Status of the X-Ray Absorption Spectroscopy (XAS) Beamline at the Australian Synchrotron

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Abstract. We present herein the current status of the X-ray Absorption Spectroscopy (XAS) Beamline at the 3 GeV Australian Synchrotron. The optical design and performance, details of the insertion device (Wiggler), end station capabilities and construction and commissioning timeline are given.

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INTRODUCTION

The XAS Beamline at the Australian Synchrotron aims to deliver a bright and highly stable scanned monochromatic photon beam. The design goals of the beamline, as dictated by the user community, are to cover ~ 4 – 65 keV to enable EXAFS measurements of all elements from Ca - U. The provision of standard XAS experiments, as well as specialized equipment setups involving extreme sample environments etc, place requirements on the flexibility of the XAS Beamline, especially in terms of control over the final beam spot and focus and energy resolution of the incident beam. Different modes of operation of the beamline allow it to be optimized for particular experiments.

The beamline will occupy sector 12 in the 3 GeV Australian Synchrotron. It will consist of a collimating mirror, liquid Nitrogen cooled double crystal (Silicon) monochromator and dual toroid refocusing mirror. The source will be a 1.9 T wiggler. Two experimental stations, in two different hutches, will be served by the beamline; the first will be a 'standard' XAFS setup, offering transmission and fluorescent XAFS on 'standard' samples between room temperature and 10 K. The second station is designed to be flexible to offer opportunities for non-standard experiments that may require specialist instrumentation with longer setup times.

INSERTION DEVICE

The XAS beamline will utilize a multipole wiggler as its source. As the beamline will not share the Wiggler radiation fan, the Wiggler parameters have been optimized to yield a high critical energy and maximized on axis radiation. The magnetic deflection parameter, K, is constrained to < 19 from the front end. A limiting aperture of 0.5 (v) x 2.2 (h) mrad is present in the front end to limit the total power delivered to the beamline components.

TABLE 1. Parameters of the XAS Beamline Wiggler

Parameter	Value
Period Length	10 cm
Number of Full Periods	20
Magnetic Length	~ 2 m
Total Length	2.4 m
Minimum Gap	14 mm
Maximum Effective Field	1.9 T
Critical Energy	11.6 keV
Total Power	8.5 kW
Power in 2 x 0.24 mrad	2.5 kW

Along with 1.9 T field, it is intended to operate the Wiggler with lower field (1.6 T) for experiments requiring ~ 10 KeV photon energy and less. This will aid thermal management of the beamline optics. The relevant Wiggler parameters are given in Table 1, and the spectral performance simulated with SPECTRA [1] is shown in Figure 1.

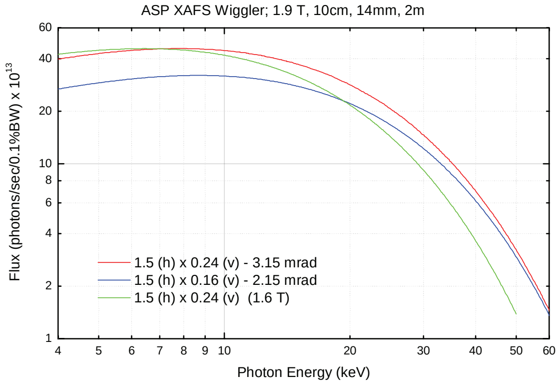

FIGURE 1. Simulated spectral performance of the XAS beamline Wiggler for 1.9 T and 1.6 T peak fileds. The given vertical apertures correspond to the acceptance of 1.2 m long optical surface at the given angle of incidence.

OPTICAL LAYOUT

The first mirror, to vertically collimate the incident beam, will be a cylindrically bent flat Silicon mirror with 1.2 m optical length, 16.1 m from the source and operating in the bounce up configuration. It will possess three stripes – Si, Rh and Pt. Each stripe will be sized to accept a 2 mrad horizontal fan, however it is expected that a maximum of 1.5 mrad will be able to be utilized due to the high thermal load at 200 mA storage ring current. Based on competing requirements for a large energy range, minimum slope errors induced from thermal distortions, harmonic rejection and ease of use, two angles of incidence are planned for the mirrors: ~ 3.15 and 2.15 mrad. For energies greater than ~ 36 keV the mirrors can be removed from the beam. A natural consequence of this is the monochromator, at ~ 18.5 m from the source, will require vertical translation of its rotation axis depending on the position of the collimating mirror.

The monochromator will be a liquid Nitrogen cooled Si(111) and Si(311) double crystal monochromator, with the crystal set selectable by an in-vacuum translation. All crystals will be indirectly Nitrogen cooled. The second crystals of each pair will be 'long' allowing the beam footprint to walk along the crystals length. A single perpendicular translation will maintain a fixed 25 mm offset. The monochromator is planned to be operated in fixed offset, pseudo channel cut, step-acquire-step and slew scan modes of operation. Directly after the monochromator a 1 m spool piece will occupy space reserved for a future secondary monochromator eg for Quick-EXAFS or high resolution.

Focusing to 2 experimental positions at 32 and 37 m from the source will be achieved with a bendable dual toroidal refocusing mirror at 22 m from the source. This will consist of two cylinders of minor radii ~ 35 and ~ 46 mm coated with Pt and Rh, respectively on a nominally flat ULE glass substrate with optical length 1.2 m. The mirror will be mounted in a cylindrical bender.

