example, the MMC beamline can address critical issues with respect to solar, high-temperature and nuclear energy materials, can enable novel studies of pollutants in the environment, can help understand mining and mineral recovery processes and can even provide new information on biological materials. The reality is that the world at all size scale is heterogeneous and that micron scale is an important length scale where heterogeneities start to resolve themselves into homogeneous crystals and structures. Such intrinsic variability in samples can be used to advantage, *e.g.* as a means for carrying out combinatorial materials science on a single bulk sample. The ability to non-destructively study samples with micron scale 3D resolution has the potential to fundamentally change the way we understand a wide range of minerals and materials!

The list below of applications, proposed by Australian researchers, demonstrates:

- The potential value-addition to be created by the MMC beamline to the fundamental, strategic and applied sciences in Australia;
- The direct application of the MMC beamline to core and growing export areas central to Australia's continued economic health;
- The broad fields of application of the MMC beamline promoting multidisciplinary world leading research including the training and longevity of internationally competitive post-graduate students and researchers.

Frontier Technologies for Building and Transforming Australian Industries:

Breakthrough science: 2D and 3D understanding of crystal grain growth, crack propagation, plastic deformation and phase transformation in relation to the development of novel materials;

Frontier technologies: Stress corrosion cracking, electro-pulse crack healing, applied stresses due to ion implantation, epitaxial growth, deformation in spot, friction and fusion welds, cryogenic and heat treatments of alloys, molecular organisation of key plant organelles and components;

Advanced materials development: Corrosion resistant materials, catalyst behaviour, retardation of whiskering, thin film grain growth on patterned, textured and modified substrates, alteration and migration of toxic species in recycled ceramics; and chemical segregation in composites and ecomaterials.

Safeguarding Australia

Transformational defence technologies: Improved armouring, lightweight materials, composite armouring, reduction in electromagnetic signatures, electric drive systems, development of bioremediation strategies.

An Environmentally Sustainable Australia

Transforming existing industries: Increased mineral processing recovery, decreased acid mine drainage and toxic metal release from waste rock, decreased furnace temperatures, reduced failure rates during manufacturing, utilisation of industrial wastes, optimisation of chemical state in waste for reduced environmental transport, improved understanding of the mechanism of inclusion of impurities during industrial processing.

Overcoming soil loss and salinity and acidity: Understanding geochemical changes in soils on weathering and interactions with ground waters, understanding porosity in soils, understanding, reducing and controlling effects of acid rock drainage and acid sulfate soils.

Reducing and capturing emissions in transport and energy generation: New materials for hydrogen generation and storage, improved battery materials, improved materials of storage of nuclear waste, improved catalytic materials for greenhouse gas reduction, improved solar cells.

Developing deep earth resources: Improved ability to cross correlate mineral phase with high value trace elements, *e.g.* uranium, increased understanding of strain and grain size distribution on the distribution of high value elements and their subsequent processing, increased understanding of deep earth materials and processes.

Promoting and Maintaining Good Health

A healthy start to life: Arsenic and lead uptake in children.

Ageing well, ageing productively: Porous silicon scaffolds for tissue engineering, optimised addition of silicon to orthopaedic materials for enhanced bone growth, nanoparticles for cancer diagnosis, lipoceramic capsules: a novel delivery system for poorly soluble drugs, understanding the roles of metals in disease processes and their treatment by XRF and XAS mapping of intact tissues.

Preventive healthcare: 3D structure of enzymes, protein and membrane structures and redox chemistry, assessment of fatigue and stress induced failure controlling longevity of common Nitinol stents used in a variety of medical keyhole surgery applications.

We also provide a list of institute specific applications for the MMC beamline. The list is not exhaustive in that we are aware of many more institutions/researchers who intend to use the MMC beamline, but nevertheless serves as a guide to breadth and depth of science that will be able to be tackled.

Applications for the MMC beamline by the **University of South Australia** are diverse: environmental remediation (remediation of acid mine drainage and the transport and speciation of hazardous metals), biotechnology (bioceramics and drug delivery systems), metallurgy (heat/cryogenic treatment of alloys), minerals processing (Cu activation of metal sulfide minerals) and hydrometallurgy (leach mechanisms of chalcopyrite, mineralogy of uranium, silver and gold containing ores and nickel laterites). Research concentrations across many disciplines have voiced support for this facility: Ian Wark Research Institute, Mawson Institute for Advanced Manufacturing, Sansom Institute and the Centre for Environmental Risk Assessment and Remediation.

The MMC beamline will provide new opportunities and critical information for a large number of existing projects in earth sciences (**CSIRO Earth Science and Resource Engineering;** Earth Sciences, **University of Adelaide**). These range from understanding the links between element mobility, mineral reactions, and deformation in metamorphic and hydrothermal conditions; understanding the mobility of metals and contaminants in soils, with applications to mineral exploration and water quality; tracking the role of micro-organisms in scavenging metals*, e.g.* during formation of calcrete.

The applications of the MMC beamline in the world of biological macromolecules (Waite Campus and the School of Agriculture, Food and Wine, **University of Adelaide** and **CSIRO**) will provide novel insights into the structure of crystalline and partly crystalline products of i) enzymic reactions, such as cellulose and starch; ii) bio-composites, for example barley β-D-glucan in complex with arabinoxylan or any other polysaccharide that represent a fibre component, and is extractable from cereal plants and iii) organisation and order of large protein complexes and protein assemblies arranged in polycrystalline states in biological membranes. Descriptions of structural and functional relationships of plant transporters will create opportunities for basic and applied research that could improve crop yields and quality, and the environmental sustainability of crops in low input agricultural production systems.

Curtin University's Centre for Materials Research focuses on microstructural characterisation of a diverse range of materials. Conventional XRD and XRF are combined with TEM and SEM but there is currently no convenient way of obtaining sensitive elemental analysis at the same time as phase analysis (XRD) at the micron level. For materials such as geopolymers there is a critical need to understand the extent of the alkaline reaction to enable optimisation of elemental composition. This can only be resolved via micron resolved elemental analysis in conjunction with phase analysis offered by the proposed MMC beamline.

Southern Cross University's research capability will be greatly enhanced in one of its main area of research strengths (*i.e.* geoscience) by the establishment of the proposed MMC beamline. Areas of intended application range from environmental remediation of degraded acid sulfate soil landscapes to the transport and speciation of hazardous metals within estuarine and riverine environments. Adequate examination of many of the clay sized minerals that mediate and control the geochemistry in these environments requires the advanced capabilities afforded by the proposed facility. Examination of both phase and composition at the micron scale is necessary to underpin the formulation of management techniques for such landscapes.

La Trobe University is seeking to expand its synchrotron capability in the area of X-ray microprobe studies, in particular, those involving XAS. Projects that will benefit greatly from regular local access to microprobe facilities include (i) micro-analyses of arsenic in lake sediments, (ii) investigation of embedded micro-crystallites in meteorite and mineral materials, (iii) *in situ* investigations of zinc distribution and speciation in plant roots, (iv) *in situ* investigations of antimony in solid industrial wastes upon leaching tests, (v) microprobe analyses of the chemistry and crystallography of paint particles in automotive paints for forensics investigations, and (vi) microprobe studies of samples of cultural heritage objects (paint flakes, metal fibres, etc; verification and historical identification of artwork).

There is a broad range of applicability of the MMC beamline within the various business units of **CSIRO**. Applications include (i) investigating the deportment of valuable metals in various mineralogical suites in both the mineral exploration and minerals processing context, (ii) investigating tribochemical effects to better understand wear mechanisms in biomaterials used in human prosthesis, (iii) understanding and controlling the arrangement of cellulose in plants would open the way for the development of many novel and interesting materials no further away than planting a seed, (iv) the development of hexagonal close packed (hcp) structures of, for example, Ti and Mg to produce new light weight metal alloys (v) development of high performance polymer composites for aerospace applications, and (vi) cultural heritage studies in connection with authentication of artworks, *etc*.

AMIRA International considers the development of the MMC beamline capability as an important adjunct to the range of mineral science techniques currently available. As it is a unique capability, the micro-XRD/XFM allows the minerals industry to address problems that could only be approached by indirect experimentation in the past. The microprobe adds an important new capability that enhances the minerals industry's ability to develop new processes and solve existing problems providing another mechanism to create strong links, ongoing interaction and research activity between the research community and the industry.

The MMC beamline will have widespread application across many applied research fields of strategic importance to **ANSTO**, including advanced materials science, environmental research and mineral processing. It should be noted that the X-ray capabilities to be provided by micro-XRD/XFM will complement the neutron scattering techniques available at the OPAL research reactor. The capabilities of the MMC beamline in the materials area in particular are unmatched, and will be applied across the whole spectrum of ANSTO's materials research for example: investigation of micro stress/strain in welds and other metal/allow systems; the micron-scale thermo-mechanical properties of alloys and intermetallics and micro-crystallinity and spatial distribution of grains in glass-ceramic waste form materials. Minerals and environmental applications include mineral processing and mine remediation *e.g.* the role of arsenic; and metal uptake in hyper-accumulating plants.

3. Demonstrated demand for the Micro Materials Characterisation beamline

Three specific groups of users have been identified that will benefit from the availability of this beamline:

- The considerable sections of the materials science community that specifically requires micro-diffraction either by itself or in conjunction with XAS and XFM. At present, there are no micro-diffraction mapping facilities at the Australian Synchrotron and thus, where a heterogeneous crystalline system is to be examined, the scientific proponents must travel overseas. It may be noted that heterogeneity may take several forms *e.g.* phase, solid solution series, grain orientation, strain etc.
- A considerable number of studies being undertaken on the PD beamline would also benefit from micro-diffraction where the samples being studied are heterogeneous and the phase of interest is a minor component and not resolvable by a bulk analysis *e.g.* the examination of uranium containing ores.
- The MMC beamline could also address the requirements for higher energy XFM. A wavelength shifter or wiggler X-ray source (discussed in Section 5.2) will enable examination of excitations (either XFM or XAS) in the high energy range not accessible to the undulator based XFM beamline. For applications where broad bandpass XFM is relevant considerable higher energy flux will also be available. Feedback from Dr. David Patterson (Principal Scientist – Microspectroscopy Beamline at the Australia Synchrotron) suggests that 3-4 XFM users per cycle would benefit from micro-diffraction. In addition a further 4-5 user per cycle would benefit from accessing a higher energy for XRF and approximately 50% of these would also like to conduct micro-diffraction on their samples.

