

Chapter 3. Beamline Science and Application

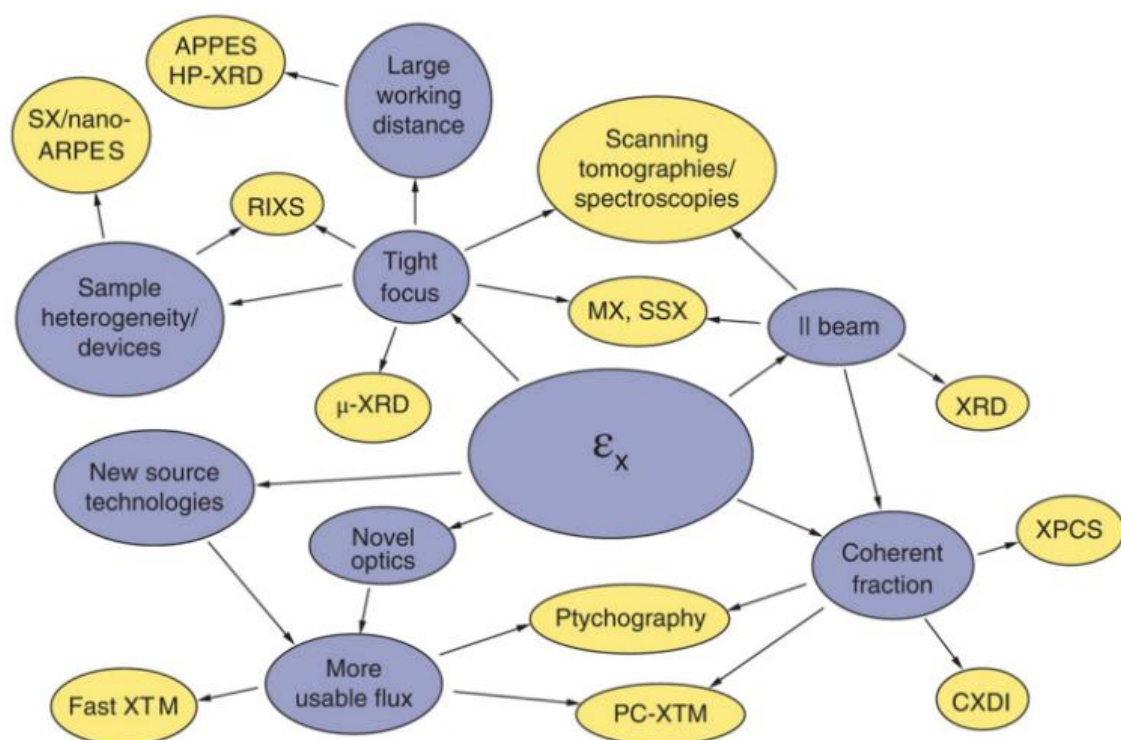
3.1 Introduction

The Multipurpose Synchrotron Accelerator (hereafter referred to as Korea-4GSR) is currently under construction in Ochang, Chungbuk, with commissioning targeted for 2025. Korea-4GSR is designed as a next-generation light source that succeeds the Pohang Light Source-II (PLS-II) and incorporates a Multi-Bend Achromat (MBA) lattice system. The adoption of the MBA lattice, in place of the Double Bend Achromat (DBA) or Triple Bend Achromat (TBA) systems used in third-generation facilities, enables a substantial reduction in the electron beam emittance.

With this design, Korea-4GSR is expected to achieve photon brilliance in the range of 10^{22} – 10^{23} photons/mm²/mrad²/0.1% bandwidth, and an electron beam emittance of approximately 100 pm·rad. While the exact performance depends on photon energy, these parameters represent an improvement of nearly two orders of magnitude compared to existing third-generation sources. This level of performance will allow significant advancements in both spatial and energy resolution.

The core beam properties of Korea-4GSR include small beam size, ultra-high brightness, and enhanced coherence fraction. These parameters have been defined as key performance targets of the facility and form the basis for its experimental capabilities. The improved beam quality will support a wide range of experimental techniques, including high-resolution spectroscopy, scanning-based experiments, Resonant Inelastic X-ray Scattering (RIXS), Coherent Diffraction Imaging (CDI), X-ray Photon Correlation Spectroscopy (XPCS), ptychography, and various in-situ and operando measurement techniques.

As summarized in <Figure 3.1.1>, the expected performance improvements of Korea-4GSR will provide direct benefits to existing synchrotron-based methods while simultaneously enabling the development of novel experimental approaches.



<Figure 3.1.1> Mutual Influence Between Experimental Methods and Technologies with the Introduction of 4GSR.

3.1.1 Initial 10 Beamlines

Globally, synchrotron radiation facilities are advancing toward the development and operation of fourth-generation synchrotron radiation sources (4GSRs), building upon the extensive utilization and experience gained from third-generation synchrotrons. Representative examples include MAX IV (Sweden), Sirius (Brazil), APS-U (United States), SLS-II (Switzerland), DLS-II (United Kingdom), HEPS (China), HAFS (China) and ALS-U (United States). These facilities have either completed upgrades to achieve 4GSR performance, are currently undergoing such upgrades, or are planning transitions to next-generation accelerator technologies.

In Korea, the Multipurpose Synchrotron Accelerator (hereafter referred to as Korea-4GSR) is under construction in Ochang, near Cheongju, Chungbuk Province, with completion scheduled for December 2029. The Phase-I beamline portfolio comprises ten beamlines strategically selected through an extensive review process. The selection was informed by the current utilization patterns of the Pohang Light Source-II (PLS-II) beamlines, as well as the unique beam characteristics of Korea-4GSR. The Beamline Technology Review Committee—consisting of experts from diverse scientific and technological disciplines—played a central role in defining the priorities and ensuring alignment with national research needs.

The initial ten beamlines to be constructed at 4GSR are listed in <Table 3.1.1>. Among them, three beamlines, ① BioPharma-BioSAXS (Bio-Pharmaceutical and Bio Small-Angle X-ray Scattering), ② Material Structure Analysis, ③ Soft X-ray NanoProbe, are designated as industry-priority beamlines, focusing on high-throughput technologies required by industrial users.

The remaining seven beamlines, ④ Nanoscale Angle-Resolved Photoemission Spectroscopy (NanoARPES), ⑤ Coherent X-ray Diffraction (CoXRD), ⑥ Coherent Small-Angle X-ray Scattering (CoSAXS), ⑦ Real-Time X-ray Absorption Fine Structure (Real-Time XAFS), ⑧ Bio-Nano Crystallography (BioNC), ⑨ High Energy Microscopy (HEM), ⑩ Nano-Probe, are planned as leading-edge fundamental research beamlines.

<Table 3.1.1> Specifications of the Initial 10 Beamlines of 4GSR

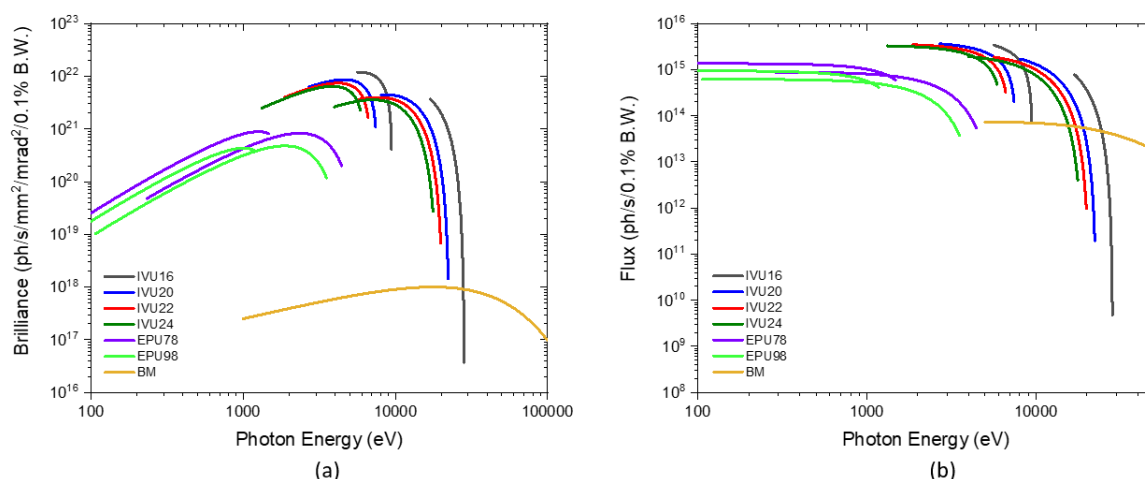
	Preliminary Feasibility Report Specifications	Detailed Design Specifications	Application	Remarks
1. BioPharma-BioSAXS (Industry-Priority)	- Beam Energy: from 5 to 20 keV - Experimental Method: Bio-SAXS	- Beam Energy: from 5 to 20 keV (Same) - Experimental Method: Solution SAXS - Resolution: from 8 to 4000 Å (SAXS) * $\Delta E/E < 2 \times 10^{-4}$ - Light Source: IUJ24	Bio	- Optimized from 8 to 25 keV - SDD (Sample-to-Detector Distance) secured up to 6 m - Automation system implemented
2. Material Structure Analysis (Industry-Priority)	- Beam Energy: from 5 to 40 keV - Experimental Method: XRD (Powder XRD), XAFS	- Beam Energy: from 5 to 40 keV (Same) - Experimental Method: Powder XRD, XAFS - Resolution: $\Delta E/E < 2 \times 10^{-4}$ - Light Source: IUJ24	Material, Energy	Implementation of HRPD and XAFS Experimental Methods
3. Soft X-ray NanoProbe (Industry-Priority)	- Beam Energy: from 0.1 to 5 keV - Beam Size: Must be $\leq 1 \mu\text{m}$ - Experimental Method: XPS, XAS	- Beam Energy: from 0.1 to 5 keV (Same) - Beam Size: from 100 nm to 10 μm - Resolution: $\Delta E/E < 1.5 \times 10^{-4}$ @ 400 eV, 4 keV - Experimental Method: XPS, XAS - Light Source: EPU78 + IUJ24	Semiconductor, Material	- EPU + IUJ Tandem → from 0.1 to 5 keV - Designed with two branch beamlines - Beam Size: * $\leq 100 \text{ nm}$ (Soft X-ray) * $\leq 10 \mu\text{m}$ (Tender X-ray)
4. NanoARPES	- Beam Energy: from 0.1 to 2 keV - Beam Size: $< 100(\text{H}) \times 100(\text{V}) \text{ nm}^2$ - Spatial Resolution: $\leq 30 \text{ nm}$ - Experimental Method: Nano-ARPES	- Beam Energy: from 0.05 to 2 keV (Range Satisfied) - Beam Size: from 100 nm to 10 μm - Spatial Resolution: $\leq 100 \text{ nm}$ - Resolution: $\Delta E/E < 10^{-4}$ - Experimental Method: ARPES - Light Source: EPU98	Semiconductor, Material	- Optimized from 50 to 200 eV - Designed with two branch beamlines - Beam Size: * $\leq 100 \text{ nm}$ (NanoARPES) * $\leq 10 \mu\text{m}$ (MicroARPES)
5. CoXRD	- Beam Energy: from 3 to 30 keV - Beam Size: $\leq 1 \mu\text{m}$ - Experimental Method: XRD, CDI	- Beam Energy: from 3 to 30 keV (Same) - Beam Size: 1.5 μm - Experimental Method: XRD, CDI - Light Source: IUJ22	Semiconductor, Material, Geology, Chemistry	Micrometer beam Focusing
6. CoSAXS	- Beam Energy: from 4 to 40 keV - Experimental Method: SAXS/WAXS (Including GI Method), XPCS	- Beam Energy: from 8 to 30 keV (Satisfies Experimental Methods) - Beam Size: * $< 5 \mu\text{m}$ (XPCS) * $< 50 \mu\text{m}$ (SAXS/WAXS) - Resolution: $\Delta E/E < 1 \times 10^{-4}$	Material, Chemistry	Securing Coherent Beam. (Wave front preserve)

		• Experimental Method: SAXS/WAXS (Including GI Method), XPCS • Light Source: IU20		
7. Real-Time XAFS	• Beam Energy: from 5 to 40 keV • Experimental Method: XAFS	• Beam Energy: from 4 to 40 keV (Range Satisfied) • Beam Size: $< 100 \mu\text{m}$ • Resolution: $\Delta E/E < 2 \times 10^{-4}$ • Experimental Method: XAFS • Light Source: IU24	Energy, Environment, Material, Geology	• Consideration of XES-Based Real-Time X-ray Absorption Spectroscopy Experimental System
8. BioNC	• Beam Energy: from 5 to 20 keV • Resolution: $\leq 1 \text{ \AA}$ • Experimental Method: MX	• Beam Energy: from 5 to 20 keV (Same) • Beam Size: from 1×1 to $13 \times 13 \mu\text{m}^2$ • Resolution: from 0.7 to 3.5 $\text{\AA}$ • Experimental Method: MX • Light Source: IU20	Bio	• Optimized from 8 to 25 keV • NanoMX • Supports Drug Development
9. HEM	• Beam Energy: from 5 to 100 keV • Resolution: $0.1 \mu\text{m}$ (at 100 m reference) • Experimental Method: Projection Imaging	• Beam Energy: from 5 to 100 keV (Same) • Resolution: from 0.3 to $0.5 \mu\text{m}$ • Experimental Method: Projection Imaging • Light Source: Centerbend • Sample Position: 100 m (Experimental Hutch: 120 m)	Material, Energy, Bio	• Bending Magnet • Excludes Near-Distance Hutch (Uses White Light)
10. Nano-Probe	• Beam Energy: from 5 to 25 keV • Experimental Method: Ptychography, XRS, XRF	• Beam Energy: from 5 to 25 keV (Same) • Beam Size: $\leq 50 \text{ nm}$ @ 10 keV • Resolution: $\Delta E/E < 1.5 \times 10^{-4}$ • Experimental Method: Ptychography, XRF • Light Source: IU24	Semiconductor, Material, Energy, Environment, Chemistry	• Pursues Nano Beam Focusing • Designed for 5f-Block Elements and RI Materials → Experiments Possible After Radiation Safety Protocol Preparation

3.1.2 Photon Source

Based on these characteristics, the Korea-4GSR Photon Source is expected to open new possibilities across academic and industrial fields, including materials science, energy and catalyst research, life sciences, new drug development, and quantum material research.

In Phase I of Korea-4GSR, photon sources have been strategically configured to support ten beamlines, comprising one bending magnet, eight in-vacuum undulators (IVUs), and two out-vacuum elliptically polarized undulators (EPUs). The distribution of these sources is summarized in <Table 3.1.2>, while the corresponding photon brilliance and photon flux characteristics are illustrated in <Figure 3.1.2> This configuration is designed to provide broad spectral coverage and high brilliance, thereby addressing the diverse requirements of both fundamental research and applied sciences.



<Figure 3.1.2> Photon brilliance and photon flux depending on BM, IVU, and EPU.

