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ENGINEERING CHALLENGES IN BIOSAXS FOR AUSTRALIAN SYNCHROTRON

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Abstract

The Biological Small Angle X-Ray Scattering (BioSAXS) beamline is the third beamline designed, developed and soon to be installed as part of the BRIGHT Program at the Australian Synchrotron. The BioSAXS beamline will deliver a high flux beam at sample position and will be optimised for time resolved experiments and low concentration/low scattering samples. This paper presents the various engineering challenges in this high flux design, including thermal management of critical components, design developments to accommodate the various operational modes and various stages of the Photon Delivery System and Experimental Station components. The paper aims to present details of design, Finite Element Analysis results and approaches taken to solve problems.

INTRODUCTION

The Biological Small Angle X-Ray Scattering (BioSAXS) beamline is the third beamline designed, developed and soon to be installed as part of the BRIGHT Program at the Australian Synchrotron. The BioSAXS beamline will deliver a high flux beam at sample position and will be optimised for time resolved experiments and low concentration/low scattering samples. The beamline will offer increased efficiency, and data quality, for all liquid phase scattering experiments, allowing measurement of new and novel samples, and experiments, that otherwise would not be possible. The BioSAXS beamline will accommodate a wide range of experiments by offering a q-range of ~ 0.001 – 4 Å-1 and an optical design optimized for high flux (~$5x10^{14}$ ph/s) x-rays. At this flux rate, BioSAXS will offer users one of the highest flux beamlines in the world.

To achieve this, the beamline will use a superconducting undulator insertion device, double multilayer monochromator, and vertical and horizontal bending mirrors, providing flexibility in optical configurations. The beamline will primarily collect data in a vertically unfocussed mode. BioSAXS will also be able to achieve a fully focused and a fully unfocussed beam.

The beamline is designed in 8 vacuum sections. The first contains a fixed mask, a bremsstrahlung collimator, cooled filter rack and a fluorescence screen. Vacuum section 2 is designed for the Double Multilayer Monochromator, two bremsstrahlung elements in each of the ports and a QBPM. The third vacuum section houses diagnostics and the attenuators. These are used to determine any shift in the beam location and enable correction for the beamline. The fourth vacuum section is design for the KB mirror system with horizontal and vertical focussing mirrors. This is followed by another group of diagnostics, formed by a grouping of QBPM and Fluorescence screens for real time analysis and correction, when combined with F460 electronics and in-flange slits, as well as a fast closing valve in the fifth vacuum section and the safety shutter in the sixth vacuum sections respectively. A beam conditioning table to manipulate the beam to sample is designed in vacuum section 7 and the end station as vacuum section 8. The beam conditioning table consists of a NanoBPM, two guard slits, XBPM and a Sample Camera for the visualisation of the sample at 29 m from the source and a mica exit window. The end station is formed by a sample table to carry samples in various environments, a vacuum vessel to house the in-vacuum Dectris detector, a detector actuation system for in-vacuum manipulation of detector position, the Beamstops and the vacuum vessel actuation.

The design of the beamline is shown in Fig 1.

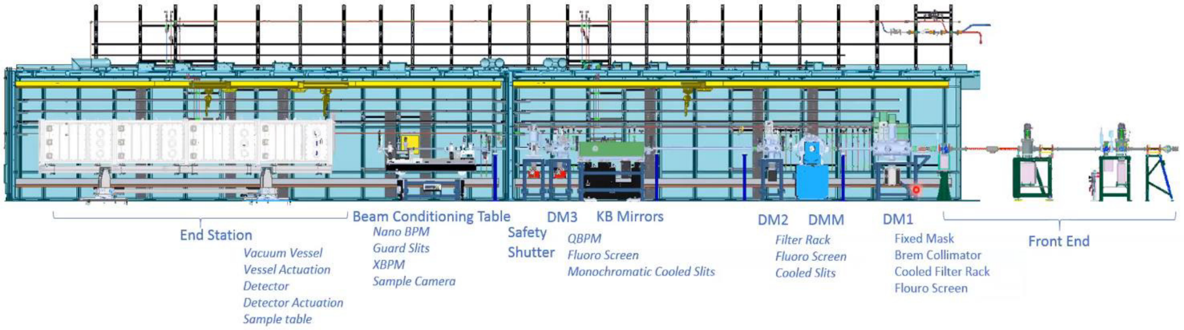

Figure 1: BioSAXS beamline schematic.