Evidence for the high level of demand for diffraction based synchrotron methodologies is provided by statistics compiled across 2009 and part of 2010 via the International Synchrotron Access Program (ISAP). Fig. 2a clearly indicates that diffraction and scattering facilities comprise a significant proportion of the funding demand. On further analysis of demand versus capability (Fig. 2b) it appears that the MMC may also play a significant role in terms of providing access to capabilities other than micro-diffraction where a greater energy range is required than is currently possible both with and without spatial resolution.

However, a much more realistic assessment of the potential user community can be made by surveying the Australian community, most of who do not currently access micro-diffraction but who can clearly see that this capability would enhance their scientific capacities. The MMC beamline will offer significant potential to attract new users with interests in materials modelling, for example the MMC beamline offers unique potential for validation of crystal plasticity models in both 2D and 3D. Furthermore, this can be done in various *in situ* environments. It should be noted that the ASRP did not offer readily available access to micro-diffraction facilities and therefore the user community cannot draw on this historic developmental foundation.

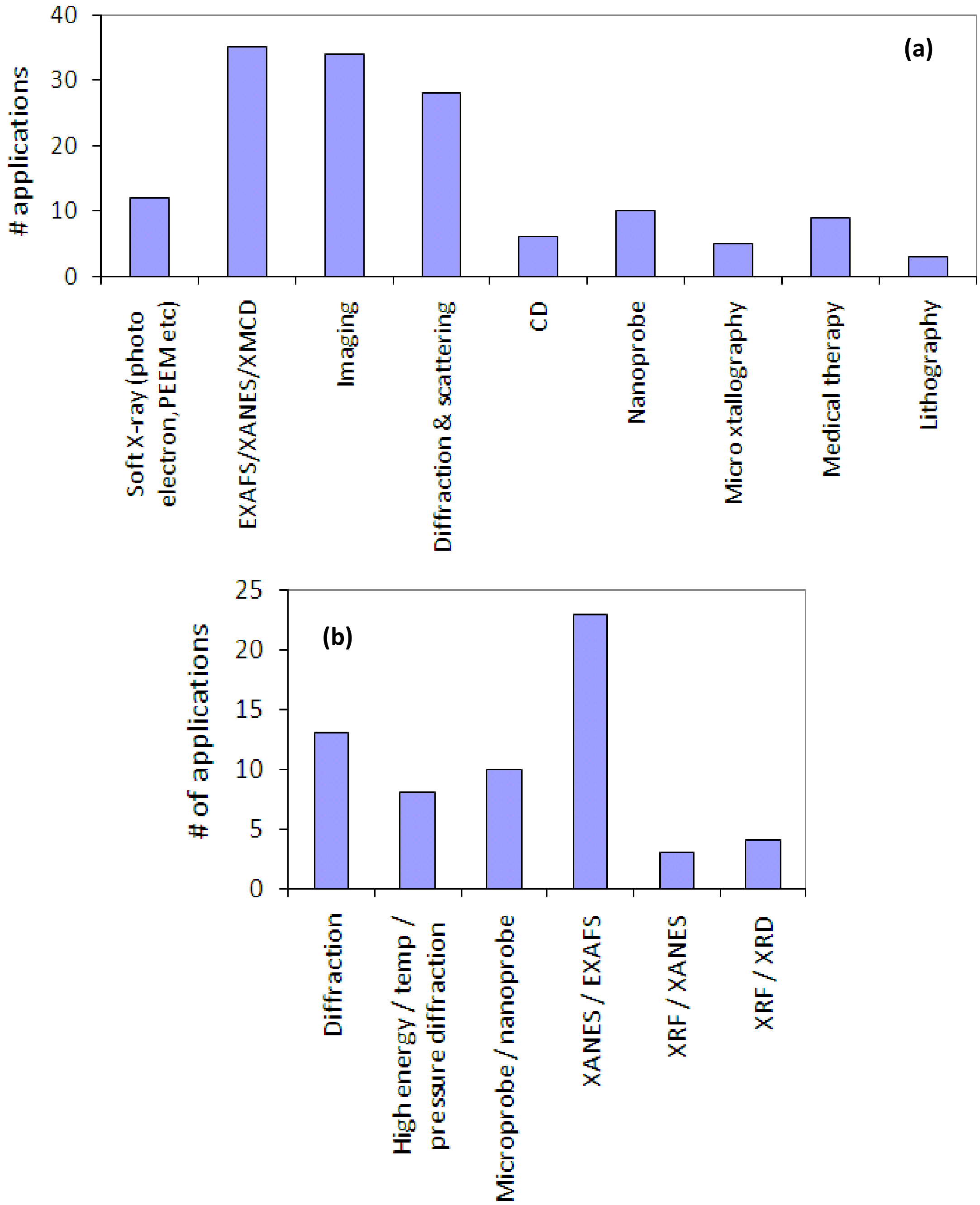


Figure 2 (a) Coarse distribution of applications for international travel funding as a function of generic technique area. (b) Applications for which the MMC beamline is likely to be applicable.

Evidence of the very high level of demand for the MMC beamline is demonstrated by Table 1 which has been developed from a survey of a *limited* number of organisations and only those that specifically require micro-diffraction. It should be noted that the number of organisations who have voiced support of this development far exceeds those listed in Table 1. It is clear that the MMC beamline will be fully utilised from the day of commissioning.

Table 1 Estimated demand for the MMC beamline across a limited selection of Australian Institutions.

Organisation	Number of users	Average number of days per month
University of South Australia	17	6
The University of Adelaide	10	4
Curtin University of Technology	5	2
Southern Cross University	8	3
La Trobe University	8	3
CSIRO	30	7
AMIRA International Ltd	5	2
ANSTO	8	3
TOTAL	91	

4. Complementarities (and minimisation of overlap) with existing and proposed beamlines at the AS

There are currently two existing and one proposed beamlines at the Australian Synchrotron to which the MMC is related. However, in both cases there exist profound differences in terms of the measurements, and therefore the science, enabled. Table 2 provides an overview of the complementary capabilities to be provided by these facilities.

The Powder Diffraction (PD) beamline provides 'bulk' monochromatic powder diffraction analysis on a spatial scale of, at the smallest, 0.5×0.5 mm. At this scale it is not possible to examine the properties of individual crystallites, for instance orientation and strain, on a crystallite by crystallite basis, an essential scientific justification of the MMC. Moreover, these properties cannot be coupled directly to composition (XRF) or local structure (XAS), a capability vital for integrated understanding.

The X-ray Fluorescence Microprobe (XFM) provides highly spatially resolved XAS and XRF analysis with an effective upper energy of approximately 25 keV. This facility does not provide diffraction analysis, either monochromatic or polychromatic. The latter requires a polychromatic X-ray beam which necessitates the adoption of appropriate achromatic optics, *e.g.* as discussed below depth graded multilayers and Kirkpatrick-Baez (KB) mirrors, as part of the initial conceptual design. The micro-diffraction capability is essential for spatially resolved diffraction characterisation and therefore understanding of minerals, materials and other crystalline systems.

The MMC is also complementary to the proposed Advanced Diffraction and Scattering (ADS) beamline which will provide a minimum incident X-ray beam size of approximately 30 µm and hence will not generally be able to probe samples on a size scale equivalent to or smaller than that of individual crystallites. Moreover, while the large accessible energy range (30-120 keV) will enable considerable depth penetration into samples 3D spatially resolved diffraction analysis on a grain by grain basis will be problematic and the resulting measurements will be effectively of the 'bulk'.

Table 2 Existing and proposed facilities at the Australian Synchrotron and the relationship of their capabilities with the Micro Materials Characterisation beamline.

Beamline	Diffraction		XAS	XRF	Spatial resolution	Energy range
Micro Materials Characterisation	✓	mono Laue	✓	✓	1×1 µm	5 - 60 keV
Powder Diffraction	✓	mono	✘	✘	0.5×0.5 mm	5 - 30 keV
X-ray Fluorescence Microprobe	✘		✓	✓	100×100 nm	4 -25 keV
Advanced Diffraction and Scattering	✓	mono Laue	✘	✘	20 x 100 µm	30 – 120 keV

5. A summary of basic performance parameters required to achieve the target outcomes

5.1 Performance Parameters

The definition of the technical requirements for the MMC beamline are well advanced and have been developed in collaboration with an international team from Oak Ridge National Laboratory (Gene Ice), NSLSII (Ruben Reininger), Advanced Photon Source/University of Chicago (Mark Rivers) and the Canadian Light Source (Renfei Feng, Emil Hamil, Stewart McIntyre).

The technical requirements to achieve the desired scientific goals as defined by this international team and the Beamline Scoping Group are provided in Table 3.

Table 3 Micro Materials Characterisation beamline technical requirements.

Minimum beam size	1 × 1 µm or less (FWHM)
Maximum beam size	5 × 5 µm using KB mirrors
Energy range	≈ 5 – 60 keV
Divergence	<2.5 mrad H, 2.0 mrad V
Band pass options	1. White light (broad-band); 2. ≈ 10% bandpass (multilayer: two bounces); 3. ≈ 1% bandpass (crystal optics: two bounces) for highly diffracting samples; 4. Si(111) or other suitable monochromator, for monochromatic diffraction, elemental/oxidation state specific fluorescence and XAS;
Change of band pass options	Ability for rapid change between bandpass options that samples exactly the same sample volume, *i.e.* the beams arising from the different bandpass options must be coincident and collinear to within the focal spot size;
Flux	$>10^{10}$ photon·s^{-1} for 10% band pass at 15 keV 1 × 1 µm (200 mA); $>10^{8}$ photon·s^{-1} for Si(111) at 15 keV 1 × 1 µm (200 mA);
Detectors	Fast CCD or multi pixel array for diffraction measurements and MAIA detector for XRF mapping

The requirement for a large energy range, *e.g.* 5 to 60 keV, with reasonable flux is worth describing more fully. Clearly, high flux results in a better signal-to-noise ratio (S/N) for both XFM and micro-XRD, enabling reduced measurement times and hence the possibility of increased range or area of sample analysis.

For XFM, greater flux at higher energies, than can be provided by a bending magnet or undulator, would enable access to a greater range of K-edge fluorescence emissions, *i.e.* for higher Z elements, than is currently available via the XFM beamline. We have found, for instance Ag Kα is not measurable in practice on the XFM beamline, even for Ag containing mineral standards, due to the low flux at the required incident energy of approximately 26 keV. Thus the K-edge of even heavier elements will also not be accessible. However, measurement of Ag Lα fluorescence resulted in considerable overlap with K Kα emission lines. More generally, the use of L-edge fluorescence emissions for XFM frequently results in overlap of fluorescence data resulting in considerable difficulty in locating and examining trace elements. At greater fluorescence energies, only accessible via the availability of higher incident X-ray energies, the likely overlap of fluorescence lines is considerably reduced. Too low a limit for the upper value of the incident X-ray energies can thus be a considerable impediment to the examination of high Z value and/or trace elements within complicated heterogeneous matrices. In addition the measurement of low energy florescence L-lines will limit the depth of X-ray penetration out of the sample and hence will limit the XFM analysis depth.