<Table 3.1.2> Summary of Photon sources for phase-I 10 beamlines

Undulator	(Unit)	IVU16	IVU20	IVU22	IVU24	IVU24	EPU78	EPU98	BM	PLS-II (IVU20)
Beamline #	[mm]	ID24 Mat. St. Anal.	ID04 CoSAXS ID22 BioNX	ID03 CoXRD (CDI)	ID10 NanoProbe ID21 BioPharma ID23 RealTime XAFS	ID26 SX-ray NanoProbe(I)	ID26 SX-ray NanoProbe(II)	ID25 NanoAEPES	BM10	
Period Length	[mm]	16	20	22	24	24	78	98	-	20
Periods		185	148	134	123	60	23	34	-	68
Device Length	[m]	3	3	3	3	1.5	2	3.62	0.186	1.4
K _{max} value		1.172	1.904	2.315	2.745	2.745	K _V 6.948 K _C 4.390 K _H 5.652	K _V 9.238 K _C 6.070 K _H 8.043	-	1.811
B _{max}	[T]	0.785	1.021	1.127	1.225	1.225	B _V 0.954 B _C 0.602 B _H 0.776	B _V 1.010 B _C 0.6633 B _H 0.879	2	0.969
Gap _{min}	[mm]	5	5	5	5	5	15	15	-	5
ε _{1st}	[eV]	5628.6	2696.1	1876.0	1327.8	1327.8	77.49 [V]/ 96.0 [C]/ 114.84 [H]	35.5 [V], 40.9 [C], 46.49 [H]	[E _c] 21280.8	1,618.78
Total Power	[kW]	7.38	12.49	15.16	17.93	8.75	6.61		1,357.83	2.91
Max. Power Density	[W/mrad ²]	154.3	164.2	165.2	165.4	80.7	24.3 [V]	38.02 [V]	Lin. Pow. Density(kW/mrad) 0.216	22.5
Photon Beam Divergence	[mrad]	Σ _x ,0.00679 Σ _y ,0.00626	Σ _x ,0.00930 Σ _y ,0.00892	Σ _x ,0.01100 Σ _y ,0.01068	Σ _x ,0.01293 Σ _y ,0.01265	Σ _x ,0.01825 Σ _y ,0.01806	Σ _x ,0.06684 [V] Σ _y ,0.06089 [V] Σ _x ,0.07241 [C] Σ _y ,0.05826 [C] Σ _x ,0.07356 [H] Σ _y ,0.05489 [H]	Σ _x ,0.06833 [V] Σ _y ,0.07244 [V] Σ _x ,0.07477 [C] Σ _y ,0.05836 [C] Σ _x ,0.08590 [H] Σ _y ,0.06327 [H]		Σ _x ,0.0341 Σ _y ,0.0171

3.2 Beamline Application

3.2.1 ID21 BioPharma-BioSAXS Beamline

3.2.1.1 Introduction

The BioPharma-BioSAXS beamline performs overall structural characterization and structural transition studies of biological molecules in solution based on small angle X-ray scattering (SAXS) technique.[1, 2] SAXS measurement of samples in solution can obtain information with a resolution as low as 1-2 nm. It can be applied to a unique physiological solution environment where the physiological phenomena of biological molecules can be activated. It is possible to analyze the structural characteristics of crystalline/non-crystalline biological molecules under physiological conditions and conduct structural stability and structural transition studies under various experimental environmental conditions (temperature, pressure, pH, UV/Visible, ionic strength, ligand, electric field, magnetic field, etc.). Due to these advantages, the usability of the solution SAXS technique has greatly increased along with high-resolution structural analysis methods of biological molecules such as X-ray crystallography, nuclear magnetic resonance spectroscopy, and cryo-electron microscopy.[3] As a result, solution SAXS technique is being used as a standard analysis technique for structural characterization from biological molecules to nanostructure systems such as organic/inorganic nanoparticles, polymers, liquid crystals, colloids, and metals.

Over the past 10 years, a dedicated BioSAXS beamline has been built at a world-class synchrotron radiation facility, contributing widely to the development of basic and applied science fields such as nanoresearch, structural biology, medicine, and new drug development. Recently, the biopharmaceutical field has begun to include the BioSAXS analysis technique in the workflow for analyzing the characteristics of biopharmaceutical for the purpose of identifying the structure, function, and operating principle of bio/protein therapeutics and providing evidence to prove the biological equivalence of biosimilars compared to original biopharmaceuticals.

The BioPharma-BioSAXS beamline is classified and constructed as an industry priority support beamline to respond to **the demands of industries** in the bio and pharmaceutical fields and to promote manpower in related fields.

The main strategy of the beamline is to process **a large number of samples at high speed**

(high-throughput) in order to efficiently utilize high brilliance and low divergence X-rays based on 4th generation synchrotron radiation.[4]

B. Scientific objectives

The BioPharma-BioSAXS beamline provides a solution SAXS technique, contributing to the analysis of biopharmaceutical properties by studying the three-dimensional structure and structural transition of solution-phase biological molecules and their complexes. Examples of applications using the solution SAXS technique are as follows: (1) Quantitatively characterize the structure of multi-domain proteins linked by flexible linkers and intrinsically disordered proteins.[5-8] (2) Reveal the structural behavior and stability of proteins and protein drugs through understanding the structure of the native and denatured states of proteins.[9-11] (3)

Recently, mRNA vaccines and treatments have been in the spotlight, and lipid nanoparticles (LNPs) are being used as an effective mRNA delivery system, and the structural stability of mRNA-LNPs in solution is being studied.[12, 13] (4) Real-time SEC-SAXS technique is used to study the change in solution phase structure of monodisperse biopolymer materials through separation/purification.[14] To facilitate such research, a collimated beam with high beam flux must be irradiated onto the sample. Varying the SDD is essential due to the diversity of samples to be measured and the need for a wide q range. A variable q range vacuum chamber will be built for fast and precise SDD change (0.5 to 6 m). By introducing an automatic sample changer at a fixed sample environment location, large number of samples can be processed at high speed to collect data at high throughput.

C. Beamline Requirements for the Insertion Device

The BioPharma-BioSAXS beamline will require the highest brilliance in the energy range of 5-20 keV without energy discontinuity. The source will be in-vacuum undulator with period length of 24 mm and total length of 3 m. A detailed description of the BioPharma-BioSAXS Insertion Device can be found in the <Table 3.2.1.1>.

<Table 3.2.1.2> Source Parameter for BioPharma-BioSAXS beamline

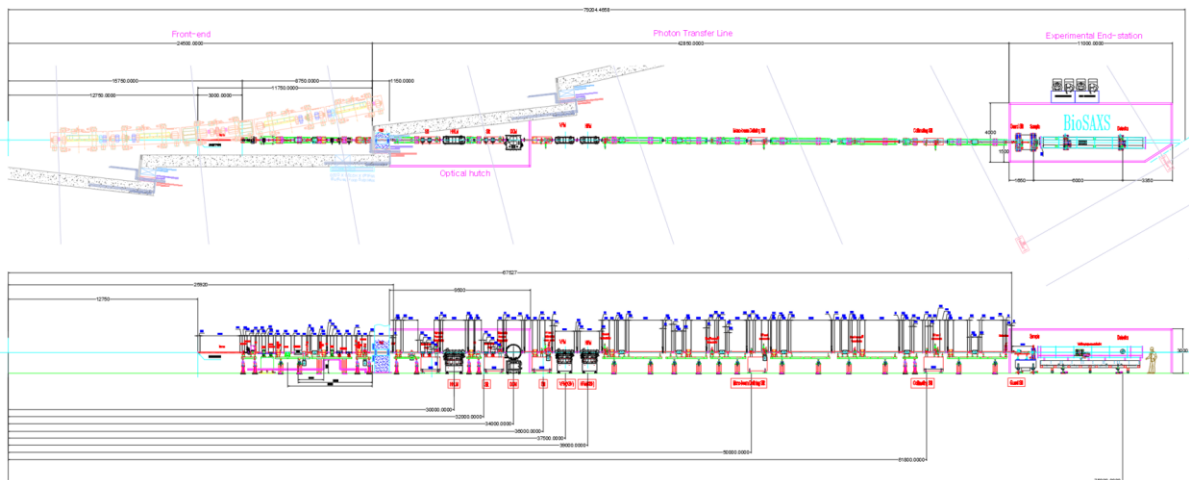
Undulator	Period (mm)	Length (m)	Ug (mm)	Kmax	Power (kW)	Power density (kW $mrad^{-2}$)	Max. power after FE (kW)
IVU24	24	3	5-16	2.747	17.9	165	0.87 Through 2(h)×2(v) mm ² FE mask

D. Beamline Requirements for the Front End

The front end of BioPharma-BioSAXS beamline will require to handle a maximum power of 17.9 kW. The output of the beam from IVU24 is appropriately attenuated using three masks in the front end to prevent damage to the optical devices in the PTL section and enable stable operation of the beam line. The BioPharma-BioSAXS beamline will utilize the standard KOREA-4GSR IVU24 front end design. Two fixed type masks and one movable type mask will control a total of 17.5 kW of heat at the front end. The beamsizes drawn from the front end will be 1.3 x 1.3 mm² at front end exit port. A detailed description of the BioPharma-BioSAXS Front End can be found in the <Table 3.2.1.2>.

E. Beamline Layout

The BioPharma-BioSAXS beamline is a SAXS-dedicated beamline at the KOREA-4GSR construction. The beamline layout is shown in <Figure 3.2.1.1>, where the beamline will consist of a front end, an optical hutch, a photon transfer line, and an experimental hutch.



<Figure 3.2.1.2> Layout of BioPharma-BioSAXS beamline.

<Table 3.2.1.2> shows major beamline components, their location along the beamline, and description.

<Table 3.2.1.2> List of BioPharma-BioSAXS beamline component

Distance from source (m)	Component	Description	Comments
27.7	Attenuator	Water cooled, CVD diamond, B ₄ C, Si	Removing low energy X-ray beam
28.3	Slit	Water cooled, 4-way slit, UHV	Eliminating heat load Mirror incident X-ray conditioning
28.8	Diagnostic	W-blade BPM	Beam position & profile defining
30.0	HHLM (High heat load mirror)	Flat mirror 2-stripe coating (Pt, Rh)	Eliminating heat load from X-ray
32.2	Slit	4-way slit, UHV	Beam conditioning
33.1	Diagnostic	W-blade BPM	Beam position & profile defining
34.0	DCM (Double crystal monochromator)	Si (111), fixed exit, NL ₂ cooled	Monochromatizing X-ray beam
35.9	Slit	4-way slit, UHV	Beam conditioning
36.3	Diagnostic	YAG + CCD	Beam position & profile defining
37.4	VFM (Vertical Focusing Mirror)	Ellipsoid Rh, PT coating	Focusing the beam in vertical direction
39.1	HFM (Horizontal Focusing Mirror)	Ellipsoid Rh, PT coating	Focusing the beam in horizontal direction
50.0	Slit	4-way slit, HV	Monochromatic beam conditioning
50.9	Diagnostic	YAG + CCD	Beam position & profile defining
57.0	Diagnostic	OFHC + YAG	Beam position & profile defining
61.8	Slit	4-way slit, HV	Monochromatic beam collimation
62.5	Diagnostic	YAG + CCD	Beam position & profile defining
67.1	Shutter	W	Blocking the beam
68.0	Slit	4-way slit, HV	Parasitic beam rejection
69.0	Sample environment	ARINAX robot	Automatic sample exchanging system
69.3 to 75.8	Variable q -range vacuum chamber	7 m long SDD 0.5 to 6.0 m	Detector position in vacuum tube SDD adjustment
69.5 to 75	2D detector	Eiger2 X 4M	Scattering pattern detection

F. Optics Overview

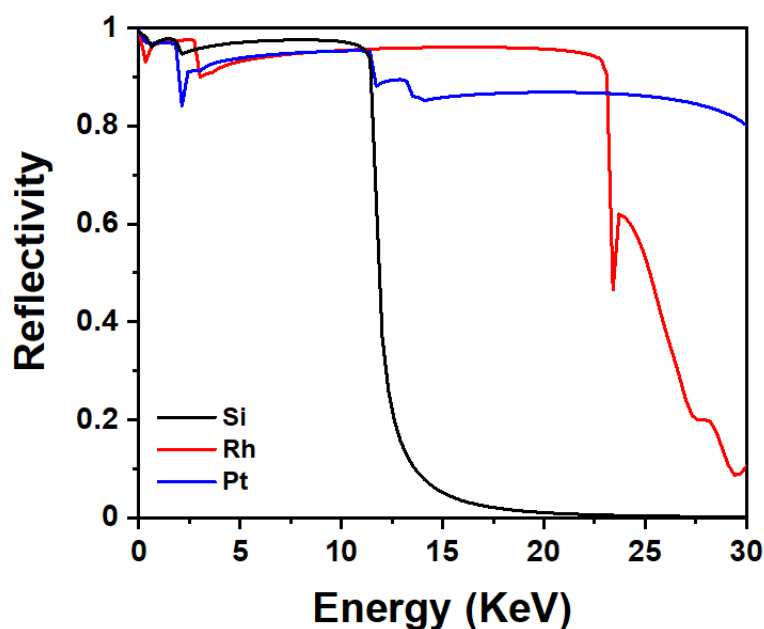
(1) Mirror Specifications

<Table 3.2.1.3> shows detailed specifications for optics.

<Table 3.2.1.3> Optics Specification for BioPharma-BioSAXS beamline

	HHLM	DCM	VFM	HFM
Installation location (m)	30	34	37.5	39
Mirror size (W x L x D, mm)	50 x 800 x 50	60 x 40	50 x 500 x 50	50 x 500 x 50
Optical footprint (W x L, mm)	1.5 x 548 (4 sigma)		1.08 x 392 (FWHM)	1.06 x 433 (FWHM)
Coating strip number	2 ea	-	2 ea	2 ea
Coating strip size (W x L, mm)	10 X 800	-	10 X 500	10 X 500
Beam size (V X H)	1.43 X 1.49 (4 sigma)	1.5 X 1.5	1.02 X 1.08 (FWHM)	1.06 X 1.13 (FWHM)
Coating material	Rh, Pt	-	Rh, Pt	Rh, Pt
Substrate material	Silicon	Silicon (111)	Silicon	Silicon
Mirror surface shape	Plane	Plane	Ellipsoid	Ellipsoid
Reflection direction	Up	vertical	Down	Ring
Cooling method	Eutectic bath	LN2	No	No
Mirror bender	Yes	No	No	No
Tangential radius (mm)	inf	inf	Ra=34,500, Rb=89.3601	Ra=34,500, Rb=88.9336
Sagittal radius (mm)	-	-	-	-
Tangential slope error (μ rad)	< 0.2	< 1	< 0.2	< 0.2
Sagittal slope error	-	-	-	-
Incident angle (mrad)	2.6 mrad	3 to 45 degree	2.6 mrad	2.6 mrad

Shot beam stability	1 μm / 30 min		1 μm / 30 min	1 μm / 30 min
Mirror surface height (mm)	1,400.0	1,400.0 at 1 st crystal	1,464.0	1,464.0
Motor axis	pitch, roll, x, y		pitch, roll, yaw, x, y, z	pitch, roll, yaw, x, y
Manual axis	pitch, roll, yaw, x, y, z		pitch, roll, yaw, x, y, z	pitch, roll, yaw, x, y, z
Max. total heat load (W)	158.8		-	-
Max. surface heat load (W/mm ²)	0.216 @ 4 keV		-	-



<Figure 3.2.1.2> Reflectivity of Si, Rh, Pt surface at 2.6 mrad of incidence angle.

(2) High Heat Load Mirror

A high heat load mirror (HHLM) will be located 30 m from the light source. This mirror receives the beam from the front end and reflects it in the vertical direction. The beam in the high photon energy is absorbed, lowering the heat load on the monochromator crystal of the double crystal monochromator (DCM) located behind it. BioPharma-BioSAXS beamline will use silicon (Si), rhodium (Rh), and platinum (Pt) mirror surfaces depending on the beam energy to be used. This mirror is coated with two lines of rhodium and platinum on a single silicon substrate, and the uncoated side is used as a Si mirror surface. The beam incidence angle of the mirror surface is 2.6 mrad, and <Figure 3.2.1.2> shows the reflectivity of each mirror surface

material. The Si mirror surface absorbs beams above 12 keV and reduces the thermal load on the DCM crystal surface. Because high reflectivity (> 0.9) occurs in the 5 to 10 keV region, a Si mirror surface is used when using beams in this region. According to a similar principle, the Rh-coated side is used when using a beam in the 10 to 20 keV range, and the Pt-coated side is used when using a beam of 20 keV or higher.

