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A Level-2 Biosafety Beamline for Macromolecular Crystallography at SSRF

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Abstract. A biosafety level-2 beamline for macromolecular crystallography is constructing at SSRF, which is one of the beamlines in phase-II beamline project approved at 2016 by the central government of China. This beamline will provide the capability of conducting the experiment on determination of the virus-related protein structure from crystals. To fulfill this aim, the end station is emphasized on the biosafety design which must meet the Chinese laws and regulations. For the limited source of insertion section in the storage ring, the beamline will be one of the canted beamline, sharing the insertion with the ultra-small angle X-ray scattering beamline. The photon source will be a 1.6 m long, in-vacuum undulator with period of 22 mm. The optics will consist of a deflection flat mirror to increase the distance of two canted beamline, a cryogenically cooled Si(111) double-crystal monochromator and focusing mirrors. The focus scheme is realized with two-stage focus scheme in horizontal and one stage focus in vertical direction. At the sample position the focused beam is 20 micron in horizontal and 10 micron in vertical. The beam size could be changed by inserting the compound refractive lens. The beamline will deliver a high flux beam in the 7-18 keV energy range, with the energy resolution of $\Delta E/E \sim 2\times10^{-4}$. In addition to the main beamline, the endstation will be negative pressure control and be functional divided to meet the biosafety regulations. This report shows the current status of the beamline design.

Keywords: Macromolecular Crystallography, Biosafety, SSRF

INTRODUCTION

Currently the Phase-II beamline project which includes sixteen beamlines and auxiliary facilities is under construction at Shanghai Synchrotron Radiation Facility (SSRF). SSRF is an intermediate-energy third generation light source based on a 3.5 GeV storage ring. It has been operated for users in top-up mode since 2012 [1]. Although there are totally four macromolecular crystallography (MX) beamlines at SSRF in operation already, a P2-level biosafety MX beamline will allow the user community to carry out the data collection from the virus-related targets. To fulfill this aim, a flexible optical design has been considered to cover the energy range and the beam size. Meanwhile the biosafety combined with the radiation safety endstation is specially designed according to the national laws and regulations.

The parameters to be achieved by this beamline are listed in table 1. The principle in the optical design is the simplicity of the components to make the beamline is operated efficiently with the suitable beam monitor and feedback system. The endstation will offer the negative pressure environment for the biosafety requirement, and the *in-situ* data collection which will reduce the biohazard risk further. The beamline is now in the procurement phase, and the commissioning is planned in the fourth quarter of 2019.

TABLE 1. Designed Parameters of the Beamline

PORT	10-ID
SOURCE	Undulator (IVU-22)
Energy Range	7-18keV
Energy Resolution	$<2\times10^{-4}$
Beam Size	$20\times10\mu m^2$
Flux	2×10^{12}ph/s
Biosafety	Level-2

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SOURCE

The beamline, called BL10U2, is canted with the Ultra Small-Angle X-ray Scattering (USAXS) beamline. These two beamlines share one standard straight section of SSRF. The in-vacuum undulator of this beamline is located at the downstream and the beamline is deflected outward from the storage ring. The deflected angle of these two beamlines is 6mrad.

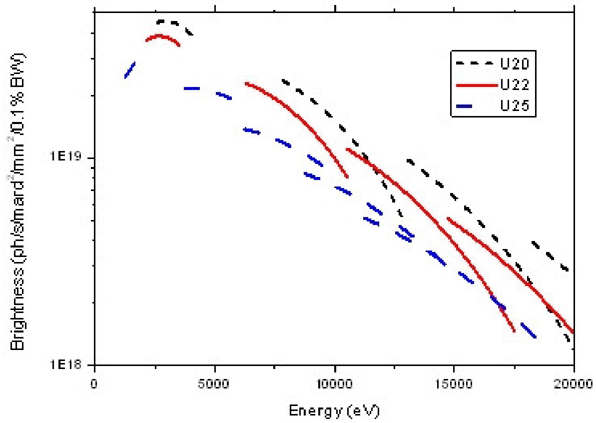

FIGURE 1. Calculated tune curve of three different periods Undulator.

Based on the layout of the straight section and the requirement of the experiment, the source of this beamline is an in-vacuum undulator. The period length is 22mm and the number of period is 72. The selection of this U22 undulator makes the beamline covers the energy range in MX experiments, and provides high brilliance and good tunability at the same time. The parameters of the IVU are listed in Table 2.