For micro-XRD an increased upper value for the incident energy range enables an increased range of diffraction data to be accessed for both monochromatic and Laue diffraction cases. Thus the amount of data measured can be tailored to the requirements dictated by the system under examination. The accuracy of measurement of strain using polychromatic radiation is directly dependent on the number of diffraction peaks that can be accessed for any given crystallite. An increased number of diffraction peaks for any given sample volume will result in increased strain resolution. For 3D DAXM diffraction higher incident energies will enable increased depth of penetration into the sample and therefore result in a more complete understanding of the surface versus bulk crystalline environment.

While usable flux obviously plays a central role in beamline viability this is generally not an issue for pink light applications, for instance a 10% band pass will provide, by definition, a factor of ≈×250 flux (reflectivity of 50% from one bounce from multilayer) over the light transmitted by Si(111). Our aim is therefore to maintain a reasonable X-ray flux while maximising the accessible energy range. All of the three groups of users identified above in Section 3 would benefit from a greater usable energy range. We have attempted to list below the advantages and disadvantages of each possible X-ray source; undulator, wiggler, superbend, bend and wavelength shifter.

Their is strong consensus among the Beamline Scoping Group for the MNC beamline that there is significant new and better science could be done by going to higher energy than may be available via a bend magnet and that there is a strong scientific motivation for exploring design strategies for achieving this.

5.2 Possible X-ray Sources

It is clear that an undulator source would not provide significant scientific advantage, in terms of access to high energy X-rays, for micro-XRD as compared to either a wiggler or WLS, and that a superbend cannot be physically implemented on the Australian Synchrotron. We therefore consider the application of either a wavelength shifter or wiggler X-ray source as a means to achieve increased X-ray energies as compared to a bend magnet source.

Fig. 3 shows the estimated flux of an existing bend magnet at the Australian Synchrotron (1.3 T) as compared to various wavelength shifters of varying magnetic field (Table 4). These X-ray flux profiles have been generated per horizontal and vertical 0.1 mrad, equivalent to the proposed front end acceptance apertures of the MMC beamline. The horizontal source size has also been taken into consideration (σ_x for a dipole of 87 µm *cf* 320 µm for an insertion device) by division of the flux values generated for the WLS by a factor of 3.7[4]. It is clear that the bend magnet performs better at smaller energies with greater flux generated by the WLS only above approximately 24 keV.

4 Comments on the Micro Materials Characterisation (MMC) Beamline Interim Report, by Bruce Cowie,16-8-2011

Table 4 Critical energy (E_{crit}), useful upper range of energy for monochromatic measurements ($E_{max} = 3 \times E_{crit}$), period (where applicable), magnetic field and total power, for an existing Australian Synchrotron bend magnet and a range of wavelength shifters. In all case for the WLS *K* (0.934 × period (cm) × magnetic field (T)) has been kept constant at a value of 20 and the stored current was 0.2 A.

E_{crit} (keV)	E_{max} (keV)	Period (cm)	Magnetic Field (T)	Total power (W)†
Bending Magnet				
7.8	23.4		1.301	30‡
Wavelength Shifter				
32.1	96.3	4.0	5.355	1306
25.6	76.8	5.0	4.284	1045
21.4	64.2	6.0	3.570	871

† WLS not normalised
‡ per mrad

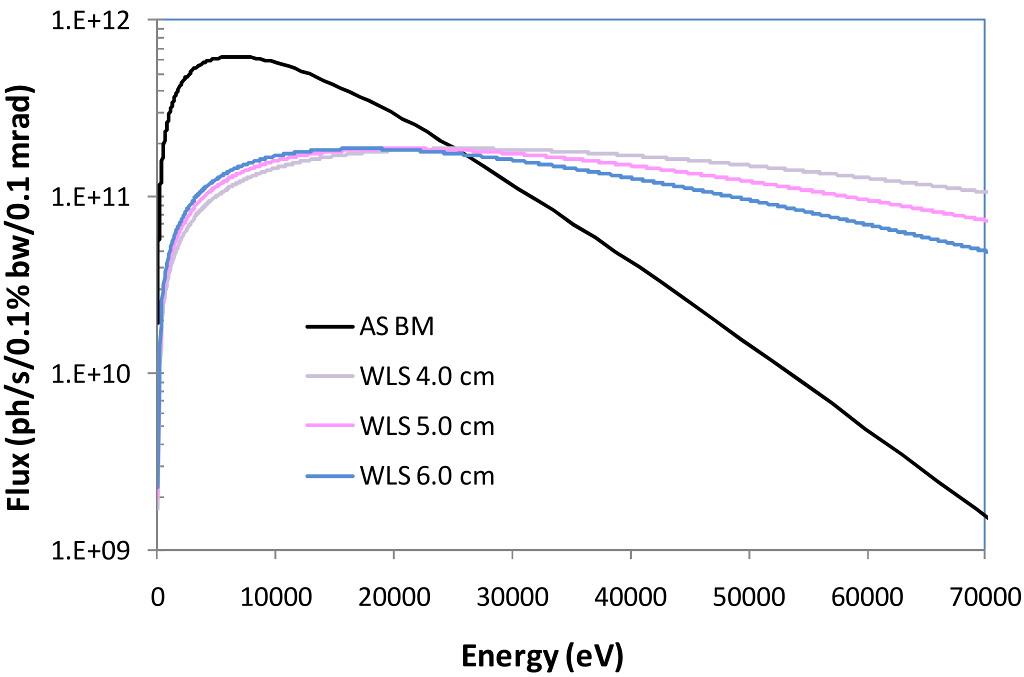


Figure 3 A comparison of the estimated flux from an existing bend magnet at the Australian Synchrotron and various wavelength shifters of different magnetic period. The stored current is 0.2 A. WLS shifter flux, as generated by XOP, is divided by a factor of 3.7 to normalise the horizontal source size of an insertion device as compared to a dipole.

At 40 keV, the 50% cut-off for a Pt coated mirror at 2 mrad X-ray incident angle, the calculated flux (ph/s/0.1% bw/0.1 mrad) for the various sources examined is:

4.0 cm period WLS	1.72×10^{11}
5.0 cm period WLS	1.51×10^{11}
5.0 cm period WLS	1.29×10^{11}
BM	4.0×10^{10}

The increased flux, of the WLS shifters examined, as compared to a bend magnet source, at 40 keV is improved by approximately a factor of 2.5.

We are therefore considering the implementation of a super conducting wiggler X-ray source. To this end Ruben Reininger has been contracted to carry out extensive ray tracing (the scope of work is provided in Appendix 2) which will, amongst other tasks, compare superconducting wiggler sources of various lengths against a standard Australian Synchrotron bend magnet with the aim of fully analysing the advantages/disadvantages a wiggler source may provide. Implementation of such a source would require a cryogenically cooled monochromator and water cooled first collimating mirror.

5.3 Design Concepts

A beamline design has been proposed previously, shown schematically in Fig. 4, which consists of:

- A single axial aperture for both 'monochromatic' and 'white' beams;
- A Pt coated toroid at 11 m from source which will deflect the beam by 4 mrad;
- Small gap monochromator (≈6 mm) with Si(111)/Si(311) and depth graded multilayers before and after the Si crystals with the second crystals tracking the beam in each case to maintain a fixed beam height;
- The toroid will provide 1:1 focus onto intermediate slits 22 m from source;
- A pair of Pt KB mirrors (elliptical cylinders) which will deflect the beam by 4 mrad (two other strips of Pd and Si will also be available to alleviate transmittance of harmonics). The first KB mirror is 7 m from the intermediate slits, deflects vertically and is 200 mm long. The second KB mirror deflects the beam horizontally and is 150 mm long. The mirror centres are 180 mm apart and their focus is 150 mm from the centre of the second KB.
- Sample stage and KB mirror pair to be mounted on a height adjustable stage, *e.g.* miCos GmbH LS-270[5] (capacity up to 150 kg and unidirectional reproducibility of 0.05 µm). This will enable the sample to be moved up and down so that white and monochromatic light are coincident and co-linear on the sample.

A complete design description is available in[6]; however, at that time our instrument design and related discussion were based on the use of a superbend which is not implementable on the Australian Synchrotron. The design will be updated on completion of further ray tracing to be carried out Ruben Reininger on commission by the Australia Synchrotron.

It is clear that the possible implementation of a super conducting wiggler will have some important repercussions in terms of beamline design. For instance to access 60 keV radiation the angle of incidence on the toroidal mirror will need to be in the order of 2 mrad or less rather than 4 mrad as was previously proposed. As a consequence of this the length of the mirror will need to be doubled to be in the order of 800 mm long to maintain the required X-ray flux. It is likely also that 2 pairs of KB mirrors will be required to access the entire energy range proposed.

5 http://www.micos.ws/web2/en/1,4,040,ls270.html.
6 Updated Design Report, October 2009, A.R. Gerson, R. Reininger.