The specifications of HHLM are listed in <Table 3.2.1.3>. When the white beam size is 1.43 mm X 1.49 mm (V x H) and incident angle is 2.6 mrad on HHLM, the foot print is 1.5 mm x 548 mm. The size of the coating surface is set to 10 mm x 800 mm to accommodate the entire incident beam. The amount of heat absorbed by the mirror surface was predicted using the SRW code in OASYS. The maximum total heat output was calculated to be 158.791 W, and the maximum heat output was calculated to be **0.216 W/mm²**. The silicon substrate size of the mirror is 50 mm x 800 mm x 50 mm. The shape uses a cooling method using indium foil, Cu pad, and cooper pipe by digging a notch groove on the side of the mirror.

(3) Focusing mirrors

To focus the beam at the sample location, place a vertical focusing mirror (VFM) at 37.5 m from the light source and a horizontal focusing mirror (HFM) at 39 m. Both of these mirror devices are curved in the beam direction (tangential ellipse). The beam is focused at 69 m, which is the sample location, and the distance between the focusing positions from the focusing mirror is 31.5 m for VFM and 30 m for HFM. As with HHLM, the incident angle is set to 2.6 mrad, and two lines of Rh and Pt coating are applied, respectively. Through this, harmonics are removed once more. <Table 3.2.1.3> shows the specifications of the beam focusing mirror device. The size of the focused beam at the sample location of 69 m is 31 μm horizontally and 9 μm vertically at half maximum.

(4) Double Crystal Monochromator (DCM)

The double crystal monochromator (DCM) for monochromator adopts a structure that reflects the beam in the vertical direction, and the monochromator crystal uses silicon with a (111) reflection surface. Since the vertical beam spread of the incident light in the 5 to 20 keV range is less than 15 μrad , the resolution ($\Delta E/E$) of the monochromatic photon energy is

expected to be less than 2.0×10^{-4} . The resolution of DCM was calculated by the following (Equation 3.2.1.1).

$$\Delta E/E = \cot \theta_B [\omega_D^2 + \phi^2]^{1/2} \quad (\text{Eq. 3.2.1.1})$$

where, θ_B is the Bragg angle (or beam incidence angle) of the first DCM crystal, ω_D is the Darwin width of the Si crystal, and ϕ is the beam spread angle.

The tilt of the crystal (pitch angle or pitch) is adjusted in the range of 5.7 to 23.3° to meet the photon energy range of 5 to 20 keV. The size of the incident beam is 1.5 mm in the horizontal direction x 1.5 mm in the vertical direction. To accommodate the beam in the entire photon energy range, the size of the first crystal is 60 mm x 25 mm, and the second crystal receives the beam reflected from the first crystal. The length is set to 150 mm so that the step can be maintained at 25 mm while accommodating it. To precisely control the direction of the emitted light, the pitch angle and roll angle of the second crystal are driven by a piezoelectric actuator. Changes in the position of DCM emitted light are checked in the diagnostic device UHV-QPBM, and a feedback system is configured to keep the beam position constant.

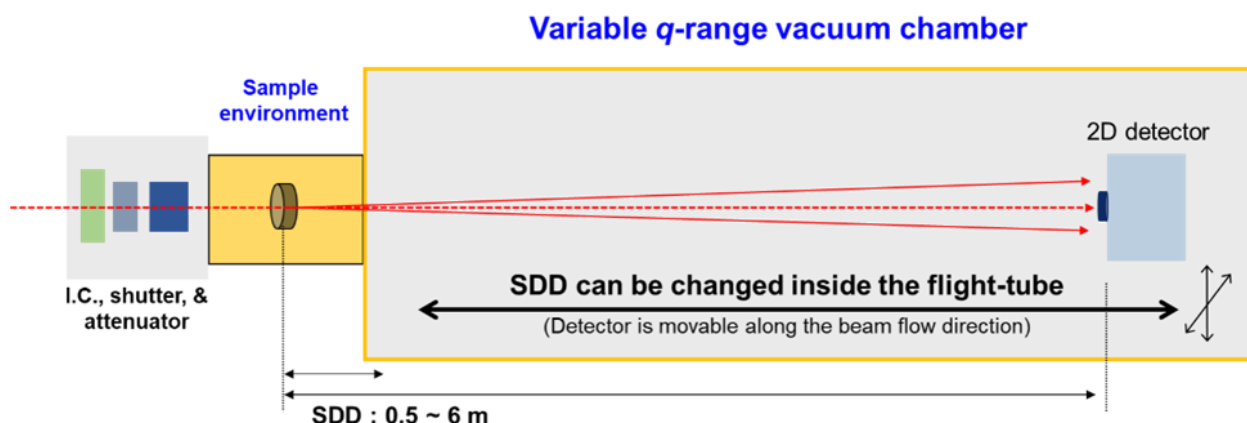
(5) Beam quality

Beam flux and beam profile at each optics.

G. Instrument Overview

(1) Variable q-range vacuum chamber

The solution SAXS technique acquires scattering patterns using a 2D large-area detector. Since the solution SAXS experimental technique requires securing scattering data in a variety of wide q-ranges depending on the sample particle size to be measured, changing sample-to-detector distance (SDD) is essential. <Figure 3.2.1.3> shows a variable q-range vacuum tube system. The 2D detector is positioned inside the vacuum tube and moved in the X-ray propagation direction through the rail, and the SDD is changed from 0.5 m to 6 m. In addition, the 2D detector can be moved vertically/horizontally based on the incident X-ray, making it easy to align the detector position. A photodiode type beam stop is placed in front of the detector to protect the detector from the direct beam, and the current value generated from the photodiode in proportion to the incident X-ray intensity is converted into voltage-frequency-count to calculate the accurate X-ray transmittance for the sample solution and (background) solvent.



<Figure 3.2.1.3> Schematic diagram of variable q-range vacuum chamber at BioPharma-BioSAXS beamline.

(2) Auto sample changer robot

In order to analyze the 3D structure of biological molecules, BioPharma-BioSAXS beamline requires high-throughput experiments and high-speed processing of a large number of samples. To this end, an automatic sample exchange robot system will be introduced. The automatic sample exchange robot will automatically place a minimum of 5 μL of sample into the quartz

capillary and irradiate it with X-rays. It takes about less than 1 minute for the robot to automatically load/unload and wash the sample, and up to 96 samples can be loaded at a time. In the case of biomolecule samples, the sample can be denatured by radiation damage from X-rays. To minimize this effect, a flow mode is additionally provided to conduct solution SAXS experiments while allowing 20 to 35 μL of the sample to flow through the quartz capillary. The storage and measurement temperatures can be adjusted from 4 to 40 $^{\circ}\text{C}$ and 2 to 60 $^{\circ}\text{C}$, respectively, depending on the characteristics of the sample. The specifications of the automatic sample exchange robot to be used in the BioPharma-BioSAXS beamline are shown in the following <Table 3.2.1.4>.

<Table 3.2.1.4> Specification of automatic sample changer robot

Performance	
Solution transfer volume	5 to 200 μL
Typical cycle time	50 s
loading/unloading	15 s / 15 s
cleaning (wash, rinse, dry)	20 s
Sample Containers	96-well microplates 96-deep well microplates 4 x 8 wells Eppendorf strips (200 μL) 4 x 3 individual 1.5 mL wells (buffers)
Control	
Sample exposure modes	1. Static 2. Flow (0.05 to 20 $\mu\text{L/s}$)
Temperature control	2 to 60 $^{\circ}\text{C}$
Exposure storage	4 to 40 $^{\circ}\text{C}$
Control panel	Video assisted automatic liquid positioning
Dimension (W x H x D)	
Main unit	550 x 800 x 1100 mm^3
Fluid management rack	837 x 576 x 900 mm^3
Control rack	712 x 576 x 900 mm^3

(3) SEC-SAXS system

For accurate structural analysis of solution samples, SAXS data acquisition from monodisperse samples is essential. The BioPharma-BioSAXS beamline will introduce an in-line Size Exclusion Chromatography (SEC)-SAXS experimental technique that allows real-time separation of samples by size and molecular weight while simultaneously obtaining scattering data for each component. Since the samples separated and purified through SEC are analyzed in real time with various detectors and small-angle X-ray scattering experiments are performed at the same time, structural information of each component in the mixture can be accurately obtained. In addition, multi-angle light scattering (MALS) and dynamic light scattering (DLS) are used in conjunction with SEC.

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3.2.2 ID24 Material Structure Analysis Beamline

A. Introduction

ID24 Material Structure Analysis beamline is a dedicated high-resolution powder X-ray diffraction beamline for crystallographic analysis of polycrystalline and crystalline materials. It has been designated as an industrial priority beamline to provide dedicated access and tailored support for industry users. This beamline takes full advantage of the synchrotron radiation's high brilliance, excellent collimation, and low divergence, enabling structure analysis of various materials. This enables diverse applications in academia and industry, including research on energy and eco-friendly materials, structural materials, functional materials, and the design of advanced materials.

While conventional synchrotron powder diffraction achieves high angular resolution with the Multi-Analyzer Crystals (MAC) detection systems, the long acquisition time - typically 1 to 2 hours per sample - limits its effectiveness in responding to increasing throughput demands and fast-paced research developments. To address these limitations, the ID24 beamline was designed to enable high-resolution measurements with substantially shorter acquisition times, thereby alleviating the throughput limitations of conventional powder diffraction experiments.

The ID24 employs an in-vacuum undulator (IVU) as its light source, intrinsically providing low beam divergence. It utilizes the shortest undulator period among the devices installed in the early phase of the Korea-4GSR project, enabling stable delivery of monochromatic X-rays even at high photon energies. Moreover, by integrating the MAC detection system with a two-dimensional detector, ID24 significantly reduces the measuring time from hours to minutes, compared to conventional systems. When necessary, it also supports in-situ/operando experiments through a system capable of time resolution on the order of seconds while maintaining appropriate angular resolution.

The ID24 beamline features two dedicated sample stages: one is a high-resolution diffractometer system (angular resolution estimated at approximately 0.005° at 33 keV) for detailed crystallographic analysis, and the other is an optical table-based stage that allows flexible experimental setups for in-situ/operando analysis with appropriate resolution ($\sim 0.05^\circ$, depending on sample to detector distance). The latter is designed as a multi-sample measurement system, enabling high-throughput data collection through rapid acquisitions. This

strategy aims to efficiently meet the growing industrial demand for the analysis of a large number of samples.

Additionally, the ID24 beamline design provides sufficient space within the experimental hutch to allow flexible configuration changes for dynamic research. It also accommodates automation systems for high-throughput sample measurements, high-speed DAQ analysis systems, and installation of compact in-situ cells. Together, these design features ensure the beamline is scalable to accommodate future upgrades in measurement technique and detector technology.

B. Beamline Requirements for the Insertion Device

The ID24 Material Structure Analysis beamline provides stable monochromatic X-rays over an operational energy range of 5.5 to 45.0 keV, utilizing an In-Vacuum Undulator (IVU) with a period of 16 mm as its insertion device. Based on the 4 GeV storage ring energy, the IVU16 is designed to deliver high photon flux – exceeding 10^{12} *ph/s* – even in the low harmonic regions (1st to 7th harmonics), while ensuring photon energies above 25 keV.

In powder diffraction, governed by Bragg's law, the accessible d-spacing range within a fixed 2θ window is linked to photon energy. Higher photon energies expand this range, enabling a broader set of lattice spacings to be measured in shorter acquisition times. Leveraging this advantage, ID24 is optimized to operate at 33.5 keV, maximizing detector efficiency and reducing acquisition times. This high-energy operation enables the beamline to efficiently accommodate the high-throughput measurement demanded by industry users, consistent with its designation as an industrial priority facility.

The key specifications of the IVU16 are summarized in <Table 3.2.2.3>. The undulator has a period of 16 mm and a total length of 3 meters, installed at the center of the straight section. The maximum power output depends on the undulator gap, with 1.07 kW at a 5 mm gap and 0.8 kW at a 6 mm gap, measured under the condition of a 400 mA storage ring current and a 2×2 mm² beam aperture located 23 meters downstream from the source. While the undulator can operate at a minimum gap of 5 mm to achieve peak performance, the beamline is configured to operate at a 6 mm gap, chosen to ensure spectral stability and reliable beamline performance under practical operating conditions.

<Table 3.2.2.4> Parameters of insertion device

Undulator	Period (mm)	Length (m)	Location	Min. Gap (mm)	Max Power (kW)
In-vacuum	16	3.0	Center of Straight Section	5	1.07
In-vacuum	16	3.0	Center of Straight Section	6	0.80

C. Beamline Requirements for the Front-End

To ensure stable performance in high-resolution powder diffraction experiments, the Front-End (FE) of the ID24 Material Structure Analysis beamline is specifically designed to meet three core requirements: thermal load management, beam position monitoring, and radiation safety. The insertion device is an IVU16, which can generate up to 7.38 kW of thermal power at its minimum operating gap of 5 mm. However, in practical operation, a minimum gap of 6 mm is expected to be applied, reducing the corresponding thermal power to 4.46 kW and contributing to improved operational stability of the optical devices.

Korea-4GSR employs a standardized Front-End system for IVU beamlines, capable of withstanding thermal loads of up to 18 kW (based on IVU24 specifications), and the ID24 beamline adopts the same system, referring to FE chapter [TBA].

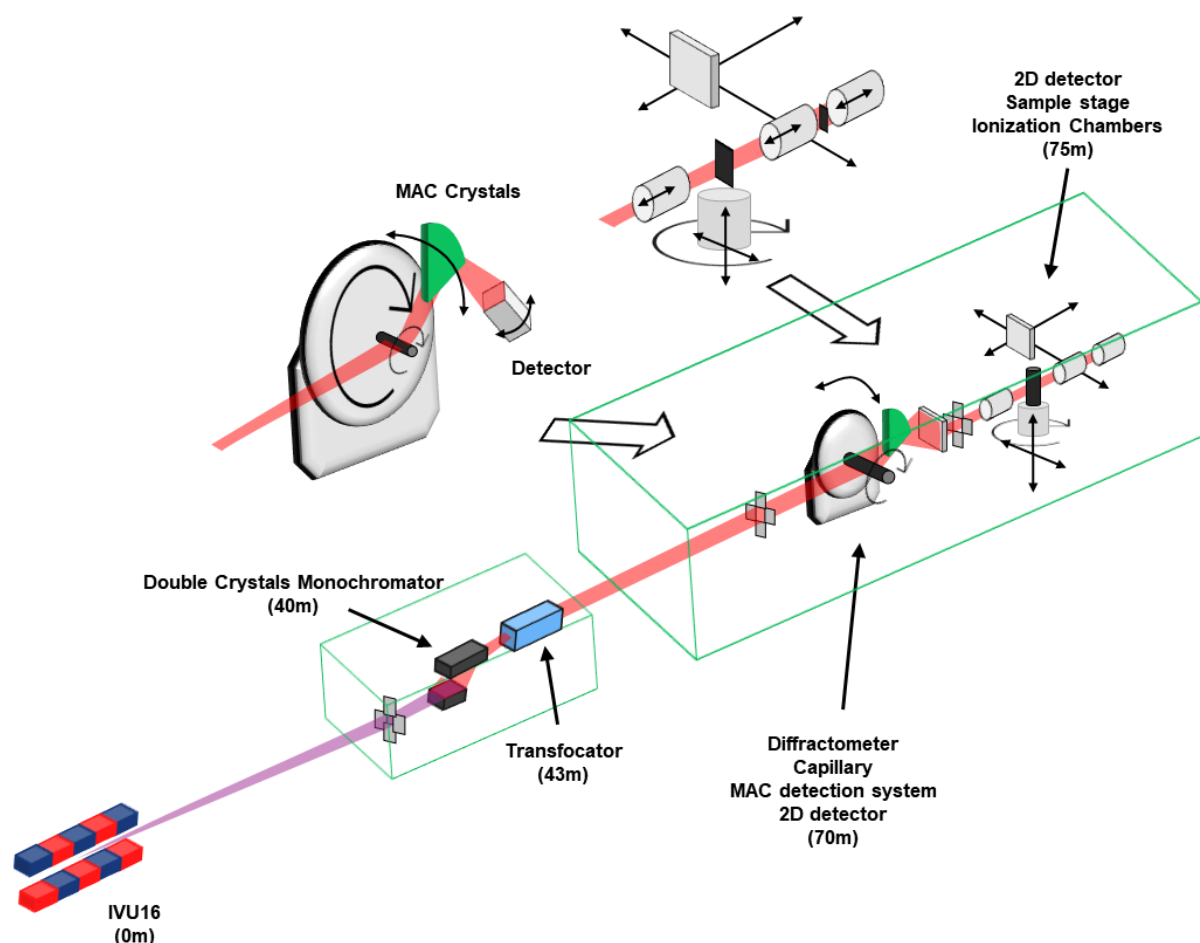
To manage the thermal load, the FE is equipped with three water-cooled masks. The first is a fixed mask with a preset horizontal aperture that allows only positional adjustment, while the remaining two are movable masks that support adjustment of both aperture size and position. Detailed specifications of each mask are provided in Section 4.2, “Vacuum Components of Front End,” of the technical design report.