TABLE 2. Source Parameters.

Type of ID	Sm_2Co_{17} permanent magnet, in-vacuum undulator
Period	22mm
Number of Periods	72
Deflection parameter (K) at minimum gap(6 mm)	1.72553
Photon source size (FWHM)	391×26 μm^2
Photon source divergence (FWHM)	81×22 μrad^2

The standard canted front-end of SSRF shown in Figure 2 will be used for these two beamlines [2]. The acceptance angle is 2.0×1.0$mrad^2$ (H×V). It transmits 959 W of power out of 2.6kW emitted by the undulator when the storage ring is operated at 300 mA. The beamline acceptance angle is further defined by the white beam slit which is water-cooled, and the nominal working angle is 0.1×0.05$mrad^2$ which can be adjusted to reduce the beam divergence from experimental requirement.

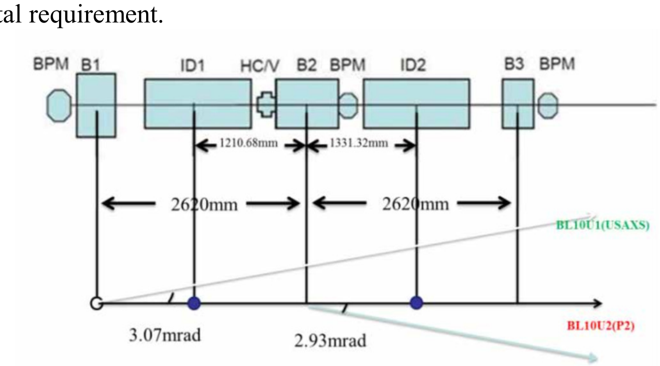

FIGURE 2. Sketch of the canted front-end.

OPTICS

To increase the lateral distance of the two beamlines, a set of back-to-back horizontal deflecting mirrors (HDM) locate at 21.5 meter. This flat mirror will take 32 W power load which will be deal with water-cooling to keep the slope error less than 1 µrad. The beam will be monochromated by a Si(111) double crystal monochromator (DCM) at 24.5 meter which is cryogenically cooled. The power load on the first crystal under working condition is 98 W. The monochromatic beam is focused by a vertical focusing mirror (VFM) in vertical and a two-stage scheme in horizontal respectively. The beam is pre-focused by a pre-horizontal focusing elliptical mirror (PHFM) at 26.5 meter. The horizontal pre-focal spot is at 33.85 meter. A high precision slit is placed at this position to adjust the beam. The horizontal focusing mirror (HFM) with elliptical shape at 43.1 meter produces the focused beam at 44.8 meter, namely sample position. The distance from the source to the VFM is 39.6 meters. The beam is directly focused to the sample position in vertical. All the mirrors are coated by Rh, and the glancing angle is 3.5mrad.

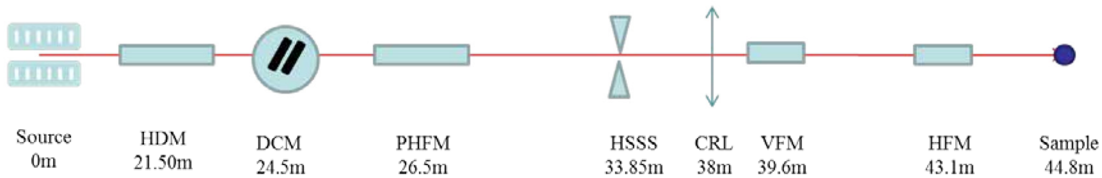

FIGURE 3. Layout of P2 beamline (Distance not scaled). CRL transfocator at 38 meter is used to enlarger the beam spot at sample position.

TABLE 3. Slope error on optical elements for simulation.