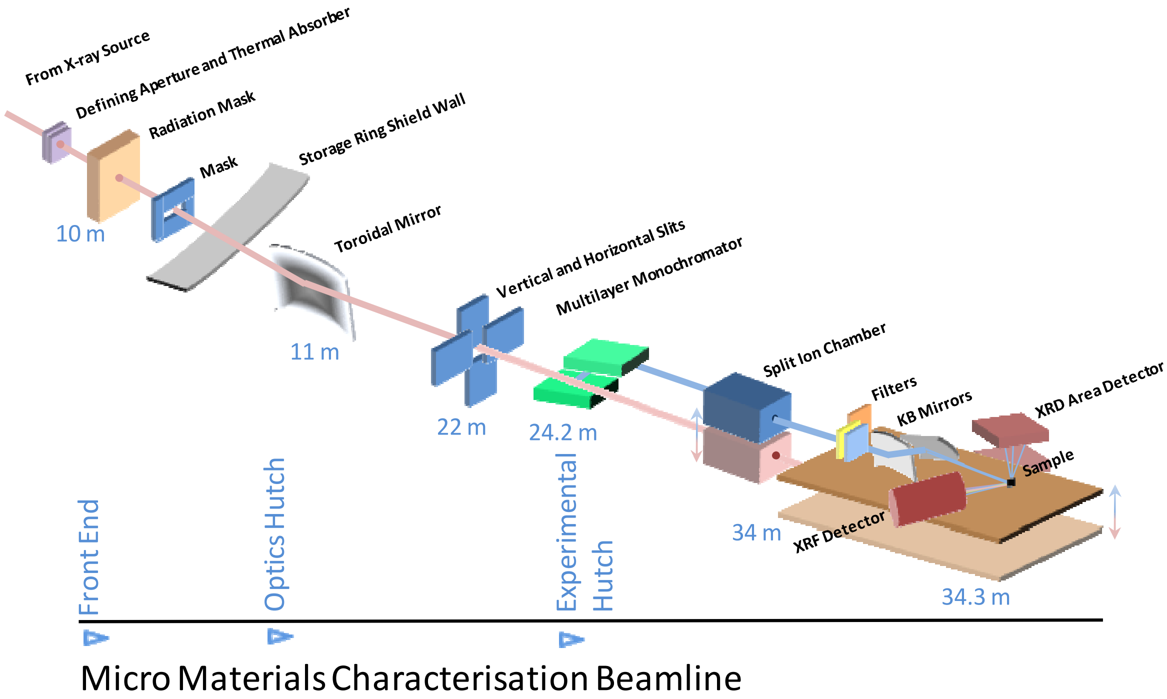


Figure 4 Schematic showing the major proposed components the MMC beamline.

In addition we assumed a vertical divergence of 57 µrad previously and had a 1:1 toroid followed by the double crystal monochromator[7]. The divergence at the monochromator is actually much larger than the width of the Si(111) double crystal monochromator at 20 keV, which is approximately 13 µrad. Therefore, the energy resolution will be dictated not by the crystals but by the vertical divergence. This will be worst at higher energies. If the intrinsic Si(111) resolution is required a vertical collimating mirror upstream of the mono followed by the 1:1 (or other demagnification) mirror may be implemented.

The optical scheme to be examined for initial examination (Appendix 2) will therefore consist of:

1. The designs will incorporate a collimating mirror as a first optical element to preserve the intrinsic resolution of Si(111);
2. The second optical element is a double crystal monochromator;
3. A focusing mirror downstream of the DCM will image the source into horizontal and vertical slits;
4. The slits will allow adjusting the spot size at the sample.5. A KB pair will focus the beam onto the sample;
5. The KB had the following approximate parameters: First mirror is 200 mm long and focuses vertically, second mirror is 150 mm long and focuses horizontally. The mirror poles are 180 mm apart and their focus is 150 mm from the center of the second mirror.

We specifically address the design questions posed in questions 1 to 19 in the Beamline Scoping Group Guidance Notes (1st June 2011) in Appendix 1.

7 Correspondence with Ruben Reininger 17-8-2011

6. A list and description of ancillary (non-beamline) support infrastructure needed to facilitate the proposed science program(s)

As the MMC beamline will be a hard X-ray beamline there will be little requirement for handling of sensitive materials (*i.e.* materials that need to be transferred to experimental facilities under vacuum) and it is likely that *in situ* cells *etc*. will be experiment specific. Our preference is for the focus to be on the beamline design with a view of maximising the useful energy range through provision of appropriate X-ray source, focussing optics and detectors.

7. A review and appraisal of other facilities with similar scope and capabilities

Relatively few synchrotron end-stations have been identified that are dedicated 2 or 3 dimensional micro-diffraction facilities. There are:

1. VESPERS at the Canadian Light Source
2. 12.3.2 at the Advanced Light Source
3. 34IDE at the Advanced Photon Source
4. BM32 at the ESRF
5. ID22 at the ESRF

JEEP at the Diamond Light Source (UK) was also suggested as a beamline that may be worthwhile for specific examination. However, the basic specifications of the beamline suggest that there is not a great overlap in terms of capabilities with the MMC beamline *e.g.* 5-150 keV, super-conducting wiggler, minimum spot size 10-20 µm, first hutch 47 m from the storage ring wall, second hutch 86 m from storage ring wall, pink light supplied by a bent crystal double Laue monochromator with additional focus (on upgrade) by compound refractive lenses (the use of which are discussed in item 7 Appendix 1).

7.1 Very Sensitive Elemental and Structural Probe Employing Radiation from a Synchrotron (VESPERS) Canadian Light Source

The VESPERS beamline in at the CLS is the closest in concept to the proposed MMC beamline. The objective of the beamline was to provide simultaneous micro-XRD and -XRF mapping with the option of subsequent XAS analysis of selected areas. Several different band pass options are available with the aim of being able to carry out Laue as well as monochromatic diffraction.

7.1.1 Specifications[8]

Source:	bending magnet;
Energy Range:	6-30 keV (note: upper energy range probably not practicably achievable);
Resolution:	Si(111) – 10^4; Multilayer mirror 2 – 10^{-1}; Multilayer mirror 1 – 10^{-2}; Pink beam
Flux (γ /s/0.1%BW) @ 100 mA):	Si(111) ≈ 2 × 10^5 @ 15 keV; MLM1 ≈ 1 × 10^{11} @ 15 keV MLM2 ≈ 4 × 10^{11} @ 15 keV
Spot size:	(2-4) µm x (2-4) µm
Endstation(s):	Microprobe Diffraction (CCD Camera) Fluorescence (Solid State Detector) Ion Chambers
Techniques:	Microprobe

8 http://www.lightsource.ca/experimental/vespers.php

	X-ray Laue diffraction X-ray fluorescence spectroscopy X-ray Absorption near edge structure Differential aperture X-ray microscopy Multi-bandpass and pink beam capability
Optics:	Compounding focusing, multi-stripe mirrors, crystal and multilayer monochromator, KB mirrors

7.1.2 Function[9]

Fig. 5 shows a schematic of the layout of the optical components of the VESPERS beamline. The front end (FE) area, the primary optics enclosure (POE, also called FOE) and the secondary optical enclosure (SOE, also called experimental hutch) are indicated in the Figure.

The first element in the POE is a mask having four rectangular apertures that define the beams accepted by VESPERS and the branch beamlines. The mask is located at a distance of 9.736 m from the bending magnet source. The left and right pairs of apertures in the mask pass the radiation for the VESPERS line and for the branch line, respectively. The two lower apertures transmit the beams that will go through the monochromator (“monochromatic”) and the two upper apertures the beams bypassing the monochromator (“polychromatic”). The mask is designed to be slightly larger than the acceptances of VESPERS and of the future branch, a total of 0.47 mrad horizontal by 0.17 mrad vertical.

Further downstream are two vertically focusing mirrors in tandem, M1a and M1b. M1a is designed to focus, along the vertical direction, the VESPERS “monochromatic” beam at the intermediate slits. M1b focuses along the vertical direction the VESPERS “polychromatic” beam at the intermediate slits. Since the mirrors are wide enough, they also focus vertically the beams going into the branch line. M1a and M1b deflect the beams upwards by 5.2 and 5.1 mrad, respectively. The distance between the poles of M1a and M1b is 405.88 mm and the pole of M1b is 1.09 mm higher than that of M1a. After these two mirrors the beams collected above and below the ring plane are parallel, make an angle of 5.15 mrad with the horizontal plane, and are vertically separated by 1 mm.

After the two vertically focusing mirrors, there are two horizontally deflecting mirrors, M2a and M2b, facing each other and intercepting the beams at an angle of 2.6 mrad. The mirror poles are separated by 4.8 mm. Each mirror accepts the corresponding “monochromatic” and “polychromatic” beams. M2a is used for the VESPERS experimental station and focuses its two beams along the horizontal direction at approximately the intermediate slits. M2b has the same focal distance as M2a and focuses the two beams for the future experimental station of the branch line. The beams reflected by M2a and M2b cross each other at a distance of 480 mm downstream from the mirror poles. The horizontal angle between the beams after the mirrors is 10 mrad.

The shape initially thought for M1a, M1b, M2a, and M2b is that of a meridian cylinder. However, due to the large meridional radius of these mirrors, they can be replaced by spherical mirrors. This has two advantages: lower cost and mirrors with smaller slope errors. A significant additional savings is possible by using identical mirrors for M1a, M1b, M2a, and M2b.

The next optical component in the POE is the monochromator. It has three different alternative pairs of diffracting elements (one pair of Si(111) and two pairs of Mo/B4C multilayer mirrors) for 0.01%, 1.6% and 10% bandpass, respectively. The “polychromatic” beam will go through the

9 Edited selected text from Preliminary Design Report for the VESPERS Beamline at the Canadian Light Source Inc. CLS Design Note 28.2.1.2 - Rev 0 Date: 2005-11-22

monochromator without touching any diffracting elements. The "monochromatic" beam will be deflected by one of diffracting pairs of optical elements, producing a vertical shift of 1 mm lower to the incident beam, thereby making it collinear with the "polychromatic" beam.

Horizontal and vertical intermediate slits are located in the POE at 10.3 m from the M1a mirror at the horizontal and vertical foci. This intermediate focus is then imaged at the sample position of the VESPERS beamline by a KB pair of meridional plane elliptical mirrors (M3 and M4) in the SOE (Secondary Optical Enclosure). These mirrors will intercept the beam at angles of incidence between 2.6 and 4.0 mrad. The first mirror of the KB pair, M3, focuses the beam along the vertical direction and the second, M4, along the horizontal direction.

The last component (not shown in the Figure) in the POE hutch is an integration of two photon shutters (one for each branch) and a bremsstrahlung stop. The bremsstrahlung stop will stop miss-steered bremsstrahlung and let synchrotron beams pass through. All beamline components except for the second KB pair (M3 and M4) are in the vacuum that is open to the ring. A beryllium window is placed in the SOE to terminate the vacuum. The second KB pair (M3 and M4) is in a helium environment.

A number of ion chambers, slits and filters are used to monitor, shape and filter the X-ray beam. A bendable KB system (M3 and M4) is used to focus the X-ray beam to micron scale in both vertical and horizontal directions. The experimental sample is mounted on a sample stage whose motions in X, Y, Z, θ and ψ directions are controlled. A precise one dimension scan stage is used to control a thin platinum wire traversing across the surface of the sample in order to obtain the three-dimension phase distributions within the sample using Laue diffraction. A CCD camera and a solid state Si detector are located 90° with respect to the incoming beams (45° to the sample) in perpendicular to and in the plane of the storage ring to measure the diffraction pattern and fluorescence spectrum, respectively. An optical microscope with machine vision is used to monitor the sample and define the area of interest on the sample. All these components are mounted on an optical table.