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KEY TECHNICAL CHALLENGES

BioSAXS Beamline had a preliminary design to deliver a flux of 1.8 x 10^{14} photons/sec. The source for BioSAXS is a Super Conducting Undulator (SCU) with period length of 16mm, 98 full periods and magnetic field strength of 1.084 T (on axis). Constrained by the length fo the straight in the storage ring, the design of the SCU was adapted to suit, leading to a drop in performance. With design changes in the SCU, BioSAXS Beamline needed to adapt to deliver a high performance. In order to accommodate this, changes were initiated in the design of the beamline.

The key change initiated into the beamline design to adapt to the source, were an increase in the aperture of the fixed mask to allow for more photons entering the beamline. The change to a 3.5 mm (H) x 2 mm (V) aperture allowed for a higher than anticipated performance, albeit with some challenges.

The Key challenges in the beamline and end station design were

1. Thermal load management from the increased flux
2. Management and mitigation of Bremsstrahlung radiation, and
3. Design flexibility in end station components to allow for three key operational modes in the beamline.

APPROACH TO PROBLEM

Thermal Management

The design change of increasing the aperture of the fixed mask still allowed for the capture and management of this thermal load with water cooling. Using a flow rate of 5 L/minute, a total power load of 1.98 KW. This was verified trough FEA.

However, there was still a high amount of heat going through to the beamline. In order to offer an added layer of protection for the optics, a cooled CVD diamond filter rack was added to the beamline design. CVD diamond allows for the reduction of heat while remaining transparent to the Xray going though to the monochromator, in the energy range that BioSAXS is aiming to work in.

While this reduced the thermal load on the first crystal of the monochromator, there was still a need to manage, up to 400 W of thermal loads in this area. The approach taken by the design team at the Australian Synchrotron and FMBO, our design partners, was to increase the footprint of the beam on the substrate. While this meant a larger substrate, the design of the monochromator would be simpler, with the need for a translation stage removed. This thereby, reduces the size of the vacuum vessel and directly reducing the cost of the device. In addition to the change in size of the substrate, the method to manage the thermal loads was to reduce the offset of the crystals in the crystal cage. The initial offset of 15 mm between the crystal was changed to 10 mm to allow for the spread of the incoming beam, thereby increasing the beam footprint. In addition to increasing the surface area on the substrate, this also enabled the design team to increase the performance of the beam at sample position.

For the thermal management at the monochromator, the options available for the team included water cooling and cryo-cooling. Cryo-cooled multilayer monochromators have been built and tested in the recent past by several synchrotron facilities. However, the long-term impact on the multilayers from thermal loads and the lack of long-term performance data presented a risk to the project. The design team undertook the option of pursuing water cooling, to minimise the risk and also generate cost savings.

Finite Element Analysis of the crystal substrate was undertaken to ensure that the requirements of slope errors could be met. With the addition of the cooled filters, upstream of the monochromator, the power load on the first crystal substrate was reduced to a maximum of 402 W. With a beam footprint of 4.3 mm x 121 mm, the results from the analysis showed that there was a maximum deformation of 1.8 µm, on axis. With the correction from the mirrors, further downstream, the slope errors were then maintainable within an acceptable limit. The results for the deformation from the analysis are given in Fig. 2 and Fig. 3 shows the slope errors from the monochromator.

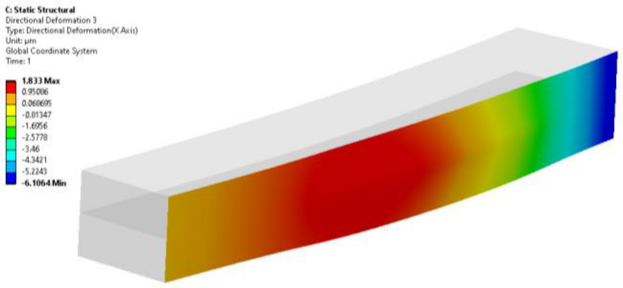


Figure 2: Deformation on the first crystal substrate of the DMM.