Optical Element	HDM	1^{st} Crystal	PHFM	VFM	HFM
Slope Error （µrad）	1	1.5	0.5	0.3	0.5

Based on the power load and the finite element analysis of the optical components, the feasible requirement on the slope error on the mirrors and DCM are listed in Table 3.The focused spot size is simulated by OASYS [3]. Regarding to the spot sizes with the simulated slope error, ray tracing calculations show that the focal spot size is around 20×10 μm^2 FWHM, and the corresponding divergence is 1.5×0.2 $mrad^2$ FWHM. The horizontal divergence can be limited by the slits furtherly. The flux of at the spot position is simulated to be above 2×10^{12}ph/s in the energy range, and the energy resolution in the whole energy range is less than 2×10^{-4} (not shown). Apertures will be used for smaller spot size, while the larger spot size will be obtained by inserting the compound refractive lens (CRL). The CRL transfocator include three group N=1,4 and 6 with the R=2000 µm 2D Be lenses [4]. The enlarged spot size is expected be around 45µm at 12.7 keV, which is the typical energy setting at MX beamline.

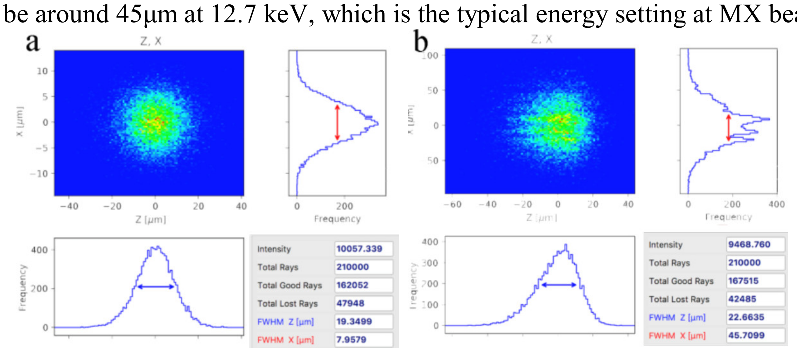

FIGURE 4. Simulated beam spot at sample position with the mirror focusing (left). The beam can be enlarged at 12.7keV by inserting CRL (right).

ENDSTATION

To carry out the data collection from virus-related targets, the endstation will offer the necessary biosafety facility. In addition to the safety equipment and laboratory facilities, such as biosafety cabinet (BSC) and autoclaveare required. The negative pressure gradient between different function areas is required according to the national and local laws and regulations also.

There will be a hutch in hutch for this endstation to implement the biosafety and radiation safety. To built the hutch-in-hutch structure, the height of the endstation radiation hutch is increased to 3.8 meters. The equipment for the negative-pressure and ventilation system will be installed inside. The maximum negative pressure is around the sample position, can be set at minus 45 Pa. The gradient is 15 Pa to the next function area. The biosafety standard operating procedures (SOP) will be established for this endstation before user operation.

The end-station consists of beam-conditioning devices and a dual-head diffractometer. The dual-head diffractometer will support the *in-situ* data collection and normal pins experiment. The *in-situ* goniometer head hold the crystallization plate in horizontal geometry, while the pin goniometer is in vertical geometry. The data collection by *in-situ* method will reduce the risk of the biohazard furtherly. The sample will be observed by an on-axis camera for centering. For the pin experiment, the sample environment will be cooled by a cryostream 800 series. A Si-drift fluorescence detector will be used for the MAD scan and X-ray excitation experiment. The cryostream and the fluorescence detector are driven pneumatically. The sample changer based on the industrial robotic arm will be equipped to support the pin and plate exchange. Diffraction data will be collected using an Eiger detector from Dectris Ltd. which is mounted on a three-axis positioning stage. On the whole, the endstation will include all the equipment which is necessary to perform automated MX experiments. Construction of the end-station is planned at this summer and the endstation is being designed by in-house engineers.

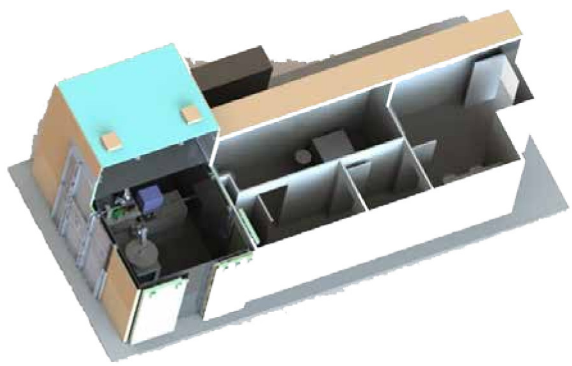

FIGURE 5. Layout of the Endstation. Except for the typical hutch, the biosafety hutch will be inside the radiation hutch. There are several function areas to support the biosafety standard operation procedure.

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