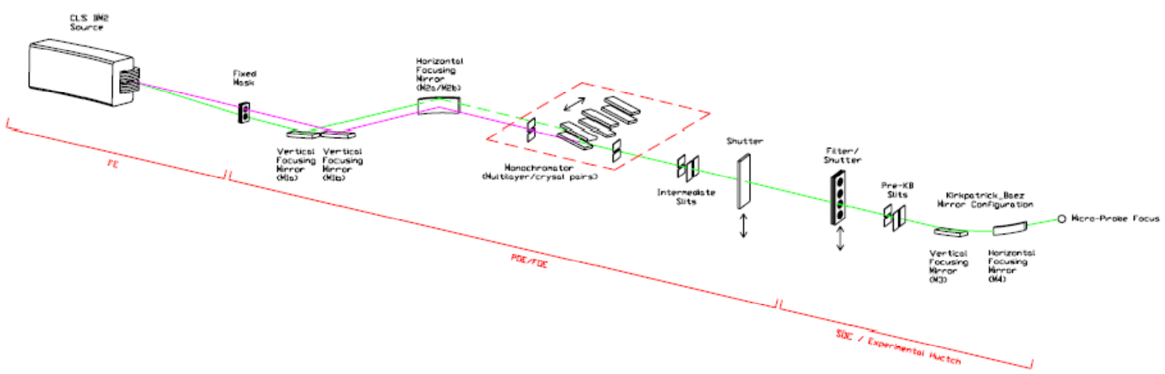


Figure 5 A schematic layout of the optical components of the VESPERS beamline. The front end area, the primary optical enclosure and the secondary optical enclosure are also indicated. It should be noted that only M2b is shown in the Figure.

7.1.3 Aspects of the design worth considering:

- Apertures above and below the beam meridian lead to a small degree of elliptical polarisation in the resulting X-ray beams which is not ideal for XAS measurements;
- The inclusion of the components for a second beamline add a degree of complexity and cost to the beamline design;
- The mode of achieving the offset between the 'pink' and 'mono' requires very precise adjustment of mirrors M1a and M1b, however, with this achieved they should not require further adjustment;
- The fixed offset monochromator offers cost advantage however there is a small vertical 'walk' of the beam of approximately 30 µm across the entire energy range;
- If the energy is changed for XRF purposes this change in height could be offset by a high precision movement of the sample in the *z*-axis. This could also theoretically be done on a continuous basis for XAS measurements;
- A more straightforward approach may be the use of suitable monochromator with tracking second crystals. Note: Three sets of monochromator 'crystals' are required, one set of Si(111) or suitable alternative(s) and two sets of depth graded multilayers;
- At this time on the VESPERS beamline it is not possible to shift between pink and monochromatic band pass options and for the beam to stay in the same place. This seems to be partly because the depth graded multilayers were deposited as strips onto the Si(111) crystals and require a considerably different incident X-ray angle to the Si(111) crystals. This ability to swap readily and reproducibly between band pass options was a central design feature of the VESPERS beamline and should be a focus of the MMC design;
- There is limited manoeuvrability of the sample stage and detectors that limits the sample geometries available, for instance transmission XRD measurements do not seem possible. Considerably greater flexibility should be ensured in the MMC beamline.

7.2 Endstation 12.3.2, Advanced Light Source

This end-station is also similar in concept to the MMC beamline and the VESPERS beamline with similar aims to provide a dedicated white and monochromatic micro-diffraction end-station for application of materials and earth sciences, with simultaneous XFM mapping capability.

7.2.1 Specifications[10]

Source:	Superbend magnet
Energy range:	6–22 keV
Monochromator:	White light and monochromatic [four-crystal Si(111)]
Calculated flux (1.9 GeV, 400 mA) 8.5 keV:	1×10^9 photons/s/µm^2/3x10^{-4}BW (1 × 1 µm spot)
Resolving power (E/ΔE):	1000–7000 depending on vertical convergence accepted
Detectors:	MAR 133 CCD, Dectris Pilatus 1M Pixel detector, Silicon drift detector
Spot size at sample:	16 × 2 µm^2 down to 0.5 × 0.5 µm^2
Sample format:	Typically less than 1 cm^2 × 1 mm thick

10 http://www-als.lbl.gov/index.php/beamlines/beamlines-directory/135-1232.html

Sample environment: Typically air

7.2.2 Function[11]

Fig. 6 shows the outline of the beamline in elevation and plan views.

The first optic encountered by the X-ray beam is a horizontally deflecting toroidal mirror that conveys the beam to a virtual source just after the experimental hutch entrance. The Pt (25 nm) and Rh (8 nm) coated silicon toroidal mirror operates at a grazing angle of 3.5 mrad cutting off the energy spectrum at about 22 keV. Water-cooled tungsten roll slits are used to adjust the virtual source size and therefore the size of the focused beam onto the sample. Final focusing is achieved using a Kirkpatrick- Baez (KB) mirror assembly contained in a vacuum box. The KB mirrors assembly is Peltier-cooled to compensate for the heat load on the mirrors inside the optic box vacuum chamber. The demagnifications to obtain a 1×1 um^2 size beam are approximately 16:1 and 8:1 for the vertical and horizontal KBs respectively. The choice of using KBs is directed by the use of polychromatic radiation, as they are to date the most efficient achromatic optics available.

The beamline can switch between white and monochromatic beam by way of a 2 channel-cut - 4 bounce Si(111) Bartels monochromator arrangement. This particular design is aimed at having the capability to illuminate the same spot on the sample with either white or monochromatic beam independent of energy. The two channel-cuts are mounted on roll-bearing rotation stages that are independently driven by linear motors via a sine bar mechanism, replacing the previous end-station 7.3.3 technology that used a tape-drive system.

The sample stages are placed on a high precision XYZ stage for accurate positioning. A χ stage defines the incident beam angle onto the sample. Diffraction patterns are collected using a Pilatus 1M X-ray detector and X-ray fluorescence signal by a Vortex Si-drift detector coupled with a XIA multi channel analyser. The design is flexible to allow for both reflective and transmitting sample geometries. Precise positioning (within a few microns) of the sample into the focal point of the beam is obtained via a Keyence laser triangulation tool.

11 Extracted from http://www.osti.gov/bridge/purl.cover.jsp;jsessionid=6C78B96C66C57A197E9AAADA9EB2DEF7?purl=/953690-RCC4dp/

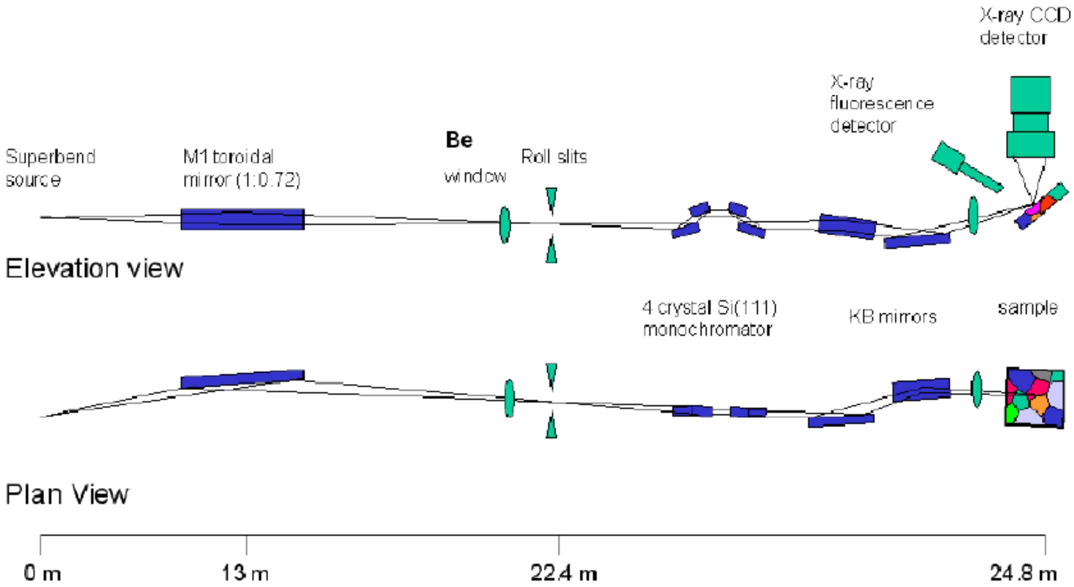


Figure 6 Elevation and plan view of the 12.3.2 micro-diffraction beamline at the Advanced Light Source.

7.2.3 Aspects of the design worth considering

- This is a considerably simplified design as compared to VESPERS with a single front-end aperture, a single toroidal mirror rather than three spherical mirrors (required for one beamline, *i.e.* one horizontal and two for vertical focus) and two band pass options, monochromatic and white, as opposed to four on VESPERS;
- The fixed off set two crystal monochromator is replaced by a four bounce (two channel cut) monochromator to ensure the incident beam stays in the same location regardless of wavelength or band pass. This results in some loss of flux of the monochromatic beam due to the increased number of 'bounces' off optics, however this loss may be marginal as the number of upstream focussing optics is considerably reduced;
- The resultant incident sample beam size seems to be considerably smaller than for VESPERS however the reasons for this are not clear in terms of the optics and may be due to superior alignment strategies;
- The feedback from this beamline to date has been quite positive, at least for white light experiments, although there were some initial teething problems regarding the alignment of the 4 bounce monochromator.
- This is a relatively straightforward and cost effective beamline design with proven results for the materials most likely to be studied at the proposed MMC beamline.

7.3 Endstation 34IDE, Advanced Photon Source

This beamline is located on an undulator X-ray source at the Advanced Photon Source. This intense X-ray source in combination with the considerably longer beamline length of 64 m means that many of the design concepts utilised may not be ideal for the shorter lower flux MMC beamline.

7.3.1 Specifications[12]

Source	Undulator A
Energy range	7-30 keV
Beam size	300 nm $\times$ 300 nm
Energy resolution	1×10^{-4}
Flux (photons/sec)	1×10^{11} white 1×10^{9} mono

7.3.2 Function

It is not clear that there are any publications in which the entire set of optics for beamline 34ID encompassing end-station E has been produced. Most publications focus on the novel nature of the monochromator[13] or the measurements that can be carried out[14].