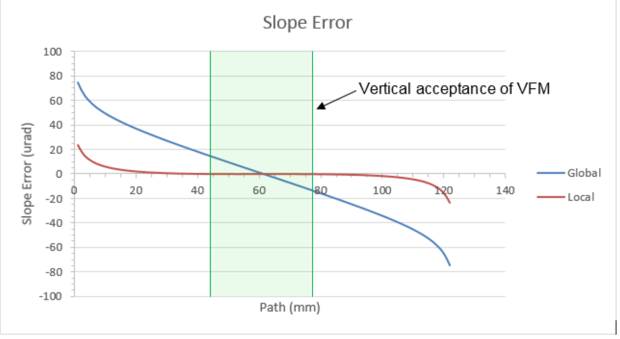
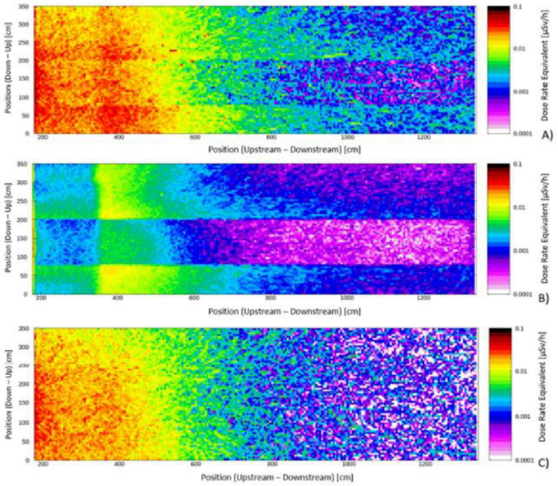


Figure 3: Slope error resulting from water cooling of the first crystal in DMM.

Bremsstrahlung Radiation Management

One of the challenges arising from a low-offset monochromator design is the subsequent radiation issues arising from the close distance of the optical aperture to the Bremsstrahlung rays. The guidelines at the Australian Synchrotron recommend a minimum of 3 Moliere radii from the edge of the optical ray to the edges of the Bremsstrahlung components or in the presence of an optical aperture in the component, a minimum of 1 Moliere radius to the optical aperture, followed by 2 Moliere radii after the optical aperture. This has shown to reduce the scatter of the radiation going downstream from the component, by up to 95%. Since the Moliere radius for the materials vary, Tungsten was selected as the suitable material, providing a needed clearance of ≈ 8 mm. The low offset design in the monochromator allowed for a clearance of 1.9mm to start with. One new Bremsstrahlung collimator was included in the beam in-port of the DMM and the downstream stop was relocated to the beam out-port of the DMM to create an increased distance. With the design changes, a maximum aperture-to-aperture clearance of 6.5 mm was achieved (0.7 Moliere Radius). A Montecarlo analysis was performed by B. Bewer of the Canadian Light Source to investigate the effect of this clearance not meeting the required guidelines. The results from the analysis showed that the radiation dose rates on the outside hutch walls were able to meet the required specification of <0.5mSv/hr. This was achieved through ray tracing and identifying the scatter directions through the optical aperture. By increasing the need from a minimum of 20 radiation lengths (3.5 mm for Tungsten/ length) to a total of 200 mm thickness, there was sufficient material through the aperture to absorb the scatter through the optical aperture. This enabled the team to meet the radiation dose rate requirements. Typical results, for this general arrangement in BioSAXS beamline, is show in Fig. 4.



Dose rate equivalent distribution along the FOE outboard wall along the downstream portion of the wall: A) Total dose rate equivalent, B) photon dose rate equivalent, and C) neutron dose rate equivalent.

Figure 4: Results from Montecarlo analysis for Bremsstrahlung radiation dose rates.

Design Flexibility

The BioSAXS beamline aims to provide users three main modes of operation, enabled by design flexibility provided through the optics. The modes are

1. Fully focussed
2. Vertically unfocussed
3. Fully unfocussed

While the beamline anticipates the majority of users would prefer the vertically unfocussed mode, the option of having all three modes of operation addresses the needs for future users, expanding the outreach of the beamline. In order to enable experiments in these modes, the end station of the beamline had to adapt to the beam positions in all the three modes, while also accommodating a variety of sample environment. To achieve this, the BioSAXS end station is designed as two major components. The beam conditioning table, as part of the photon delivery system, provides five axes of movement. This includes vertical, transverse, pitch, roll and yaw motions. The end station aimed to accommodate the beam through these different positions.