The FE also includes a Beam Position Monitor (BPM) system. During the initial phase of operation, this BPM enables real-time monitoring of the X-ray beam position, and the data are used to control the slit position, thereby ensuring consistent beam intensity at the sample.

For radiation safety, a safety magnet with a field strength of 0.5 Tesla is installed to address potential scenarios in which the electron beam might unintentionally enter the Front-End region. This magnet deflects the electron beam horizontally, preventing it from reaching the Optical Hutch.

D. Beamline Layout

(1) Beamline overview



<Figure 3.2.2.3> Beamline schematic of Material Structure Analysis beamline.

As part of the Korea-4GSR project, the ID24 Material Structure Analysis beamline was designed with the shortest undulator period, using IVU16. The IVU16 delivers low beam divergence and high photon flux, making it particularly advantageous in the low harmonic range. This configuration optimizes the beamline for high-energy X-ray experiments, particularly powder diffraction, at energies exceeding 25 keV.

The ID24 beamline provides a stable, fixed-energy X-ray beam via a monochromator. To support a wide range of experimental configurations and techniques, the beamline provides a transfocator system equipped with configurable sets of Compound Refractive Lenses (CRLs). This optical system allows for full operational flexibility, including beam collimation, vertical

and horizontal focusing, or complete bypass to transmit the natural beam without optical intervention.

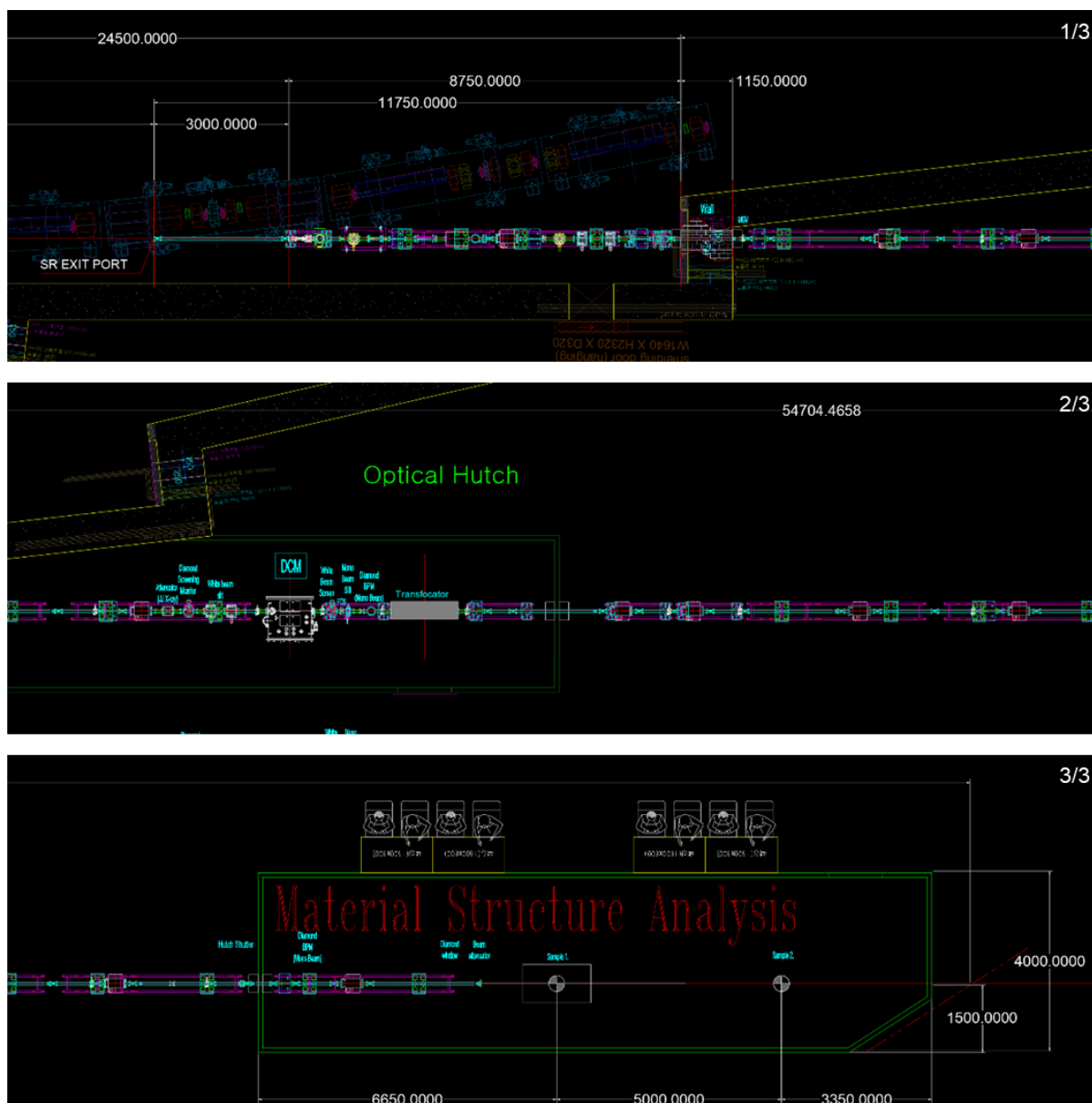
The conditioned X-ray beam is directed to a single experimental hutch housing two independent sample stages, positioned at approximately 70 m and 75 m from the source. This configuration allows for selective beam delivery tailored to distinguish experimental objectives, maximizing the versatility and performance of the beamline.

<Table 3.2.2.2> lists the main components of the Material Structure Analysis beamline and their distances from the source.

<Table 3.2.2.2> Main component list of Material Structure Analysis beamline.

Distance	Location	Component name	Description
0	Front W-End	In-Vacuum Undulator	Period 16 mm, Device Length: 3 meters
39.0	Optical Hutch	White beam slit	Up to 4 kW heat load
39.5		Diamond monitor	Resolution <1 um, Diamond thickness 30 um
40.0		DCM	Vertical bounce, LN2 cooled, Max heat load < 200W, Offset: 25 mm
41.0		DBPM	Resolution beam size <0.1%,
42.0		Beam monitor	Diamond screen monitor, 1 um resolution, Removable
43.0		Transfocator	Transfocator, CRLs
64.5	Experimental Hutch	DBPM	Resolution beam size <0.1%,
65.0		Beam monitor	Diamond screen monitor, 1 um resolution, Removable
66.0		Monochromatic slit	Parasitic scattering rejection
66.5		Ion gas chamber	I0 monitor
67.0		Attenuator	I0 adjustment
70		Sample stage #1	Diffraction set up
75		Sample stage #2	Flexible XRD set up

(2) Beamline Floor Plan



<Figure 3.2.2.2> Beamline drawing of Material Structure Analysis beamline.

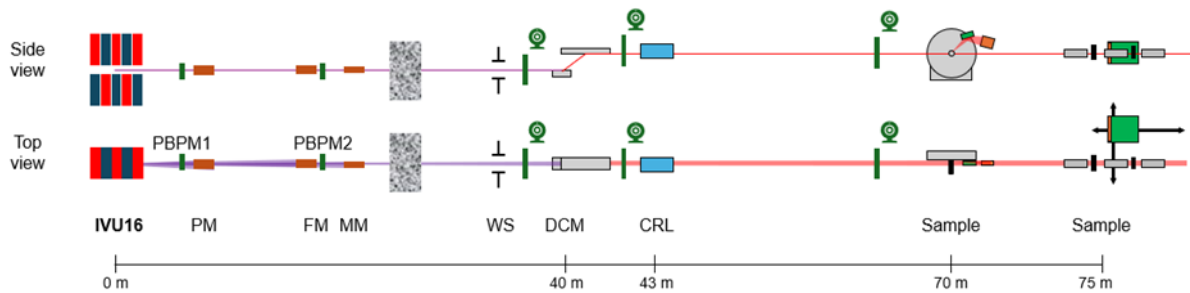
E. Optics overview

(1) Optical Layout Consideration and Simulation

The optical simulation of the ID24 Material Structure Analysis beamline was conducted with the goal of operating in a stable fixed-energy range above 25 keV, under conditions where the undulator gap is set to 6 mm or greater. At a gap of 6 mm - where maximum photon flux is

achieved - the highest attainable energy in the low harmonic range corresponds to the 5th harmonic at 33.5 keV, and this energy condition was used as the baseline for the simulation.

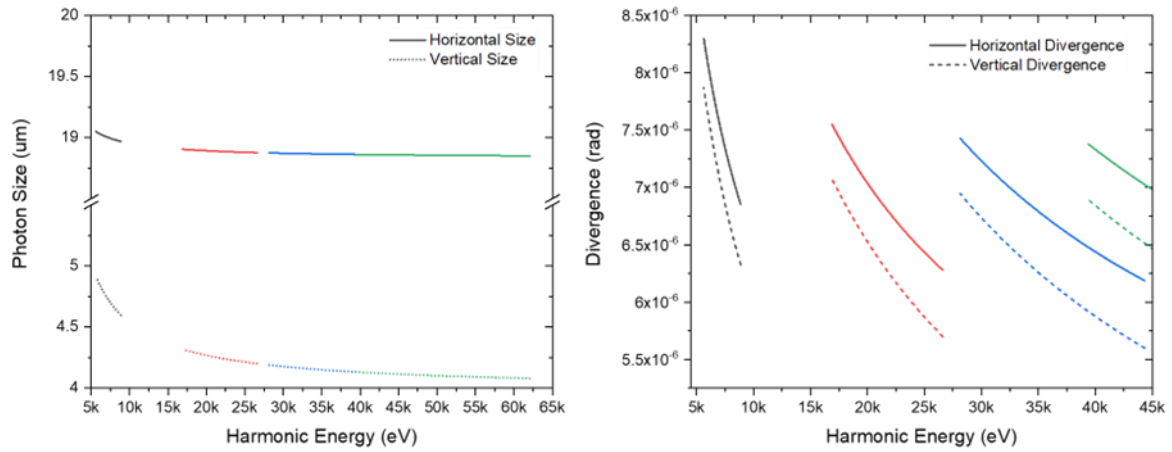
The optical layout, as shown in <Figure 3.2.2.3>, was designed to deliver an X-ray beam with a vertical divergence of less than $10\ \mu\text{rad}$ and a total photon flux exceeding $10^{12}\ \text{ph/s}$ at the sample position. These beamline characteristics are intended to enable high angular resolution, temporal resolution, and a reduction in total measurement time, thereby supporting efficient and high-quality data acquisition. The simulation was performed using ShadowOui in the OASYS environment, with undulator source parameters provided by SPECTRA [1-3].



<Figure 3.2.2.3> Optical layout of Material Structure Analysis beamline. DCM is Vertical deflecting Double Crystal Monochromator. PM: Parasitic mask, FM: Fixed mask, MM: Movable mask, WS: White beam slit, DCM: Vertical double crystal monochromator, CRL: Transfocator including Compound Refractive Lens (CRLs).

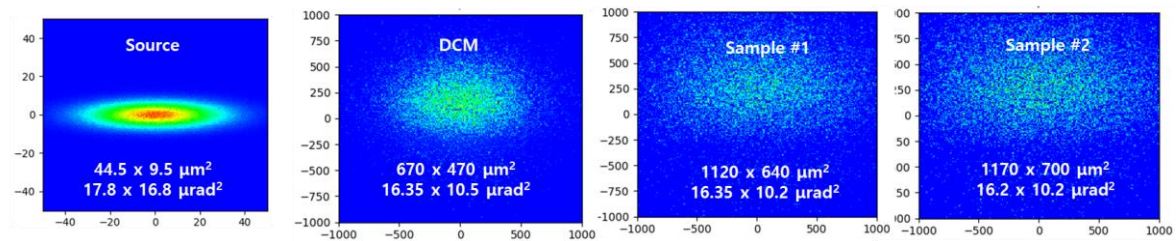
<Figure 3.2.2.4> illustrates the photon source size and divergence of the IVU16 in both vertical and horizontal directions. The 5th harmonic beam at 33.5 keV exhibits a divergence of less than $10\ \mu\text{rad}$, resulting in an approximate beam size of 1 mm (horizontal) $\times$ 0.5 mm (vertical) at the sample position. This low divergence characteristic suggests that the beamline can support direct beam delivery to the sample without the need for additional optical collimation via mirrors. In addition, to address the growing demand for spatial and temporal resolution in sample analysis - driven by evolving research paradigms - the beamline has been designed to support flexible beam focusing conditions using CRLs. This allows the delivery of beams tailored to various experimental requirements.

The beam size evolution along the optical path, as simulated using the OASYS environment, is shown in <Figure 3.2.2.5> and listed in <Table 3.2.2.3>.



<Figure 3.2.2.4> Photon size and divergence in vertical and horizontal direction, σ and σ' , of IVU16.

@33.5 keV, FWHM & FWHM'



<Figure 3.2.2.5> Beam size and divergence evolution along the beamline simulated by using ShadowOui.

<Table 3.2.2.3> Photon size and divergence in vertical and horizontal direction, σ and σ' , at different locations

Energy (harm.)	K	Position (σ and σ')			
		Source	DCM	Sample #1	Sample #2
20 keV (3 rd)	0.91	18.9 x 4.5 μm^2	290.5 x 240.0 μm^2	500.0 x 390.0 μm^2	540.0 x 420.0 μm^2
		8.2 x 7.8 μrad^2	7.2 x 6.0 μrad^2	7.2 x 5.7 μrad^2	7.2 x 5.7 μrad^2
33.5 keV (5 th)	0.91	18.9 x 4.3 μm^2	284.0 x 220.0 μm^2	490.0 x 350.0 μm^2	530.0 x 360.0 μm^2
		7.1 x 6.5 μrad^2	7.1 x 5.5 μrad^2	7.1 x 5.1 μrad^2	7.1 x 5.1 μrad^2

(2) Heat Load Consideration

Efficient heat load management is essential for maintaining optical stability and minimizing spectral distortion in high-brilliance beamlines. In ID24, the heat load introduced by the IVU16 undulator was analyzed to ensure safe and stable operation.

As described in Section 3.2.2.B, when operating at a 5 mm gap, the IVU16 delivers approximately 1.07 kW of power through the $2 \times 2 \text{ mm}^2$ beam aperture of the FE, and about 0.80 kW at a 6 mm gap. These values correspond to approximately 80% of the heat load generated by the IVU24 - an in-vacuum undulator having the highest total power currently in Korea-4GSR construction project - having a distinct advantage in heat load management for this beamline. Based on this analysis, a white beam can be directly incident on DCM without the need for additional upstream heat load reducing optics. This configuration simplifies the beamline design while ensuring stable performance under thermal conditions.

In DCM design, a primary consideration is suppressing thermal deformation (thermal bump) and preventing rocking curve distortion on the first crystal surface. To mitigate these effects, the peak power density on the crystal is limited to below 40 W/mm^2 . To achieve this, DCM is installed approximately 40 meters downstream of the source, allowing spatial dispersion of the incoming photon beam and reducing the total heat load delivered to the optics. DCM crystals are cryogenically cooled with liquid nitrogen, maintaining the surface temperature at approximately 120 K to further suppress thermally induced distortions.