The following text extracted from[15]
"*The experimental station is located about 64 meters from an APS type A undulator source. A non-dispersive total-external-reflecting Kirkpatrick-Baez (K-B) mirror pair is used to focus either polychromatic or monochromatic x-ray beams. An 80 mm long primary mirror with focal length of 130 mm for focusing in the vertical plane and a 40 mm long secondary mirror with focal length of 60 mm for focusing in the horizontal (ring) plane are combined to achieve typically about 300 nm x-ray beam in both directions. The mirror enclosure to sample working distance is about 30 mm, which gives sufficient space for in-situ experiments with various environmental stages and chambers. Slits can be used when focal size is more important than flux. For example, a slit at 28 m was placed to control the total power in the beam and to reduce the undulator horizontal source size from ~ 700 µm down to < 100 µm. This also acts to create a new effective object. In the vertical plane, the undulator source, with FWHM of about 40 µm serves directly as the object.*

On beamline 34-ID-E, a specially designed small-displacement Si (111) double-crystal monochromator allows rapid switching between monochromatic and polychromatic modes. The monochromator displaces the x-ray beam by about 1 mm but is designed to take the beam to be monochromated from a lower portion of the incident beam, and the angular displacement is corrected by heating the second crystal to tilt the monochromatic beam, so that the monochromatic beam is parallel and coincident to the polychromatic beam. The energy can be tuned over a wide range of about 7 - 30 keV."

---

12 http://www.aps.anl.gov/Sectors/33_34/microdiff/

13 G.E. Ice., J.-S. Chung, W. Lowe, E. Williams and J. Edelman (2000) Small displacement monochromator for microdiffraction experiments, Review of Scientific Instruments, **71**, 2001-2006.

14 G.E. Ice, B.C.Larson (2004) Three-dimensional X-ray structural microscopy using polychromatic microbeams, MRS Bulletin, March 2004, 170-176

15 W. Liu, P. Zschack, J. Tischler, G. Ice, B. Larson (2010) X-ray Laue Diffraction Microscopy in 3D at the Advanced Photon Source, Proceedings of the 10th International Conference on X-ray Microscopy, Chicago, August 2010.

7.3.3 Aspects of the design worth considering

This beamline utilises a fixed small-gap monochromator (on which the VESPERS monochromator was based). The monochromatic and polychromatic beams are co-aligned through use of pre-monochromatic slits to select different portions of the incoming X-ray beam, *i.e.* the portion of the beam selected for transmission through the monochromator is off-set by the gap of the monochromator from the portion of the beam selected for monochromatisation. It is assumed that the post-monochromator beam will be substantially larger than the post-monochromator slits and hence the displacement of the beam on changing X-ray energies will not be apparent on the sample. Moreover the incoming beam must be at least as large as the gap of the monochromator (1 mm) so an appropriate portion of the white beam can be selected for transmission. Due to the use of the undulator source it is possible to 'slit down' the out-going post-monochromator beam while maintaining reasonable flux.

For our purposes, where we also wish to access pink light and to carry out XAS over a broad energy range, a more conventional monochromator encompassing various sets of crystals and depth graded multilayers with a small but variable gap ('tracking' second crystal) is likely, to be more costly, but to also be more robust and flexible.

7.4 BM32 ESRF

As for 34ID-E at the APS BM32 at the ESRF is a considerably longer beamline than the MMC, being approximately 60 m, however in contrast to 34ID-E, BM32 utilises a bend magnet X-ray source. Two different sets of optics are used for the monochromatic and white beam as detailed below under Function. Pink beam mode is used for Laue micro-diffraction and while the beamline can deliver both pink and monochromatic X-ray beams the intent of the optics design was to use these two sources for different types of measurements and not to be able to analyse the same sample volume using both monochromatic and pink beam modes.

7.4.1 Specifications[16]

Monochromatic mode:

Beam size at sample	position (1:1) 0.5×0.3 mm^2 (H $\times$ V)
Spectral range	7 – 30 keV
Energy resolution	$\approx 0.5 \times 10^{-4}$ for Si(311) $\approx 2 \times 10^{-4}$ for Si(111)
Flux at sample	$\approx 5 \times 10^{11}$ ph s^{-1}(10^{-4} rbw, 0.1 A at 20 keV)

Pink mode

Beam size at sample	0.5×0.7 µm^2 (H $\times$ V) FWHM Typically 0.8-0.9 µm
Spectral range	5 – 25 keV

16 http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM32/Beamline

7.4.2 Function[16,17]

BM32 was initially designed to provide monochromatic X-rays to two diffractometers, one designed for *in situ* UHV growth studies and the other to provide a range of sample environments. To carry out pink beam studies the monochromator is removed from the beam by widening the crystal gap and the two beamline mirrors are used for vertical focussing providing a secondary source in the experimental hutch (Fig. 7 and Table 5).

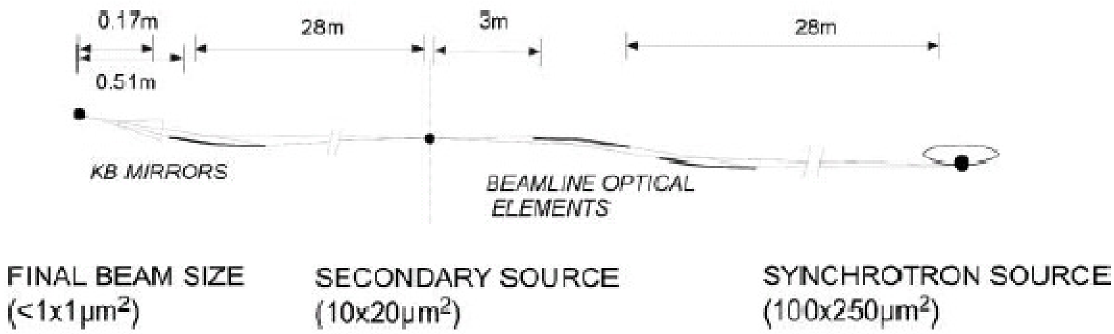


Figure 7 Demagnification of the pink beam using two vertical focussing elements focussed onto a secondary source. (Figure 1 from footnote 17.)

Table 5 Details of the optical arrangement used for pink beam mode.

Optical elements	**Mirror 1**	**Mirror 2**	**Secondary source**	**Two Kirkpatrick-Baez (Pt) mirrors**
distance from source	26 m	30 m	35 m	60 m
Optical function	vert. foc. Ir-coating	vert. foc. Ir-coating	20×20 µm^2	vert.+horiz. foc.
working angle	3.65mrad	3.65 mrad		2.9 mrad

Mirror 1 provides a parallel beam in the vertical plane and mirror 2 focuses the white beam on the secondary source which is located 3.2 m from mirror 2 achieving a demagnification ratio of 10. The source, composed of high precision slits is generally opened to 20 µm to match the synchrotron source size. Further demagnification is achieved using a KB mirror pair.

The brilliance of the bend magnet sources is approximately 10^{14} ph/s/0.1%BW/mrad^2 (at 200 mA ring current). The angular acceptance of the KB mirrors is 150×300 µm) resulting in a calculated flux at the sample in the order of 10^{10} ph/s.

Of note is the current detector which is a 16 Mpixel fast read-put 12 bit CCD detector (VHR), 81 mm circular active field, 31 µm pixel size) from Photonic Science Ltd. This detector provides simultaneous integration and readout with single exposure longer than 1.5 s (an order of magnitude slower than pixel array technology).

17 O. Ulrich, X. Biquard, P. Bleuet, O. Geaymond, P. Gergaud, J.S. Micha, O. Robach and F. Rieutord, A new white beam X-ray micro-diffraction setup on BM32 beamline at the European Synchrotron Radiation Facility, Review of Scientific Instruments, 82 033908 (2011)

7.4.3 Aspects of the design worth considering

- In monochromatic mode it appears that mirror 2 is used for horizontal focus through sagittal bending. However, there appears to be no horizontal focus in pink beam mode prior to the KB mirrors. As the horizontal divergence would presumably be quite large from a bend magnet source this apparent lack of horizontal focus would suggest a considerable lose of flux.
- It appears that the use of two vertical focus mirrors is in part due to a requirement for the beam to remain horizontal.
- The focal lengths of the optics and sample position have been in a large degree determined by the pre-existing beamline capabilities.
- The beamline does not attempt to provide co-linear and co-incident pink and monochromatic beams. Changes in the wavelength range can only be achieved by changing the tilt of mirrors 1 and 2.
- Due to the more limited capabilities of the beamline as compared to those planned for the MMC, and limitations on beamline optics, the optics are not particularly relevant with respect to the MMC.

7.5 ID22 ESRF

ID22 provides micro- fluorescence, diffraction and absorption capabilities. While this beamline was initially conceived as monochromatic microprobe recently a pink-mode has also been introduced. It is one of the few beamlines that aims to provide similar capabilities to MMC but whether the pink (or white) beams are co-linear and co-incident with the monochromatic beam onto the sample is not clear. The microprobe setup is approximately 45 m from the source.

7.5.1 Specifications[18]

The main beamline components and specifications for ID22 are as follow:

Flat Si mirror with 2 coatings
    Horizontal deflection: 2.6 mrad
    Cut-off energies:
        Si strip: 12 keV
        Pd strip: 24 keV
        Pt strip: 32 keV

Vertical double flat crystal monochromator, fixed exit cam system (Kohzu)
    Angular range: 3-30°
    Energy range:
        4-37 keV for Si(111) crystals
        7-72 keV for Si(311) crystals

Micro-focusing elements
    Kirkpatrick-Baez (KB) Mirrors

Size of beam at the sample location (V x H)
    Experimental hutch 1 (microprobe): 1.5×3.5 µm
    Experimental hutch 2: 150 x 150 nm

18 http://www.esrf.eu/UsersAndScience/Experiments/Imaging/ID22/BeamlineHandbook

Detectors

Si(Li) detector
Si drift diode detector
PIN diodes, ionization chambers
High resolution CCD cameras
Medium resolution CCD camera
Gas filled (position sensitive) detector

7.5.2 Function

The following text has been extracted from[18] with minor edits and some omissions:
"A classical layout has been chosen in order to provide a flexible and easy-to-use device and to keep it open for further evolutions: the beamline can be operated either with the direct beam from the undulator (white) or with a flat mirror (pink) and/or a fixed-exit double crystal monochromator (4-70 keV).

Different X-ray focusing elements are available for different experimental set-ups: Bragg-Fresnel optics and Fresnel Zone plates are used with high demagnification factors (20 to 100). Compound Refractive lenses (CRL) allow either pre-focusing of the beam – front end location - or focusing - experimental hutch location. The machine provides a low emittance beam (0.04 nm.rad vertically) and the particularly low divergence of the beam in the high-beta section is an advantage considering the small acceptance of the focusing elements.