The detector is housed in a rectangular vacuum vessel with a cross section of 1.1 m (H) x 1 m (V) and a length of 8 m. With a three degree of freedom actuation system for the detector, the detector stage can transverse the entire length of the vessel, allowing for fast change of the focal lengths of the camera for imaging. The detector stage, in vacuum, allows for transverse and vertical movements, driven on stages powered by stepper motors. The beamstops are also built on the same stage and allow for the positioning of four photodiodes built on a rotary stage to change between the diodes. This is then mounted on two translation stages allowing any of the diodes to be placed anywhere on the detector surface. A coarse beamstop is also included in the design to allow the users to stop the beam while the diodes are being positioned. The design of the detector stage was first built and used in the SAXS/WAXS beamline at the Australian Synchrotron by L. Adamson and N. Kirby. The design of the detector stage is shown in Fig. 5.

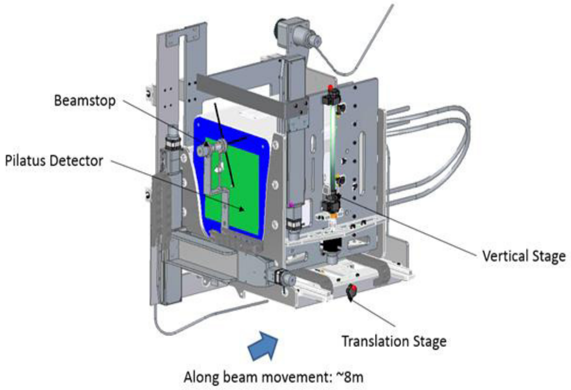


Figure 5: Detector stage.

The vacuum vessel table, carries the vacuum vessel and allows for the positioning of the vessel, depending on the beam operational mode and also accommodating differences in the sample table dimensions. To meet this positioning requirement, the table is equipped with four different axes of movement. This includes a total range of ±150 mm in the vertical axes, ±150 mm in transverse and a total range of 600 mm along the beam in the downstream direction. The travel requirements are met with an upgrade to the motions but following the same design principle of the vacuum vessel table in the SAXS/WAXS beamline. The vertical motion of the vessel is achieved four vertical jacks, powered in pairs through two high power motors, generating the capability to move the upstream and downstream ends of the vessel independently. A shoulder joint installed on the upstream side, in conjunction with linear slides on the downstream end, enable pitching motion of the vessel. The transverse and longitudinal motions are powered using a combination of stepper motors and air bearings. Eight, 300 mm air bearings support a total load of 5.57 tons, including the vessel and the table components. The design of the vacuum vessel table is shown in Fig. 6.

Figure 6: Design of vacuum vessel table.

The sample table, which accommodates samples in various sample environments is also designed to suit the motion ranges in the beam conditioning table and the vacuum vessel table. The sample table is designed over a granite block and carries an optical breadboard 450 mm x 750 mm. Similar to the vacuum vessel table, two vertical stages, on the upstream and downstream ends, provide vertical and pitch motions. The pitch motions are enabled through double flexures on the downstream side and single flexures on the upstream side. Two additional stages provide the transverse and longitudinal motion. The longitudinal motion is a total of 50 mm. Transverse motion for the breadboard is a total of 600 mm. To achieve this challenging range, a double rail, telescopic arrangement has been developed driven by a rack and pinion, with adjustments to minimise backlash. The double rail enables the moment and load management, with a total payload capability of 100 Kgs. The design of the double rail system is shown in Fig. 7 and the sample table at the extremities of the vertical motion is shown in Fig. 8.

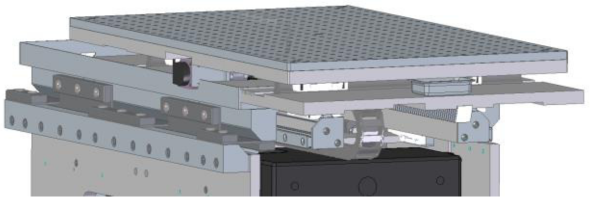


Figure 7: Sample table double rail motion arrangement.