To further refine the thermal load reaching the DCM, a white slit aperture is positioned upstream to selectively shape the beam profile and limit the maximum incident power to 120 W. This aperture plays a critical role in fine-tuning the total heat load while preserving the target photon flux of 1,012 photons/s at the sample position. The entire beamline geometry and aperture settings have been optimized to ensure both thermal safety and beam performance.

The heat load and absorbed power on the DCM across different undulator gap settings were evaluated using the SRCalc simulation tool [4, 5]. In this simulation, a beam aperture of approximately $1.45 \times 1.45 \text{ mm}^2$ at the white slit located 39 meters from the source, beam energy of 5.5 keV – corresponding to the lowest available beam energy on this beamline – at DCM located 40 meters, and a $200 \mu\text{m}$ diamond filter were applied. The results are summarized in <Table 3.2.2.4>.

<Table 3.2.2.4> Calculated the heat load of an optical component

Gap	5	6	7	8	9	10
K	1.172	0.912	0.718	0.572	0.461	0.376
Energy (keV)	5.6	6.7	7.5	8.1	8.5	8.8
DCM: Peak power density (W mm ⁻²)	19.85	12.86	8.96	6.40	4.59	3.29
DCM: Absorbed power (W)	146.6	112.4	87.6	67.1	50.2	36.9
DCM: Transmitted power (W)	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01

(3) Beam Specifications and Optics Specifications

A standard double-crystal monochromator (DCM) with a fixed exit of 25 mm is employed, equipped with a pair of liquid-nitrogen-cooled Si(111) and Si(311) crystals. The DCM ensures an angular stability better than 50 *nrad* over extended operation periods, providing reliable beam stability for continuous measurements. Detailed specifications are presented in <Table 3.2.2.5>.

<Table 3.2.2.5> Specifications for DCM

Distance (m)	Incident Angle (deg)	Shape	Type	Crystals	Dimensions (mm ²)	Figure error (nm, RMS)	Slope error (μrad, RMS)
40	2.5 to 21	Plane	Vertical deflection	Si(111), Si(311)	1st: 60×25×50 2nd:140×25×30	<1	<1

To meet the collimating and focusing requirements of the ID24 Material Structure Analysis beamline with full operational flexibility, a transfocator system is implemented. The system is initially configured for optimized operation at 20 keV and 33.5 keV, enabling vertical/horizontal collimation and focusing on these energies. In anticipation of evolving diverse research requirements and experimental paradigms, the Transfocator includes additional capacity to accommodate further CRL assemblies. This allows future expansion to adapt beam characteristics for different energies and focusing conditions without major hardware modifications.

F. Experimental System Overview

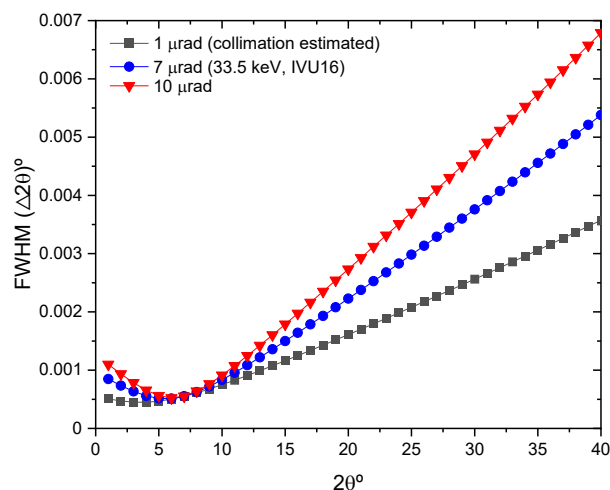
The primary technique offered by the structural materials analysis beamline is high-resolution powder diffraction (HRPD), supported by auxiliary methods such as in-situ XRD, various diffraction techniques, and X-ray absorption fine structure (XAFS). To accommodate the diverse research demands in energy materials, catalysis, and geosciences, and to enable the rapid acquisition of wide d-spacing data, the beamline is designed with two complementary operational modes, based on fixed sample environments located at 70 m and 75 m from the source.

Sample Stage #1, optimized for high-resolution powder diffraction, is located 70 m from the source and is configured for capillary sample by default. A high-angular-resolution detection system, which consists of 13 Multi-Analyzer Crystals (MAC) spaced at 2° intervals and combined with a 2D detector, is employed [6]. The Darwin width of each analyzer crystal enables precise separation of diffraction peaks, delivering excellent angular resolution. Operating at an energy of 33.5 keV, this stage covers a 2θ range of 3° to 40° (optimized for 5° to 30°), corresponding to d-spacings from 0.5 to 7.0 Å. High energy limits the small-angle range, reducing the maximum d-spacing (dmax). To address this, the system can operate at 20 keV using the 3rd harmonic, extending dmax for broader structural analysis. <Table 3.2.2.6> summarizes the measurable d-spacing ranges for different energies within the same 2θ range. For reference, the general 2θ range of 10 to 130° , corresponding to a d-spacing of 0.85 to 8.89 Å at 8 keV, is achievable by adjusting the crystal angle of the DCM without additional setup changes.

<Table 3.2.2.6> d-spacing ranges for different energies

	d-spacing (Å)	
2θ range	20 keV (Gap 6 mm, 3 rd harmonic)	30 keV (Gap 6 mm, 5 th harmonic)
3 to 40	0.91 to 11.84	0.54 to 7.07
5 to 30	1.20 to 7.11	0.71 to 4.24

The estimated angular resolution is approximately 0.005° , and typically completed in 15 minutes per sample, using a 0.02° step scan with 0.5 s exposure time. The estimated angular resolution performance across the detection range is shown in <Figure 3.2.2.6>.



<Figure 3.2.2.6> Estimated angular resolution at different beam divergences using Si(111) of DCM and MAC crystals in Sample Stage #1.

Sample Stage #2, located at 75 m from the source, is designed for multi-sample measurements, in-situ XRD, and various diffraction techniques. This stage supports a wide range of sample environments, including a gas-flow cell, hot air blower, Cryostream, heating furnace, and in-situ battery cell or customized chamber. The flexible stage design enables efficient high-throughput experiments and is expandable to accommodate additional sample environments in the future. High-throughput experiments utilize a large-area 2D detector, with sample-to-detector distances ranging from 500 mm to 2,000 mm, providing a variety of measurable d-spacing ranges. The target measurement performance includes an angular resolution of approximately $\sim 0.05^\circ$ and a measurement time of less than 1 minute per sample. Depending on the selected distance, this stage system offers adjustable trade-offs between angular resolution and angular coverage. The estimated angular resolution and d-spacing range at 33.5 keV using a 0.5 mm thick sample and the PILATUS4 X 4M detector are summarized in <Table 3.2.2.7>. This configuration provides spatial flexibility to enable user-friendly sample environments, aiming not only for high-throughput measurements but also for time-resolved measurements with second level resolution, high-precision measurement.

<Table 3.2.2.7> Estimated angular resolution and d-spacing range at 33.5 keV using a 0.5 mm-thick sample and the PILATUS4 X 4M detector in Sample Stage #2

Sample to detector distance (mm)	Maximum 2θ (degrees)	Angular resolution (degrees)	d-spacing range (Å)
500	37.47	0.074	0.5 to 4.3
1,000	18.74	0.037	1.1 to 8.6
2,000	9.37	0.019	2.0 to 16.0

Reference

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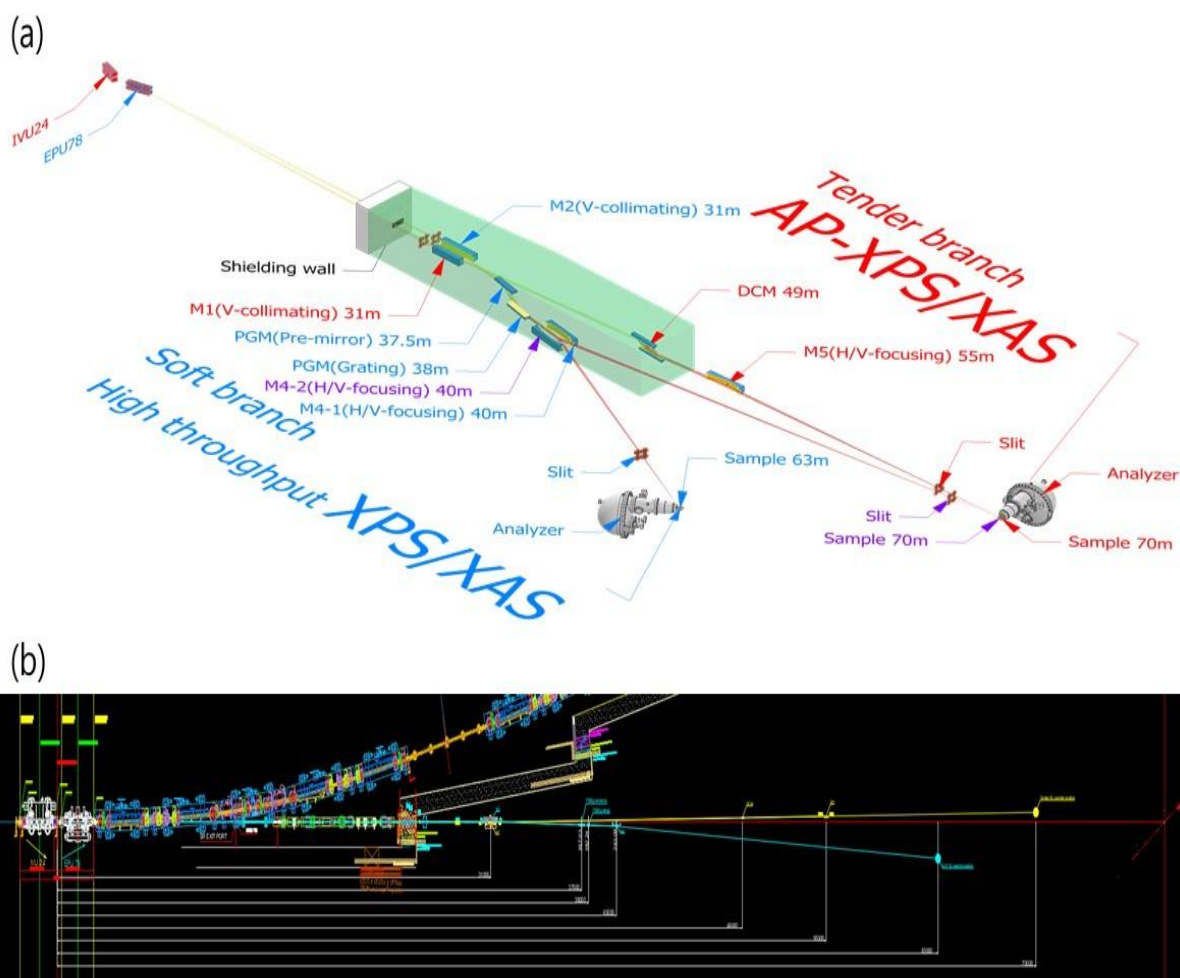
3.2.3 Soft X-ray NanoProbe Beamline

A. Introduction

(1) Beamline Outline

The Soft X-ray NanoProbe beamline, identified as a priority facility for industrial applications, is slated for establishment to provide a wide range of photon energy encompassing both the traditional soft X-ray range (a few eV to 2,000 eV) and the increasingly significant tender X-ray range (2,000 eV to 5,000 eV). This beamline aims to facilitate extensive research in basic science, as well as technology development within the industry. Experimental techniques anticipated for use with this beamline include Photoemission Spectroscopy (PES) and X-ray Absorption Spectroscopy (XAS), both of which have previously demonstrated exceptional effects in chemical and electronic property investigations. With increasing demand for advanced material studies particularly in high-density semiconductor devices, eco-friendly catalysts, and secondary batteries there is a growing need for nanoscale analyses providing high spatial resolution and significant probing depths for sub-surface (interface and bulk) examination.

The newly constructed Korea-4GSR is anticipated to serve as a powerful alternative that addresses the existing limitations, delivering advantages such as approximately 100 times the brightness of third-generation beamlines, a reduced beam size, and increased coherence. The Soft X-ray NanoProbe beamline is designed to cover a relatively wide range of photon energies, from 100 eV to 5,000 eV, and will consist of two branch beamlines, as can be seen in <Figure 3.2.3.1>. The beamline major parameter has appeared in <Table 3.2.3.1>. Branch 1 will employ tender X-rays for depth-probing XPS/XAS experimental setups in both ultra-high vacuum (UHV) and ambient pressure environments. In contrast, Branch 2 is dedicated to next-generation high-throughput XPS and XAS, enabling fast, automated analysis of large sample batches. Designed with user accessibility in mind, it aims to accelerate industrial applications and combinatorial material discovery through streamlined, scalable measurements. This dual-branch design will make the beamline a highly competitive experimental tool for various applications.



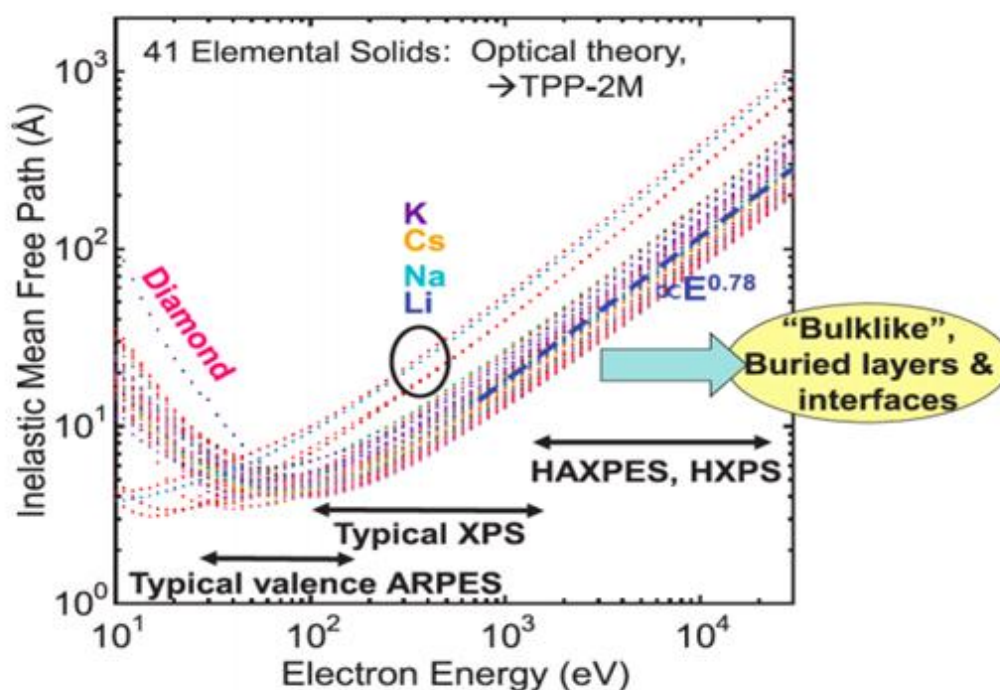
<Figure 3.2.3.1> Optical layout of the ID26 Soft X-ray NanoProbe beamline showing (a) the dual-branch configuration for Tender AP-XPS/XAS and Soft HT-XPS/XAS experiments and (b) ID26 beamline layout

<Table 3.2.3.1> Key specifications of 4 Soft X-ray NanoProbe Beamline

	Branch 1	Branch 2
Light source	IVU24	EPU78
Energy range [keV]	2.0 to 5.0	0.1 to 3.2
Techniques	(AP)XPS/XAS	(AP)XPS/XAS
Beam size (h × v, FWHM)	5 × 12 μm ²	36 × 14 μm ²
Beam flux (ph/s/0.1%B.W.)	1.5 × 10 ¹⁵ @4 keV	6.3 × 10 ¹⁴ @400eV

(2) Scientific objectives

Photoemission spectroscopy has its roots in the work of A. Einstein and K. Siegbahn and is a unique experimental technique for measuring the chemical and electronic structure of samples. The first experiment measured by K. Siegbahn involved the Cu 1s using Mo K α (K α 1=17,479, K α 2=17,374 eV), for which he was awarded the Nobel Prize in Physics in 1981, recognizing his contribution to developing high-resolution electron analysis methods. The emergence of synchrotron radiation has been a catalyst for photoemission spectroscopy experiments, and until recently, experiments have predominantly been conducted using soft X-rays (30 to 2,000 eV), which have advantages in surface sensitivity, photon flux, and photon ionization cross-section, rather than high-energy photoemission spectroscopy experiments using energies of 2 to 10 keV, successfully illuminating the chemical/electronic structure of surfaces.