Micro-analysis
The beamline provides a microprobe facility for micro-fluorescence, micro-XAS and micro-diffraction. At the sample location, the beam can be focused on a spot of few microns size with 10^9 -10^{12} phot/sec. Using the monochromator in the range 4-35 keV, measurement of all elements can be carried out with very high sensitivity (> ppb or 10^{-15} g): K edges up to xenon ($Z = 54$, $B_K = 34.6$ keV), L and M edges and lines up to uranium ($Z = 92$, $B_{L1} = 21.8$ keV, $B_{M1} =5.5$ keV).

*The recently commissioned **PINK** beam mode uses high intensity, high energy bandwidth beams obtained directly from the undulator and mirror. These beams span several full undulator harmonics and can be focused with high efficiency by CRL lenses located in the experimental hutches. The flux thus obtained is one to two orders of magnitude higher than the monochromatic one.*

Optics (shown schematically in Fig. 8)
The spectrum available at the micro-FID beamline is limited down to ≈5 keV due to the beryllium windows between the storage ring and the experimental hutches. Direct beam can be provided at the experiment location but the beam can be filtered by using the flat mirror, the double-crystal monochromator, absorption filters or any combination thereof.

The mirror produces a reduction of intensity of the high energy harmonics from the undulator. It gives a horizontal deflection (at a fixed angle of 0.15 °) in order to preserve the vertical coherence of the beam. Two different coated strips Pt, Pd and the Si substrate provide an energy cut-off respectively at 32, 24 and 12 keV.

The monochromator is based on a so-called CAM system which provides a very high stability of the beam along all the spectral range. The parallelism between the two crystals is better than few microradians and the exit beam is maintained in less than 15 mrad over the full angular range (3-30 °). Recent measurements over a range of 200 eV at 6.5 keV achieved a fixed exit of better than 2 µm on the sample. Further corrections using piezo actuators of the crystals angle can improve the fixed-exit capabilities to sub-micron range for XANES measurements.

Using Si(111) and Si(113) at first order of diffraction, the monochromator will cover the energy range 4-70 keV but it is also possible to reach up to 100 keV with higher orders of diffraction.

The direct beam is at a height of 1400 mm from the floor and the monochromatic beam is delivered 12.5 mm lower than the direct beam.

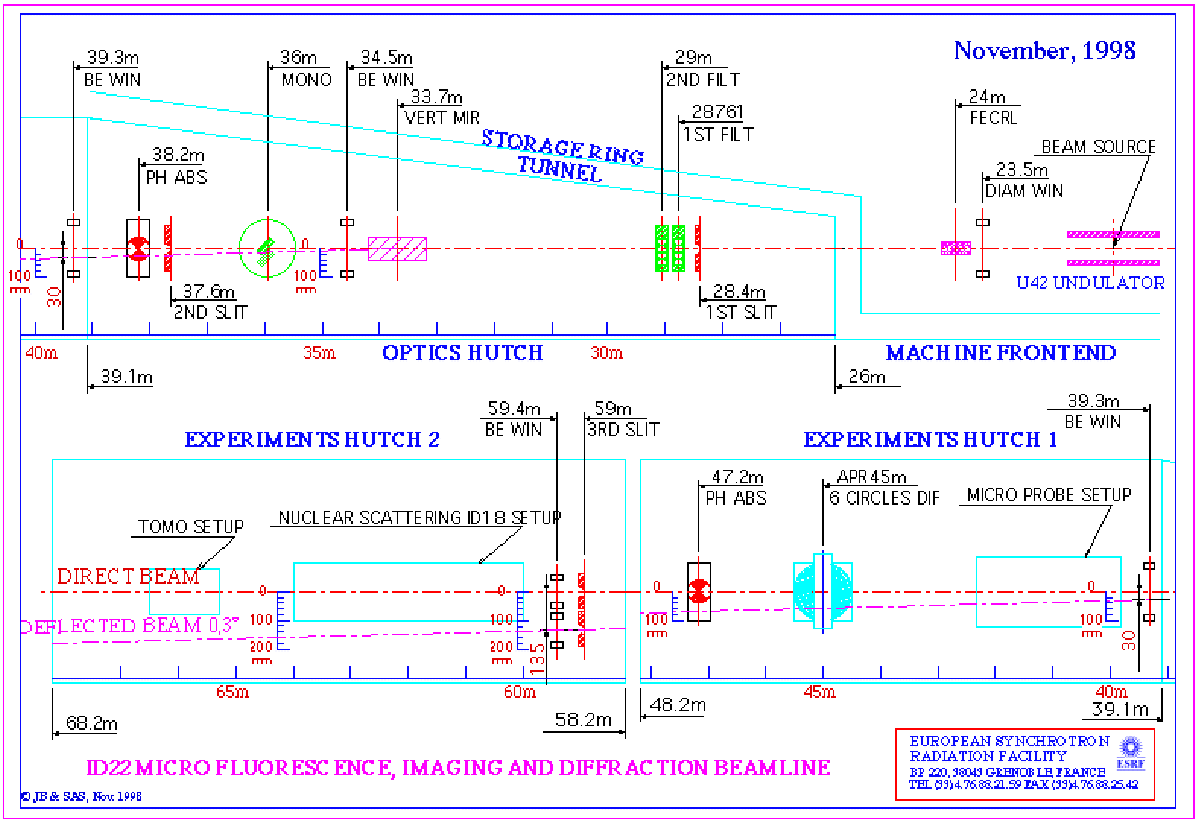


Figure 8. Schematic of the optics layout for ID22. The microprobe is located in the first experimental hutch. (from [19])

End Station

Two large experimental hutches (~30m^2 each) accept different set-ups:

- *The microprobe facility is located in the first experimental hutch on a 2.5 x 1.2 m^2 granite optical table. The set-up includes a focusing stage, a pinhole stage, a sample scanning stage with 2 sample holders (goniohead or slide holder), a video microscope, fluorescence, diffraction and normalization detectors as well as a high/medium resolution CCD camera stage. The optical table can be remotely moved in the vertical plane.*

Detectors

The micro-FID beamline is provided with different detectors for X-rays:

- *The beam is monitored by current integration detectors (silicon PIN diodes), a scintillator counter or proportional counters (ionization chambers).*
- *Spatial sensitive detectors are used for micro-diffraction and X-ray imaging by absorption or phase contrast: two dynamic (16 bits) CCD cameras for X-rays with less than 1 micron resolution will be commissioned before the end of 1998.*
- *A multiple wire gas filled detector is available for time resolved small-angle scattering experiments.*

19 http://www.esrf.eu/UsersAndScience/Experiments/Imaging/ID22/BeamlineManual/GenBemInfo/id22lay

- *X-ray fluorescence measurements are carried out with either a Si(Li) solid state detector or a Si drift detector.*
- *Further developments of the micro-spectroscopy setup will provide a wavelength dispersive system for high spectral resolution (WD-XRF) and high counting rate and a high resolution scanning sample stage using piezo motors*

7.5.3 Aspects of the design worth considering

- The minimum spot size obtainable for the microprobe is considerably larger than what we aiming for with the MMC. This is probably due to the use of compound refractive lenses (transfocator) as the focusing optic rather than KB mirrors.
- It is not clear whether the transfocator is used to focus both pink and white light. The drawback of the use of a transfocator is that it provides essentially chromatic focus so that the band pass (perhaps 1% for pink light) energy is only variable by either moving the transfocator to sample distance or by changing the number of optical elements in the transfocator. With the latter approach it appears a smooth energy spectrum is not possible.
- It also appears that there is no attempt at making the pink and monochromatic beam co-linear with the monochromatic beam being 12.5 mm lower than the pink beam.

Appendix 1 Design questions posed in Beamline Scoping Group Guidance Notes (1st June 2011)

1. **What is the required energy range of the beamline?**
   We aim is to be able to achieve as high an incident energy as possible while maintaining a **spot size of approx. 1 µm.** The approximate energy range of 5 - 60 keV is likely to be the outcome. However, this upper energy range is based on the assumption of the application of KB optics which will require a very low incident angle X-ray angle at high energies. Low end energy will be optics determined.

2. **What is the required photon flux across that energy range?**
   This is a function of reflectivity of mirrors on increasing X-ray energy and is linked, also, to the detectors that are chosen. The accessible flux as a function of energy will be determined by ray tracing which will examine different optical combinations. A decision can then be made as to the optimal choice between energy range and flux to enable the experimental conditions required.

3. **What spot size (or range of spot sizes) is required at the sample position?**
   As close to 1×1 µm as possible and up to approx. 5×5 µm.

4. **Are there any special requirements for sample temperature or pressure?**
   The beamline will be designed for ambient pressure and temperature. Down the track users may require the construction of specialised environmental cells but these will be highly varied and will need to be implemented on a case-by-case basis. The requirement in terms of end-station design is to maintain as much spatial flexibility as possible to enable ease of placement and utilisation of cells in the future.

5. **Are there any particular sample positioning, sample scanning or sample stability requirements?**
   The standard samples will need to be able to be mounted on a goniometer (or similar) to enable sample rotation. They must also be translatable in 3D for sample scanning measurements and beam focus. A key capability is the capacity to move between monochromatic and pink light options while maintaining the beam position on the sample. In the current design movement in *Z* would be required for the movement between white and monochromated light (including pink). Therefore fine control of the sample in Z would be advantageous.

6. **Are there specific requirements for beam stability, ambient temperature stability or vibration suppression at the sample?**
   The typical approach to measurement will be rapid move and settle mode (< 10 s) with scanning the sample in the horizontal and vertical (step size of approx. 1 µm). However, particularly when carrying out 3D diffraction a data set many take many hours to collect and therefore both thermal drift and vibrational sample/stage stability is extremely important.

   The observation at 34ID-E is that with their Newport optical table vibrations are limited in both the vertical and horizontal directions to a magnitude of about 50 nm. However, the preference seems to be towards granite optical tables, which provide some improvements, particularly in horizontal directions. Granite tables (or granite support blocks for conventional table tops instead of steel frame) are preferred for any critical optics support and granite is now very cost competitive (often cheaper than the steel frame). At the XFM the vibrational stability is ≈30 nm. However, vibrational stability is also a function of underfloor vibrations for which reports are available for the vicinity of the XFM.

For submicron focus, 0.5°C stability is sufficient. Below 100 nm, 0.1°C stability is required. XFM currently uses passive temperature control (wait for hutch to equilibrate – and reduce air exchange on entry to hutch). For a 0.1°C active system a soft air curtain approach to avoid strong convection air currents would need to be considered.