Control over the beam focus can be achieved by manipulating the bend and also incidence angle of the focusing mirror. The vertical beam focus can be achieved by adjusting the mirror curvature, whilst the horizontal focus size / position can be selected by varying the incidence angle of the mirror. The cylinder radii have been selected based on the chosen angles of incidence for the collimating mirror. At 3.15 mrad (i.e., lower energies) use of the Rh stripe is appropriate, with a focus at ~ 32 m (Sample position 1). To focus to Sample position 2, the incidence angle of the focusing mirror needs to be decreased to ~ 2.6 mrad. Conversely, for higher energy operation the Pt stripes and 2.15 mrad angle of incidence are appropriate. The range of the focusing mirror to focus between sample positions 1 and 2 is ~ 2.15 – 1.95 mrad.

A simple glass harmonic rejection mirror will be located on the experimental table to enable the target harmonic content of < 10^{-5} to be achieved over the entire energy range.

RAYTRACING STUDY

The optical performance of the XAS beamline has been simulated with SHADOW [2], using calculated mirror reflectivities and crystal Darwin widths, but assuming perfect mirror figures and roughness. It is clear an extra harmonic rejection mirror will be required for energies less than ~ 12 keV to meet the 10^{-5} goal (results not shown).

TABLE 2. Simulated (theoretical) performance of the XAS Beamline at several energies. Mirror reflectivities and crystal Darwin widths have been included in the simulation, but not slope errors, roughness, alignment errors etc.

Energy (KeV)	Crystal (Si)	~ resolution (eV)	Flux in focal spot	Flux in .2x1mm aperture
6	111	0.7	2.05E+13	1.64E+13
10	111	1.3	3.32E+13	2.70E+13
20	111	2.4	1.82E+13	1.50E+13
30	311	1.25	1.50E+12	4.28E+11

Table 2 shows the calculated theoretical flux. Allowing a factor ~ 10 for losses due to roughness, figure / slope errors (including thermal distortions) and misalignments etc, the beamline will meet the user community' requirements of $> 10^{12}$ photons/sec over a large energy range. Finally, Figure 3 shows simulations of the focal spot obtained by manipulating the focusing mirror angle of incidence (horizontal beam size) and bend radius (vertical beam size).

MODES OF OPERATION

Several operational modes have been proposed that allow optimization of the energy range and harmonic content, but also to maintain optimum power management for the significant heat loads. For 3.15 mrad incidence angle on the Si stripe, approximately 1000 W will be absorbed by the collimating mirror. Cooling of this mirror will be performed utilizing 3 slots immersed in Ga eutectic. For higher energies, however, C foils will be used to reduce the power component from low energy photons.

Whilst the design and operation of the XAS Beamline's multiple modes entails considerable complexity, the design of components will be flexible such that the modes can be optimized (or even fixed).

Power management of the first crystal of the DCM will be a critical aspect of beamline operation. The worst case for the DCM first crystal sees ~ 700 W incident power. Power loads of this order are known to be tolerated by direct crystal cooling with a Wiggler beam [3], however the decision has been taken to use indirectly cooled crystals as a conservative approach for maintenance, operation and installation reasons. Detailed studies of the first crystal thermal management will be undertaken during commissioning to ensure the monochromator delivers the expected monochromatic beam quality.

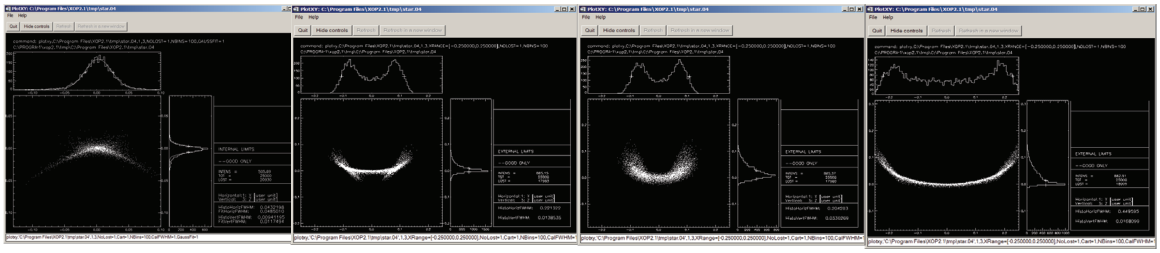

FIGURE 3. Examples of focal spot obtained from ray tracing. In the left panel, the focus has been optimized at 32m. To the right shows changing angle of incidence of the refocusing mirror but correcting the bend radius to obtain a wider spot. The last two panels illustrate the range of focus profiles possible. The characteristic 'smile' is a synonymous aberration from spherical optical figures.

CURRENT STATUS

Advanced Design Consulting (ADC) has been contracted to design and fabricate the Wiggler, whilst Accel Instruments has been contracted to design, fabricate, install and commission the Beamline components. Both are scheduled for delivery commencing in December 2006.

For commissioning and day one operations, the first experimental hutch with contain a standard XAFS setup with ion chambers, multi element solid state detector and 10 K closed cycle He cryostat. The second hutch will be commissioned at a later stage. It is expected to have beam on sample, with the optics at an advanced stage of commissioning, by April 2007, with user operations commencing later in 2007.

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