<Figure 3.2.3.2> Variation of inelastic mean free path (IMFP) as a function of electron kinetic energy for different materials.

As illustrated in <Figure 3.2.3.2>, when employing soft X-rays, the kinetic energy of photoelectrons emitted from the surface typically ranges from a few eV to 2,000 eV. The universal curve indicates that the escape depth is approximately 1 nm, thereby enabling the acquisition of precise information directly from the surface. Recently, high-energy photoemission spectroscopy (HAXPES) beamlines utilizing X-ray energies in the range of 2

to 10 keV have been constructed at various international synchrotron facilities, as summarized in <Table 3.2.3.2>. Building on the established principles of soft X-ray PES, novel techniques have emerged, increasing the probing depth to approximately 10 nm, facilitating research in catalysts and a variety of applied materials.

This advancement is particularly crucial for recently developed semiconductors and energy devices characterized by multilayer structures. The properties of these devices are governed by the chemical, electronic, and structural attributes of the surface, interfaces, and bulk materials at depths around 10 nm, emphasizing the need for comprehensive studies of surface and interface phenomena. Additionally, there is an escalating demand for investigations into the real-time changes in properties under operational conditions of these devices. Concurrently, the rapid advancements in science and technology have ushered in powerful synchrotron light sources, refined vacuum technologies, and enhanced detector capabilities, resulting in a substantial increase in photon flux in the hard X-ray domain (approximately 10^{13} photon/sec). This has led to probing depths of around 30 nm, thereby elevating the prominence of PES experiments. Consequently, as detailed in <Table 3.2.3.2>, synchrotron facilities worldwide are currently exploring experimental setups for HAXPES beamlines that utilize broad photon beams in the energy range of 0.2 to 10 keV.

Furthermore, understanding the dynamic characteristics of semiconductor devices and solar cell batteries under actual operating conditions is increasingly recognized as paramount. The performance of these devices is intricately linked to alterations in their physical and chemical properties, particularly at the surfaces and interfaces. The introduction of HAXPES beamlines enhances the utility of photoemission spectroscopy, enabling precise measurements in the in-situ environments of these samples.

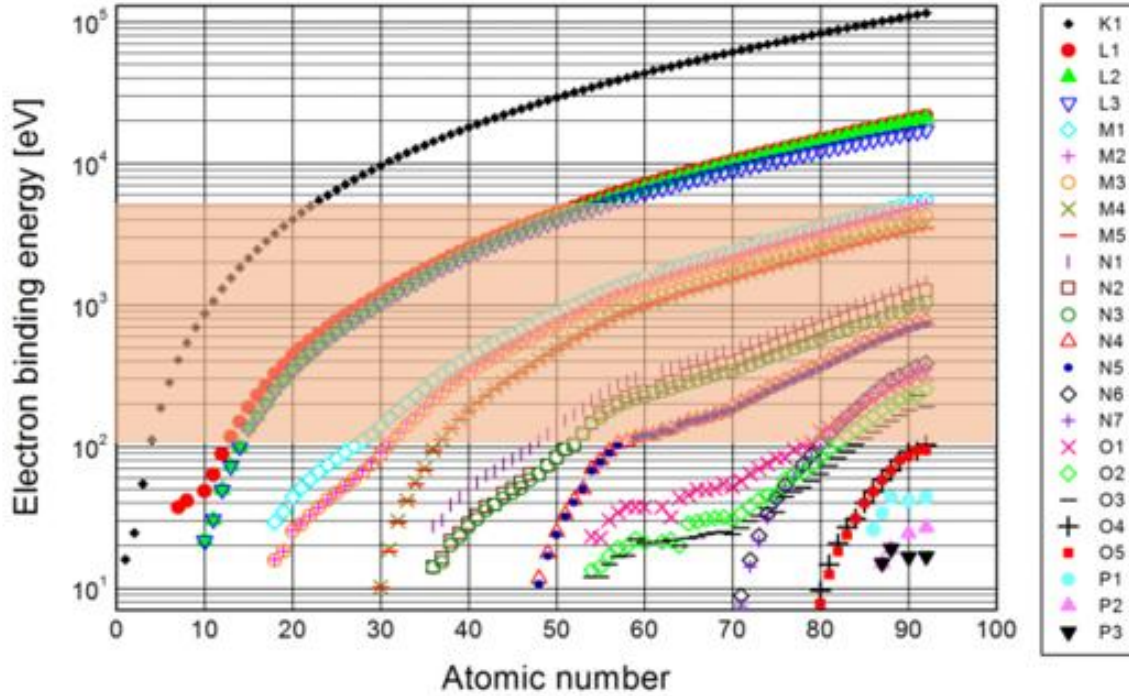
In the case of the 4GSR, the implementation of the Multi-Bend Achromat (MBA) system enables a photon brightness that is 100 times greater than that of existing third-generation sources, while also allowing for beam sizes focused at the nanometer scale. This capability supports three-dimensional imaging with nanoscale spatial resolution and facilitates measurements of spontaneous nanoscale processes over time scales ranging from minutes to nanoseconds. The Soft X-ray NanoProbe beamline will incorporate two undulators (photon sources) installed in canted array to encompass an energy range of 0.1 to 5 keV, addressing both the soft X-ray and tender X-ray regions, and will consist of two branching beamlines.

<Table 3.2.3.2> Examples of international beamlines similar to the Soft X-ray NanoProbe beamline

Beamline	Source	Energy range	Beam size	End-station
ALS, USA, BL9.3	Bending Magnet	2,300 to 6,000 eV (DCM)	$\leq 300 \mu\text{m}^2$	HAXPES, APXPS, Tender-XAS,
		200 to 900 eV (PGM)	$\leq 1.0 \text{ mm}^2$	APXPS, XAS
BESSY-II, Germany, BL13.2	U48	80 to 2,200 eV	$100 \times 80 \mu\text{m}^2$	NAP-HE-XPS, XAS
	U17	700 to 1,600 eV (PGM) 2,200 to 10,000 eV (DCM)	$180 \times 50 \mu\text{m}^2$ $150 \times 20 \mu\text{m}^2$	HAXPES, APXPS, Tender-XAS, RIXS
SLS, Switzerland, X07DB	Bending Magnet	270 to 1,500 eV	$\leq 50 \text{ nm}^2$	APXPS, Nano-XAS(STXM)
PAL, Korea, BL 8A	Undulator 6.8	100 to 2,000 eV	$50 \times 50 \mu\text{m}^2$ $150 \times 200 \text{ nm}^2$	APXPS, SPEM
ALBA, Spain, BL24	Undulator	100 to 2,000 eV	$20 \times 100 \mu\text{m}^2$ $3.2 \times 36 \mu\text{m}^2$	NAPP(APXPS), PEEM
Soleil, France, TEMPO	HU80, HU44	40 to 1,500 eV	-	NAP-XAS, XMCD
Max IV, Sweden, HIPPIE	EPU53	260 to 2,200 eV	$25 \times 60 \mu\text{m}^2$	APXPS, APXAS
SSRF, China, BL02B	Bending Magnet	40 to 2,000 eV	$\leq 7.5 \mu\text{m}^2$	APXPS
Diamond, England, B07	U56	230 to 800 eV	$40 \times 20 \mu\text{m}^2$	ARPES, NEXAFS
	U27	2.1 to 18 keV	$40 \times 20 \mu\text{m}^2$	HAXPES
NSLSII, USA, BL71D	EPU60	100 to 2,200 eV (PGM)	$40 \times 40 \mu\text{m}^2$	HAXPES, XAS
	EPU48	1,500 to 7,500 eV (DCM)		
4GSR, Korea	EPU78	100 to 3,000 eV (PGM)	$36 \times 14 \mu\text{m}^2$	XPS/XAS Tender AP XPS/XAS
	IVU24	2,000 to 5,000 eV (DCM)	$6 \times 12 \mu\text{m}^2$	

This energy range is particularly suitable for various catalytic studies aimed at addressing critical issues related to energy production and climate change. Moreover, it allows access to the absorption edges (K, L, M-edges) and core-electron binding energies of key elements found in semiconductors and life sciences, such as silicon (Si), phosphorus (P), sulfur (S), chlorine (Cl), calcium (Ca), yttrium (Y), zirconium (Zr), niobium (Nb), and molybdenum (Mo), as

illustrated in <Figure 3.2.3.3>. This capability significantly enhances the characterization of diverse materials, thereby contributing to advancements in multiple scientific disciplines.



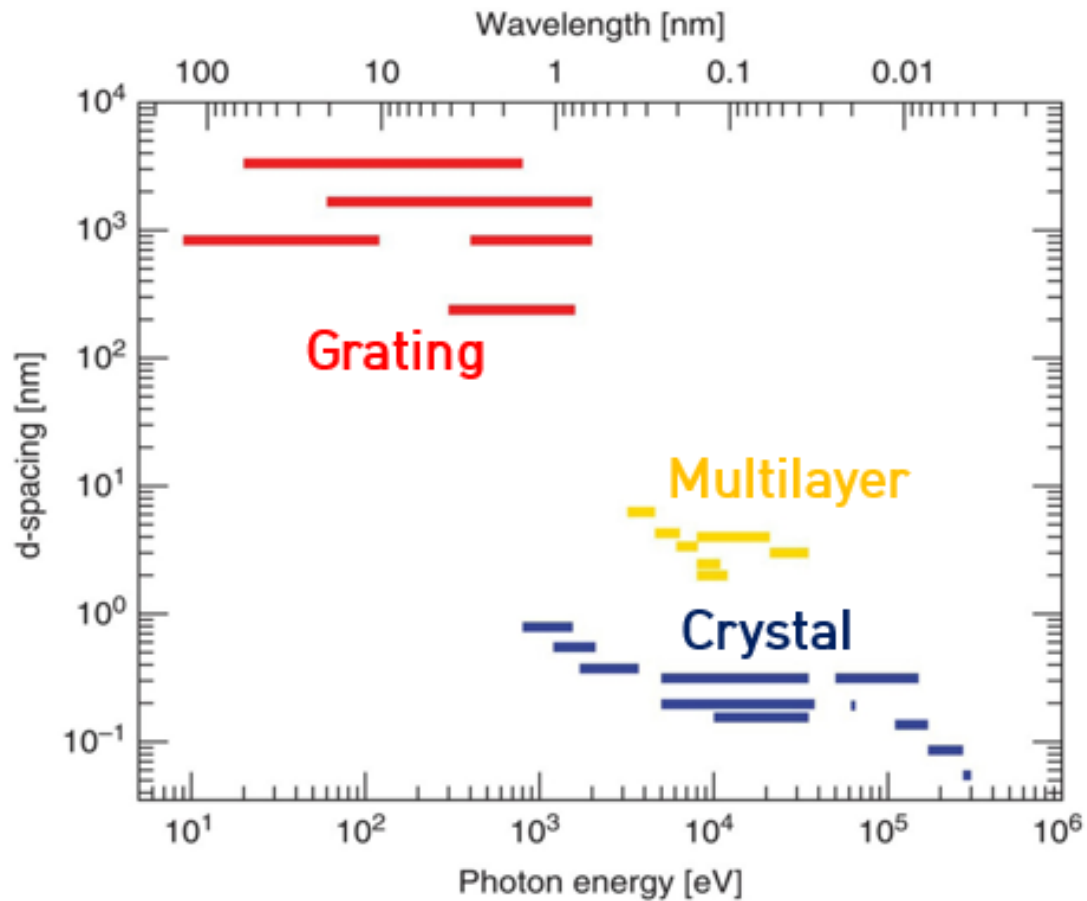
<Figure 3.2.3.3> Relation between electron binding energies, atomic number Z and electronic transition.

(3) Utilization of the Beamline

The photon energy range to be implemented at the Soft X-ray NanoProbe beamline will span from 0.1 to 5 keV. Consequently, it is advantageous to conceptualize this beamline as consisting of two distinct sections dedicated to soft X-rays and tender X-rays. As illustrated in <Figure 3.2.3.3>, the beamline will incorporate two types of monochromators tailored to the respective energy ranges: a grating monochromator for energies ranging from 0.1 to 3 keV, and either a Double Crystal Monochromator (DCM) or a Double Multilayer Monochromator (DMM) for energies from 2 to 5 keV.

Additionally, the beamline will include two types of insertion devices: the EPU78 for soft X-rays and the IVU24 for tender X-rays. Both undulators will be installed in canted array and are designed to achieve a photon flux ranging from 10^{13} to 10^{15} photons in the respective soft and tender X-ray regions. Consequently, the beamline will be configured with two independent

branch beamlines: Branch 1, designated Tender-AP XPS/XAS, will operate within the energy range of 2 to 5 keV, while Branch 2, termed High-ThroughPut XPS/XAS, will utilize the energy range of 0.1 to 3 keV, functioning in parallel with Branch 2.



<Figure 3.2.3.4> Monochromator based on light energy.

B. Photon source (EPU78 and IVU24)

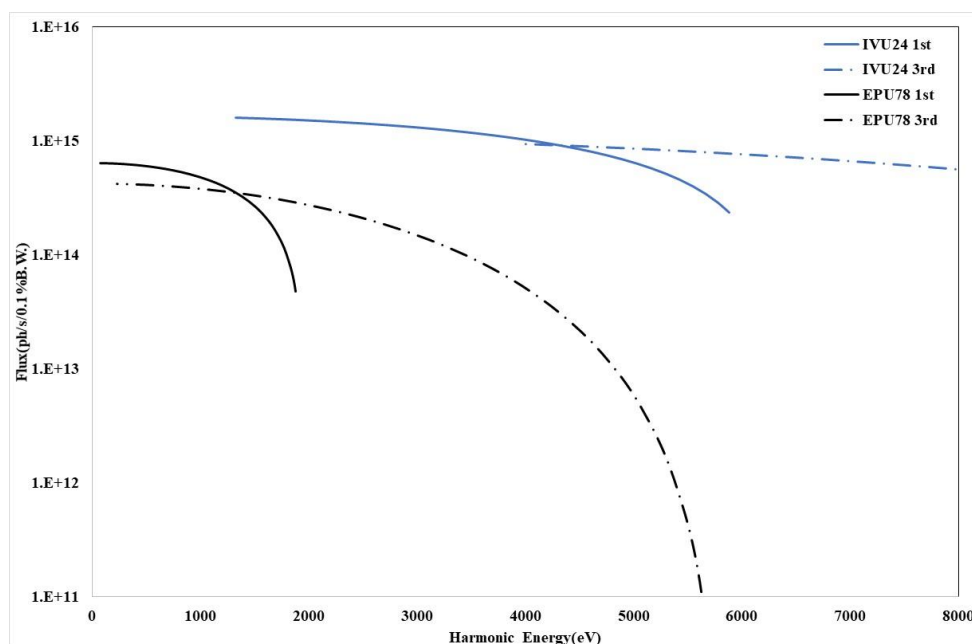
ID26 Soft X-ray NanoProbe beamline is specifically introduced canted array undulator system to meet the wide range of photon energy. This geometry accepts both current and future demands in industrial and applied research.

The beamline integrates two complementary undulator types: an Elliptically Polarized Undulator (EPU78) optimized for the soft X-ray regime, and an In-Vacuum Undulator (IVU24) optimized for the tender X-ray regime. The canted configuration enables efficient and continuous coverage across the full soft-to-tender X-ray energy window (100–5,000 eV), as summarized in <Table 3.2.3.3> and <Figure 3.2.3.5>.