7. What are expected to be the main components in the beamline?
This will be updated in detail on completion of the updated ray tracing to be carried out by Ruben Reininger (NSLS II) but the likely key components are detailed in Section 5.3.

The possibility of using transfocator optics[20] has been discussed but not at this time adopted into the design. In particular the transfocator seems to have potential application at higher energies (> 30 keV) where mirror-type optics become more problematical due to the required small incident angles required. A transfocator optic is composed of a series of compound refractive lenses. Being essentially chromatic in nature with low demagnification power it is unlikely that such an optic could be used in replace of focussing optics for the MMC beamline. However, they can also be used, when present as a single compound refractive lens optic, as an in-line broad band-pass monochromator to produce for instance 1 % bandpass. The considerable advantage of this optic in this application is that they appear to have no high-end energy limit. However, the focal length will shift as a function of energy and hence some mechanism to move the optic longitudinally along the beamline would be required. It is possible to use these optics prior to KB mirror pairs to 'condense' the beam thus reducing the foot print size particularly at high energies enabling better retention of flux and/or reduced mirror sizes. However, their focal length is extremely long (*e.g.* a single Be lens at 40 keV has a focal length of 474 m) and hence this mode of application is viable only for very long beamlines, *e.g.* ID11 ESRF.

8. What types of detectors will be used?
(1+2) More than one detector will be required to reasonably cover the available diffraction energy range.

The application of a large distortion free amorphous Si detector for diffraction measurement is at this time seen to be practical option currently available. The amorphous Si detector used for Laue at JEEP cost approximately $160,000 AUD.

Another possibility worth considering is the use of new energy resolving detector which are currently coming on line. The application of energy resolved area detectors would reduce the complexity of interpreting Laue diffraction patterns to that of analysing monochromatic diffraction data. This would make the analysis of unknown multi-phase samples far more approachable.

The pnCCD [21]is already up and running, with an active area ≈70 mm^2, an energy resolution of ≈200 eV and ≈100 µm pixel size. The ALS has also developed an equivalent detector which is being installed on the imaging end-station at the ALS in the coming months. A further possibility is the Medipix detector being developed at CERN[22] however, the spatial resolution of the pixcels is still relatively poor (*e.g.* 55 µm). Note – the energy range says 3 keV and up which would be extremely practical but the active area is actually quite small.

---

20 G.B.M. Vaughan, J.P. Wright, A. Bytchkov, M. Rossat, H. Gleyzolle, I. Snigireva, A. Snigirev (2011) X-ray transfocators: focusing devices based on compound refractive lenses, *J. Synchrotron Rad*. **18**, 125–133
21 http://hasylab.desy.de/instrumentation/detectors/projects/pnccd/index_eng.html
22 http://technologytransfer.web.cern.ch/technologytransfer/en/Technology/Medipix.html

A further point that does not get much publicity regarding the multi-pixel array (*i.e.* Pilatus) is its energy thresholding capabilities. This feature is really unique for diffraction capabilities as it is possible to effectively remove noise (fluorescence) by choice of threshold level. This is particularly effective for Fe containing samples as is typical for earth science applications. The only bad point with respect to Pilatus (apart from fairly large pixels) is the module format. This presents a bit of a problem for integration of monochromatic ring patterns, especially if you are after strain information.

Currently, at 34ID-E (APS) there are three PekinElmer area detectors for Laue diffraction measurement. They can cover angular range of about 120°. The reason PE detectors were chosen was for their speed (up to 15Hz in certain modes) at that time (3 years ago). The cost was about $350k (US) for all three. However, Dr. Wenjun Liu of the APS suggests that high speed Mar CCD detectors should be considered for the MMC beamline. Their speed is up to 100Hz for the smaller detector and the signal/noise would be much better than that of PE.

It will be necessary to readily rotate these detectors between 90 °2θ in the vertical and 0 °2θ (transmission) mode and also to move them towards, and as far away from the sample as possible to improve strain measurement resolution. There is probably no need to be able to swap detectors rapidly as users will typically want to use a specific energy range for a given instrument time allocation. The flexibility to translate the detector off axis may also be worth considering for improved strain sensitivity.

It is possible to envisage a situation where 2D detection of the transmission through the sample while simultaneously measuring the diffraction is required. This would allow techniques such as diffraction contrast tomography (DCT) and topo-tomography - both 3D grain/orientation imaging experiments, which would complement the DAXM. The major limitation of topography and DCT as being is the need for samples which are free of residual elastic strain, whilst the major limitation on DAXM is the volume which can be probed (even with optimised translation and detection 10 x 10 line scans is about the maximum which is practical at the moment).

The CCD to measure the direct signal for DCT/tomography *etc*. should probably be a reasonably spec'd fiber coupled CCD with a pixel size down to ≈1 µm, to give sufficient resolution for microstructured materials. Possible cost anywhere between $30 - $60,000 AUD.

(3) A Vortex or similar detector will be required for XRF/XAS measurements. The XRF detector will be placed to the side of the sample at the front (45°).

(4) Transmission detector for alignment (2D area detector) – monochromatic radiograph, standard CCD *e.g.* 13.5 µm pixels. This should be able to be moved in and out and across out of the way.

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?

Control software that may be readily adapted may be available from CLS or APS who both have similar beamlines and use EPICS based beamline control software. ALS does not use EPICS and uses instead a LABVIEW based system. It was suggested by Dr.Tamura (12.3.2 ALS) that adapting code can be as time consuming as writing code from scratch and it is better to develop code for specific needs and hardware.

10. Are there any items which will require a specific development program, as they are not available commercially?

No

11. **Are there specific suppliers that are preferred for certain components?**
No, not at this stage. Fraunhofer have been contacted with respect to details regarding depth graded multilayers.

12. **Do we have price estimates already for some of the components?**
No. Existing budgets are now too out of date to provide a reliable price guideline.

13. **Are there specific software packages that will be required?**
Laue diffraction analyses software is available from ALS 12.3.2 (XMAS – Windows based) or APS 34ID-E (X-ray Laue Diffraction Microscopy Data Analysis – IGOR based).

    XMAS has a windows PC version the executable of which is freely downloadable from the web and a UNIX cluster version that runs on a 48 nodes cluster. The cluster version uses a script file generated by the PC version for automated analysis. XMAS can index Laue patterns obtained from any crystal structure cubic or non-cubic in any experimental configuration (transmission/reflection, detector at 0 or at an angle), and also provides support for monochromatic powder data, and 3D reconstructions. Dr.Nobu Tamura (12.3.2 ALS), the developer of XMAS states that MMC beamline users "will be welcome to use XMAS for their data analysis but it would be advisable to have some of your staff trained with us on how to use it so that they can in turn train your users."

    UniSA have developed software specifically designed to index strained crystal systems using a Hough transform approach however, this may require some further development to make it sufficiently user friendly for general release. There has also been some software developed by Andrew Stevenson (CSIRO) which may be useful but availability is likely to be determined CSIRO policy. In particular manual clustering via Oracle VM ware removes the single thread issues and allows access to all cores in multi-core PCs. Time gains of 7-20 have been achieved at Deakin University.

    It would be useful to examine real time streaming of data into analysis programs. It may also be possible to get source codes for parallalisation and/or implementation on MASSIVE (Multi-modal Australian Sciences Imaging and Visualisation Environment)?

14. **What sample preparation or data analysis equipment will be required (that we don't have already in our support laboratories)?**
Basic optical microscopes, basic polishing gear, kinematic mounting and standard mounts – to supply to users.

15. **Are there any specific requirements for remote access to the beamline or automated sample handling and data capture?**
Remote access would be potentially a useful feature as many samples will be quite robust and entire data sets can take a number of hours to collect. An extensive development for remote access has been undertaken for the VESPERS beamline via the Science Studio initiative (see for instance http://accelconf.web.cern.ch/accelconf/pcapac2010/papers/thcoaa02.pdf). Contact with Dr. Stewart McIntyre (UWO, Canada) has indicated a definite willingness to collaborate in this regard and no anticipated difficulties regarding licensing.

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.**
    Please refer to Section 7.

17. **Who could help us with the detailed design of the beamline (we will consider paying specialist consultants)?**
    Ruben Reininger (NSLS II) carried out the first two set of ray-tracing calculations of the MMA designed and has been commissioned to provide an updated set of ray-tracing calculations plus report.

18. **Do we have sufficient capabilities for the conceptual design with the AS or the BSG?**
    Probably, with the addition of the ray-tracing report (item 17).

19. **Are some of the identified experimental capabilities "desirable" but not "essential"?**
    Having two options for pink light, *i.e.* 10% and 1%, is desirable but may be difficult to implement in terms of monochromator design. This will depend in part on the required incident angel to access high energies and the distance the second crystal is required to track to maintain a fixed offset.

Appendix 2 Ray tracing scope of work and deliverables to be carried out by Ruben Reininger

1. Comparison of two possible designs for the MMC beamline: one based on a SC wiggler and another based on a regular bending magnet (BM). This will include:
   1.1. Determining the wiggler lengths such that its power can be dealt with a water cooled first mirror and a liquid N_2 cooled double crystal monochromator (DCM) when the monochromator is tuned to its lowest energy and the cutoff of the first mirror is either 40, 50, or 60 keV.
   1.2. Calculations of the apparent photon source of the wiggler and the BM for the acceptance determined by the KB focusing system described below when its cutoff energy is either 40, 50, or 60 keV.
   1.3. Calculations of the flux at the sample position using a Si 111 DCM assuming achievable figure errors on the optical components:
      1.3.1. At 15, 30, 40 and maximum photon energies for the three angles of incidence on the mirrors.
      1.3.2. With three intermediate slits sizes.
   1.4. Optimization of the optical scheme and KB pair parameters.

2. Initial optical scheme:
   2.1. The designs will incorporate a collimating mirror as a first optical element to preserve the intrinsic resolution of Si(111).
   2.2. The second optical element is a double crystal monochromator
   2.3. A focusing mirror downstream of the DCM will image the source into horizontal and vertical slits.
   2.4. The slits will allow adjusting the spot size at the sample.
   2.5. A KB pair will focus the beam onto the sample. The KB had the following approximate parameters: First mirror is 200 mm long and focuses vertically, second mirror is 150 mm long and focuses horizontally. The mirror poles are 180 mm apart and their focus is 150 mm from the center of the second mirror.

Deliverables

1. Report in electronic format that will include:
   a. Length(s) of the SC wiggler source
   b. Total absorbed power and power density on the first mirror and first crystal for the investigated cases.
   c. Specification of the optical components
   d. Summary of the above mentioned calculations
   e. Ray tracings at the sample position for the three apertures