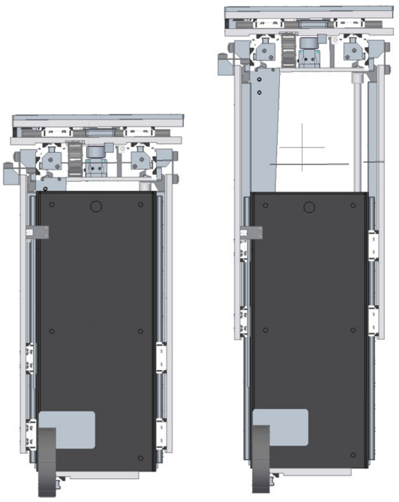


Figure 8: Sample table at heigh extremities.

In addition to the motion range requirements, the same table design is also covered by specifications for stability. In order to achieve this, the design of the upstream and downstream vertical plates was optimised for the loads and free vibration requirements. FEA was applied to analyse the deformation in a static environment and for modal analysis. The results from the analysis showed a maximum deformation of 9 µm at the breadboard. This result is shown in Fig. 9. Figure 10 shows a typical result from the modal analysis. The first Eigen frequency was calculated to be 137.3 Hz while the vertical axes was at the lowest position and 78.1 Hz at the highest position.

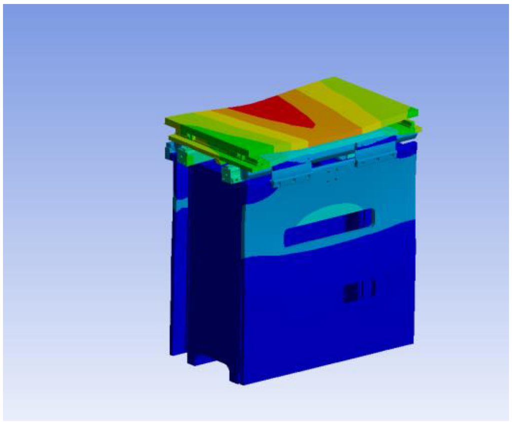


Figure 9: FEA static defection analysis results.

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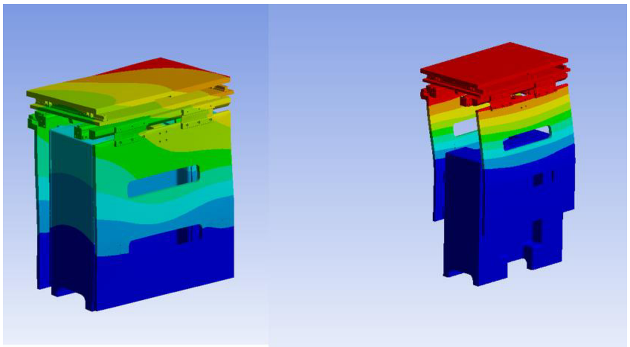

Figure 10: Typical results from modal analysis.

The complete results from the modal analysis are shown in Table 1. The results show a good stability in the design and the first Eigen Frequency falls within the specification.

Table 1: Results from Modal Analysis for Sample Table

Mode	Lowest Vertical Height	Highest Vertical Height
1	137.3 Hz	78.1 Hz
2	167.4 Hz	128.6 Hz
3	169.9 Hz	132.3 Hz
4	174.3 Hz	166.6 Hz
5	207.8 Hz	185.5 Hz
6	228.9 Hz	205.9 Hz

The results of the engineering undertaken in this beamline and end station design has delivered the needs to achieve a high flux beam at sample. With the design flexibility and effective management of thermal loads in the beamline components has kept slope errors to a minimum and achieving a flux of 8.07 x 1014 photons/sec with a beam size of 2.38 mm x 1.23 mm.

CONCLUSION

The BioSAXS beamline is currently being manufactured and installation is slated to commence for the photon delivery system in January 2022. The design of the end station components is in various stages of final design, with the vacuum vessel table currently being built for testing and the sample table in advanced final design phase. The engineering effort have achieved the goals of the beamline science requirements and it is expected that the results from the commissioning activities will be presented in upcoming conferences.

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