The EPU78 provides polarization control and high brilliance in the soft X-ray region, while the IVU24 delivers strong flux and harmonic suppression in the tender X-ray regime; together, they are optimized to support both polarization-sensitive studies and high-throughput, depth-resolved spectroscopy. This dual-undulator design reflects a strategic emphasis on experimental versatility, industrial relevance, and long-term operational flexibility of the facility.

<Table 3.2.3.3 > Parameters of insertion device

Undulator	Period (mm)	Length (m)	Max Power	Min. Gap (mm)
IVU	24	1.5	8.7 kW	5
EPU	78	2.0	6.6 kW	15



<Figure 3.2.3.5> Photon flux for IVU24 and EPU78 in first and third harmonics

○ Dual Undulator System: Canted Array

Given the critical need to accommodate a wide range of sample types and experimental requirements particularly those relevant to large-scale industrial applications the ID26 Soft X-ray NanoProbe beamline adopts a dual-undulator configuration. The beams from the two undulators, EPU78 and IVU24, respectively, separated 1 mrad canting angle.

(1) IVU24 Undulator: Extending Performance to Tender X-rays

IVU24 (In-Vacuum Undulator) is optimized to efficiently cover the tender X-ray energy range of 2,000 to 5,000 eV, making it particularly suitable for depth-resolved electronic and chemical analysis of multilayer devices and complex material systems. With magnetic period of 24 mm, a total device length of 1.5 m, and a variable gap range of 5 to 15 mm, the IVU24 delivers a peak magnetic field of up to 1.23 T at the minimum gap. <Table 3.2.3.4> summarize the key parameters and schematic design of the IVU24 undulator.

<Table 3.2.3.4> IVU24 Undulator Specification

	IVU24
No. of magnet periods (N)	60
Period length [mm]	24
B_0 @ 5 mm gap for IVU24	1.22 T
K Value @ 5 mm gap for IVU24)	2.733
Gap	5 to 18 mm
Beam size (FWHM at the sample position @hv=4 keV)	H 6 μm × V 12 μm
E 1st	1,336.4 eV
Energy range	2,000 to 5,000 eV
Beam flux (ph/s/0.1%B.W.)	1.5×10^{15} at 5 mm gap
Total Power (kW)	8.7 at 5 mm gap

(2) Branch 2 : EPU78 Undulator

Positioned in a canted array undulator configuration relative to the IVU24, the EPU78 (Elliptically Polarized Undulator) serves as the primary photon source for the soft X-ray energy range of 90 to 3,000 eV. It is engineered to provide both polarization control and wide energy tunability, essential for diverse soft X-ray applications. With a magnetic period of 78 mm, a total device length of 2 m, and a variable gap range of 15 to 100 mm, the EPU78 generates a peak magnetic field of 0.954 T at a 15 mm gap. It delivers a focused photon beam size of $36 \times 14 \mu\text{m}^2$ (FWHM) at the Exit slit(ES) position, enabling stable, high-flux photon delivery suitable for wide-area mapping, fast acquisition, and multi-mode experimental workflows. These capabilities make it particularly advantageous for industrial sample screening, combinatorial material discovery, and high-throughput studies.

<Table 3.2.3.5> summarize the key parameters and schematic design of the EPU78 undulator.

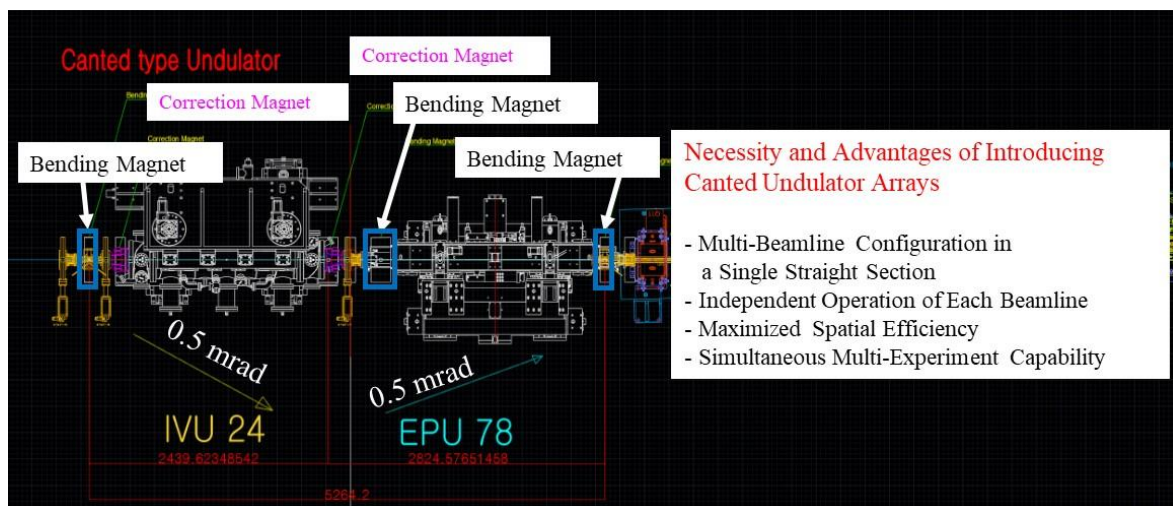
<Table 3.2.3.5> EPU78 Undulator Specification

	EPU78
No. of magnet periods (N)	23
Period length [mm]	78
B_0 @ 15 mm gap EPU78	0.954 T (V), 0.776 T (H), 0.602 T (Circular)
K Value at 15 mm gap @ 15 mm gap-EPU78	6.95 (V), 5.65 (H), 4.39 (Circular)
Gap	15 to 100 mm
Beam size (FWHM at the sample position @hv=400eV)	$36 \mu\text{m} \times 14 \mu\text{m}$ (V)
E 1st	77.45 eV (V), 96.31 eV (H), 114.73 eV (Circular)
Energy range	90 to 3,200 eV
Beam flux (ph/s/0.1%B.W.)	6.3×10^{14} at 15mm gap (V)
Total Power (kW)	6.6 at 15 mm gap (V)

(3) Canted array and Operational Flexibility

The ID26 Soft X-ray NanoProbe beamline adopts a canted array undulator configuration, where two insertion devices IVU24 and EPU78 are installed at a small horizontal angular offset (± 0.5 mrad) within a single straight section of the storage ring <Figure 3.2.3.6>. This spatial separation enables the simultaneous generation of two independently directed X-ray beams, each feeding a dedicated beamline branch optimized for distinct experimental goals.

As illustrated, bending magnets and correction magnets are symmetrically arranged on either side of the undulators to maintain beam stability and trajectory control. The physical layout minimizes mutual interference, allowing independent operation of each branch without the need for complex optical switching. This geometry supports a multi-beamline configuration within limited space, maximizes spatial efficiency, and enables true simultaneous multi-experiment capability.



<Figure 3.2.3.6> Schematic layout of the canted array undulator for Soft X-ray NanoProbe beamline.

C. Beamline Requirements for the Front-End

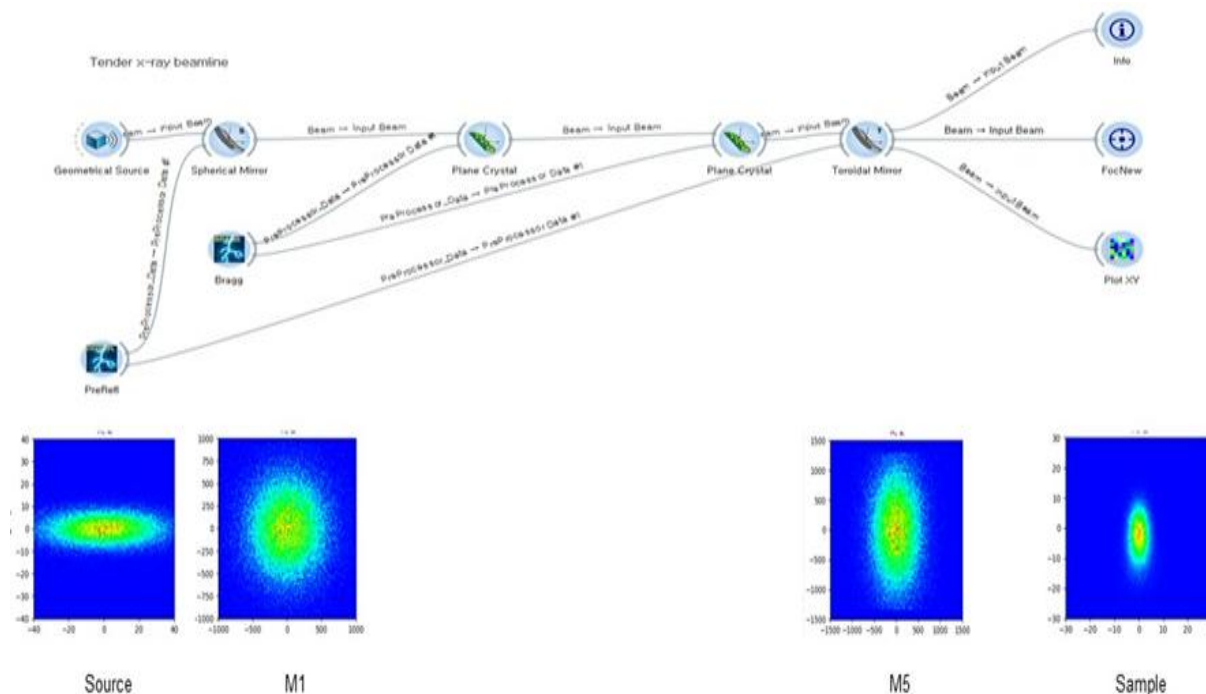
The soft X-ray beamline Front-End should be accepting the photon originated from the canted array undulators, IVU24 and EPU7. Further details will be provided in the section 4.2 ‘Vacuum components of Front-End’.

(1) Branch 1, Tender AP XPS/XAS

○ Optical system

As shown in the ray-tracing in <Figure 3.2.3.7>, the configuration of this Branch 1 beamline is consisted of a Vertical Collimating Mirror (VCM), a Double Crystal Monochromator (DCM), a Toroidal Focusing Mirror (TFM), and a Slit. The VCM utilizes a carbon (C) coating to increase the reflectivity of X-rays, and the layer is 50 nm thick. The VCM is located at a distance of 31 m from the light source and collimates the vertical divergence.

DCM with Si (111) crystal is used to cover the photon energy from 2 to 5 keV, and finally TFM is used to focus the beam at the sample location. The beam size at the sample location is $6 \times 12 \mu\text{m}^2$. The surface of the TFM is also coated with C like the VCM. <Table 3.2.3.6>



<Figure 3.2.3.7> Optical layout of the Tender branch in OASYS, illustrating the sequential optical components from the source to the sample for the AP-XPS/XAS configuration.

<Table 3.2.3.6> List of optical components for Tender AP XPS/XAS, Branch 1 beamline

	M1(VCM) C 50 nm	DCM (Si(111))	M5(TFM) C 50 nm
Distance (m)	31	49	55
Incident Angle (°)	0.3	23.3356° to 82.0087°	0.3
Shape	Cylindrical	Plane	Toroidal
Substrate	Si	Si	Si
Beam Size (mm×mm)	H 0.72×V 0.75 (FWHM)	H 1.23 ×V 0.73 (FWHM)	H 0.73 ×V 1.32 (FWHM)
Foot Print (mm×mm)	W 0.7×L 144(FWHM)		W 0.7×L 251 (FWHM)
Mirror size (mm×mm)	W 50×L 500	1 st : 40×30×20 2 nd : 170×30×20	W 50×L 500
Focus distance (mm)	∞		15,000
Radius of Curvature (tangential/sagittal) (mm)	∞ / 330	∞ / ∞	4,501,400 / 156.51
Roughness σ (nm)	0.3 rms	0. rms	0.3 rms
Slope error (tangential/sagittal) (μrad)	0.5 rms / 5 rms	1 rms / 10 rms	0.5 rms / 5 rms

○ M1, VCM (Vertical Collimating Mirror)

The VCM serves to increase the energy resolution by collimating the vertical divergence of the beam before it reaches the DCM. It also reduces the thermal load on the DCM crystals and employs water cooling. The mirror is coated with 50 nm of C for high reflectivity at a grazing incidence angle of 0.3°.

For vertical collimation, a cylindrical mirror with curvature only in the sagittal direction is used. The required radius of curvature is determined by the Coddington equations: (Equation 3.2.3.1)

$$\frac{1}{p} + \frac{1}{q} = \frac{2}{R_t \sin \theta_i}, (\text{Tangential}) \quad \frac{1}{p} + \frac{1}{q} = \frac{2 \sin \theta_i}{R_s} (\text{Sagittal}) \quad (\text{Eq. 3.2.3.4})$$

Here, p is the distance from the source to the mirror, q is the distance from the mirror to the focal point, θ_i is the grazing incidence angle, R_t is the tangential radius, and R_s is the sagittal radius.

For vertical collimation, the source is at $p=31$ m and the beam is collimated ($q=\infty$). Since the mirror is flat in the tangential direction ($R_t=\infty$), we only calculate the sagittal radius R_s :

$$R_s = 2p \sin \theta_i = 2 \cdot (31,000 \text{ mm}) \cdot \sin(0.3^\circ) \approx 324.6 \text{ mm}$$

This calculated value is Similar to the design target of **330 mm(±1%)**.

At the mirror position, the beam size is 0.72 mm (H) × 0.75 mm (V) FWHM, and the footprint on the mirror surface is 0.7 mm (width) × 144 mm (length). The clear aperture of the mirror (50 mm × 500 mm) provides sufficient acceptance. The surface roughness is specified as 0.3 nm RMS, with slope error tolerances of 0.5 μ rad (tangential) and 5 μ rad (sagittal).

At the mirror position, the beam size is 0.72 mm (H) × 0.75 mm (V) FWHM, and the footprint on the mirror surface is 0.7 mm (width) × 144 mm (length). The clear aperture of the mirror is 50 mm × 500 mm, providing sufficient acceptance for the beam footprint at an incidence angle of 0.3°. **(Rethink mirror size)**

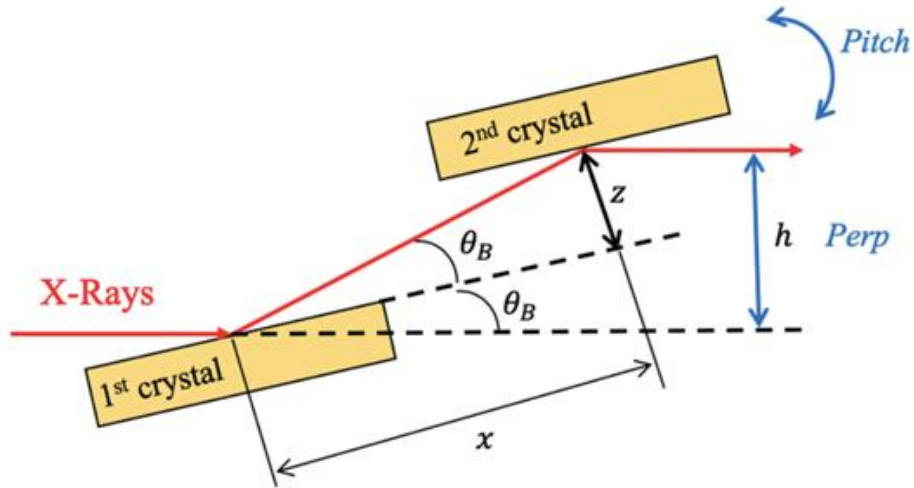
The surface roughness is specified as 0.3 nm RMS to suppress scattering and maintain wavefront quality. Slope error tolerances are 0.5 μ rad in the tangential direction and 5 μ rad in the sagittal direction, ensuring precise beam collimation and stable delivery to the DCM.

○ Monochromator, Double Crystal Monochromator (DCM)

The Double Crystal Monochromator (DCM) is designed to select the desired photon energy by varying the Bragg angle of two Si (111) crystals arranged in a fixed-exit geometry. The first crystal absorbs the primary heat load, and to minimize thermal deformation, liquid nitrogen (LN₂) cooling will be applied. The Bragg angle (θ_B) can be calculated from Bragg's law:

$$n\lambda = 2d\sin\theta_B$$

where n is the diffraction order, λ is the photon wavelength, and d is the lattice spacing of Si (111), $d=3.1356 \text{ \AA}$. For the target photon energy range of 2 to 5 keV, θ_B varies from 23.3356° to 82.0087° . This geometry ensures a beam offset of 25 mm for the Si crystal configuration, enabling smooth transition between modes, enabling smooth transition between modes.

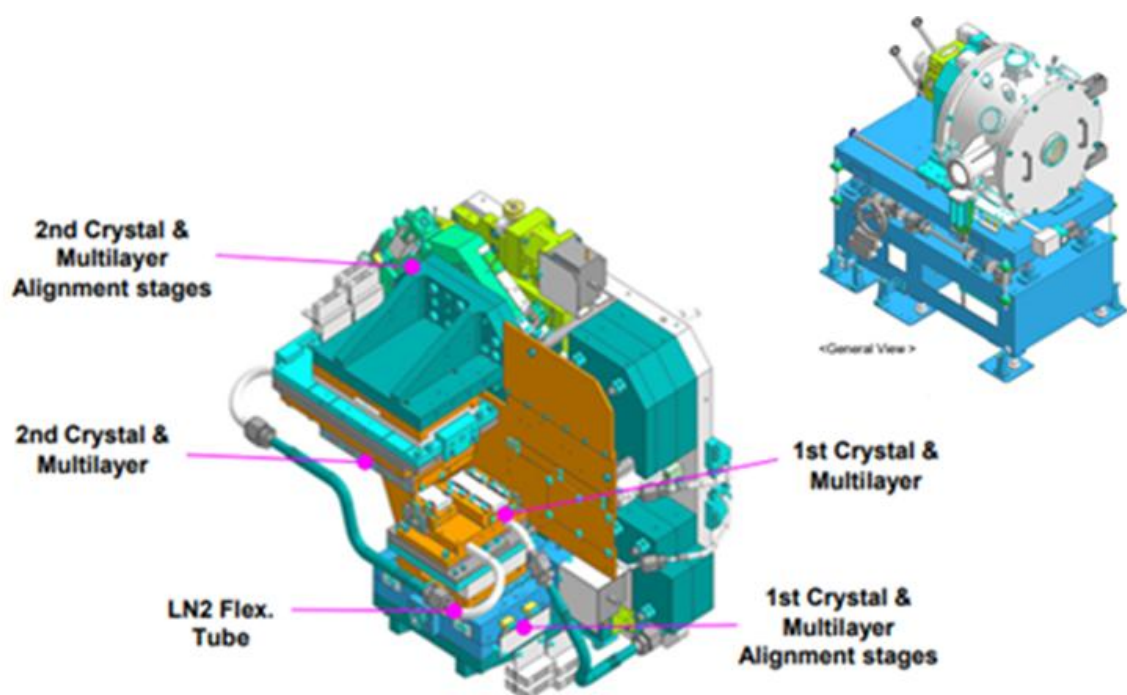


<Figure 3.2.3.8> Schematic Diagram of DCM. Crystal = Si (111).

As shown in <Figure 3.2.3.8> and <Figure 3.2.3.9>, the DCM assembly consists of two crystals mounted on high-precision alignment stages, with independent pitch, roll, and translation controls. The first crystal is directly connected to an LN₂ cooling loop, while the second crystal maintains parallelism to preserve the fixed exit height during energy scanning.

The specification for the DCM is summarized in <Table 3.2.3.7>, which is based on the expected parameters of the KOHU PHV-30 model currently used in 1C beamlines(PLS-II). A monochromator with equivalent or higher performance will be procured for the Tender branch. The design parameters include a Bragg angle range of 23 to 82° for the Si crystal configuration, crystal parallelism within ± 2 arcsec, vacuum pressure below 1×10^{-7} mbar, and a main frame height of 1,400 mm. The crystal dimensions are $40 \times 30 \times 10 \text{ mm}^3$ for Si (111) and $170 \times 30 \times 2.8 \text{ mm}^3$ for the multilayer coating, with a cooling capacity of 80 to 120 W at LN₂ temperature.

Furthermore, a dedicated dummy slot is designed to enable the future implementation of various crystal types.



<Figure 3.2.3.9> 3D model of the double crystal monochromator.

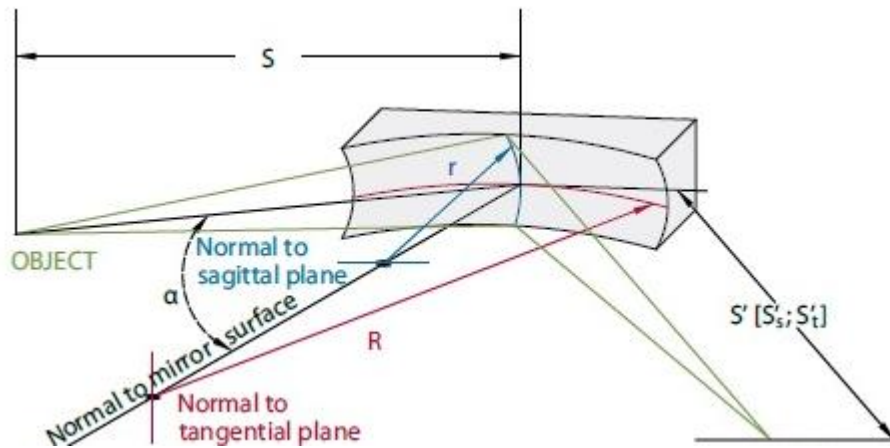
<Table 3.2.3.7> Double crystal monochromator Specification

A-Model	Specification
Main θ height	1,400 mm
Beam Offset	Si: 25 mm upward
Bragg Angle Range	Si: 23.3 to 82 deg
Main θ Rotation Center	Center of the 1st Crystal
Crystal Parallelism	10 arcsec (for full stroke), 2 arcsec (at any 3 degree)
Vacuum Pressure	$4.00 \times 10e^{-5}$ Pa
Crystal Size: Si(111), 1 st and 2 nd	40×30×20, 170×30×20 (L×W×T: mm)
Dummy for the Future	40×30×20, 170×30×20 (L×W×T: mm)
Dimension	1,100×1,550×1,850 (L×W×H: mm)

○ M5 Toroidal Focusing Mirror (TFM)

The TFM is a toroidal mirror located at 55 m from the light source, designed to focus the beam reflected from the DCM onto the sample position in both vertical and horizontal directions. The mirror, with its surface facing the experimental hall, deflects the beam with an incidence angle of 0.3° , and the surface is coated with C to provide high reflectivity in the tender X-ray energy range (2 to 5 keV). The substrate is single-crystal Si with dimensions of $50 \text{ mm} \times 500 \text{ mm}$, a surface roughness of 0.3 nm rms, and slope errors of $0.5 \mu\text{rad}$ (tangential) and $5 \mu\text{rad}$ (sagittal).

The focusing properties of a toroidal mirror are described by the Coddington equations, which relate the object distance, image distance, and radii of curvature for the tangential and sagittal planes. Using the variables shown in the figure, the equations are:<Figure 3.2.3.10>



<Figure 3.2.3.10> Schematic diagram of the focusing geometry of a toroidal (or curved) mirror.

The equation for the tangential plane, which focuses the beam horizontally in this geometry, is:

$$1/S + 1/S'_t = 2/R \cos \alpha \quad (\text{Eq. 3.2.3.2})$$

- S : Object distance (from the source to the mirror).
- S'_t : Tangential image distance (from the mirror to the horizontal focal point).
- R : Tangential radius of curvature (the major radius of the torus).
- α : Grazing incidence angle.

The equation for the sagittal plane, which focuses the beam vertically, is:

$$1/S + 1/St' = 2\cos\alpha/r \quad (\text{Eq. 3.2.3.3})$$

- S: Object distance (from the source to the mirror).
- S'_s: Sagittal image distance (from the mirror to the vertical focal point).
- r: Sagittal radius of curvature (the minor radius of the torus).
- α : Grazing incidence angle.

At the mirror position, the beam size is 0.73 mm $\times$ 1.32 mm (FWHM), and the footprint is 0.7 mm $\times$ 251 mm (FWHM). Ray-tracing calculations indicate that the focused beam size at the sample position (70 m from the source) is approximately 6 μm $\times$ 12 μm (FWHM).

Finally, the positions, specifications, and optical functions of all components in the Tender-XPS/XAS branch, including the TFM, are summarized in <Table 3.2.3.8> to guide alignment, manufacturing tolerances, and performance verification.

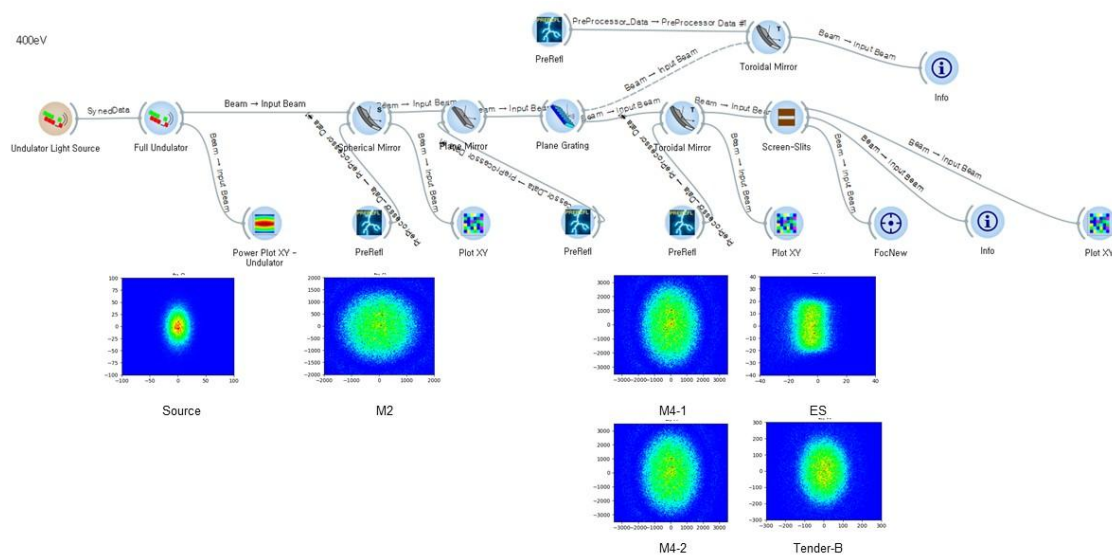
<Table 3.2.3.8> Soft X-ray Nanoprobe Beamline (Tender AP-XPS/XAS) Component Table

(m)	Component	Description
26	Movable mask	4-way slit, UHV, Water cooling
31	M1 (V-Collimating Mirror)	
34	White beam slit	4-way slit, UHV, Water cooling
35	White beam Screen Monitor	Diamond window Fluorescent metal screen, current signal output
38	M3 and PGM	Pass through
39	H/V Screen monitor	Fluorescent metal screen, current signal output
45	Attenuator	JJ X-ray
46	Pink beam monitor	-
47	Pink beam slit	JJ X-ray
48	Photon shutter	Water cooling
49	DCM	Si (111), fixed exit
51	H/V Screen monitor	Fluorescent metal screen, current signal output
53	Mono beam slit	4-way slit, UHV
54	Mono beam screen	YAG window Fluorescent metal screen, current signal output
55	M5 (H/V Focusing Mirror)	
57	H/V Screen monitor	Fluorescent metal screen, current signal output
68.5	Mono beam screen	YAG window Fluorescent metal screen, current signal output
69	Exit slit	4-way slit, UHV
69.5	Photon Shutter	
70	Sample Position	

(2) Branch 2, High-Throughput XPS/XAS

○ Optical system

As shown in the ray-tracing in <Figure 3.2.3.11>, the configuration of this Branch 2 beamline is very simple. The main optics consist of a Vertical Collimating Mirror (VCM), a Plane Grating Monochromator (PGM), a Toroidal Focusing Mirror (TFM), and a Slit.



<Figure 3.2.3.11> Optical layout schematic of the Soft branch in OASYS, showing sequential optical components from the source to the sample for the high-throughput XPS/XAS configuration.

<Table 3.2.3.9> List of optical components for the Soft X-ray XPS/XAS Branch 2 beamline

	M2(VCM) Au 50 nm	M4-1(TFM) Au 50 nm	M4-2(TFM) Au 50 nm	Exit Slit
Distance (m)	31	40	40	51.5
Incident Angle (°)	0.6	0.1	2.5	
Shape	Cylindrical	Toroidal	Toroidal	
Substrate	Glidcop	Si	Si	
Beam Size (mm×mm)	H 0.76×V 0.72(FWHM)	H 0.766 ×V 0.879 (FWHM)	H 0.1 ×V 0.072 (FWHM)	H 0.036×V 0.014 (FWHM)
Foot Print (mm×mm)	W 0.7×L 68 (FWHM)	W 0.7×L 21 (FWHM)	W 1.5×L 21 (FWHM)	W 1×L 52 (FWHM)
Mirror size (mm×mm)	W 50×L 500	W 50×L 300	W 50×L 300	
Focus distance (mm)	∞	15,000	30,000	
Radius of Curvature (tangential/sagittal) (mm)	∞ / 653.8	1,023,588.2 / 401.2	755,195.7 / 2442.6	
Roughness σ (nm)	0.3 rms	0.3 rms	0.3 rms	
Slope error (tangential/sagittal) (μrad)	0.5 rms / 5 rms	0.5 rms / 5 rms	0.5 rms / 5 rms	

The VCM utilizes a Gold (Au) coating to increase the reflectivity of X-rays, and the layer is 50 nm thick. The VCM is located at a distance of 31 m from the light source and collimates the vertical divergence.

Grating using Si is used to cover the light energy from 0.1 to 3 keV, and finally TFM is used to focus the beam at the Exit Slit location. The beam size at the Exit Slit location is $36 \times 14 \mu\text{m}^2$. The surface of the TFM is also coated with Au like the VCM.<Table 3.2.3.9>

○ M2, VCM (Vertical Collimating Mirror)

The M2 mirror in the Soft Branch serves to increase the energy resolution by controlling the vertical divergence angle of the beam incident on the plane grating monochromator (PGM). It also ensures an optimal beam size at the exit slit and minimizes aberrations in the downstream optics. The substrate material is Glidcop, coated with 50 nm of Au for high reflectivity in the

soft X-ray energy range (100 to 3,000 eV), with a grazing incidence angle of 0.6°. For vertical collimation, a cylindrical mirror with curvature in the sagittal direction is used.

The radius of curvature for the mirror is calculated using the Coddington equations, previously defined in (Equation 3.2.3.4):

$$\frac{1}{p} + \frac{1}{q} = \frac{2}{R_t \sin \theta_i} \text{ (Tangential)} \quad \frac{1}{p} + \frac{1}{q} = \frac{2 \sin \theta_i}{R_s} \text{ (Sagittal)} \quad (\text{Eq. 3.2.3.4})$$

Here, p is the distance from the source to the mirror, q is the distance from the mirror to the focal point, and θ_i is the grazing incidence angle.

For this VCM, the source distance is $p=31$ m and the beam is being collimated, so the focal distance is $q=\infty$. With an incidence angle of $\theta_i=0.6^\circ$ and a flat tangential radius ($R_t=\infty$), the required sagittal radius (R_s) is:

$$R_s = 2p \sin \theta_i = 2 \cdot (31000 \text{ mm}) \cdot \sin(0.6^\circ) \approx 649.3 \text{ mm}$$

This calculated value is consistent with the design specification of **653.8 mm ($\pm 1\%$)**.

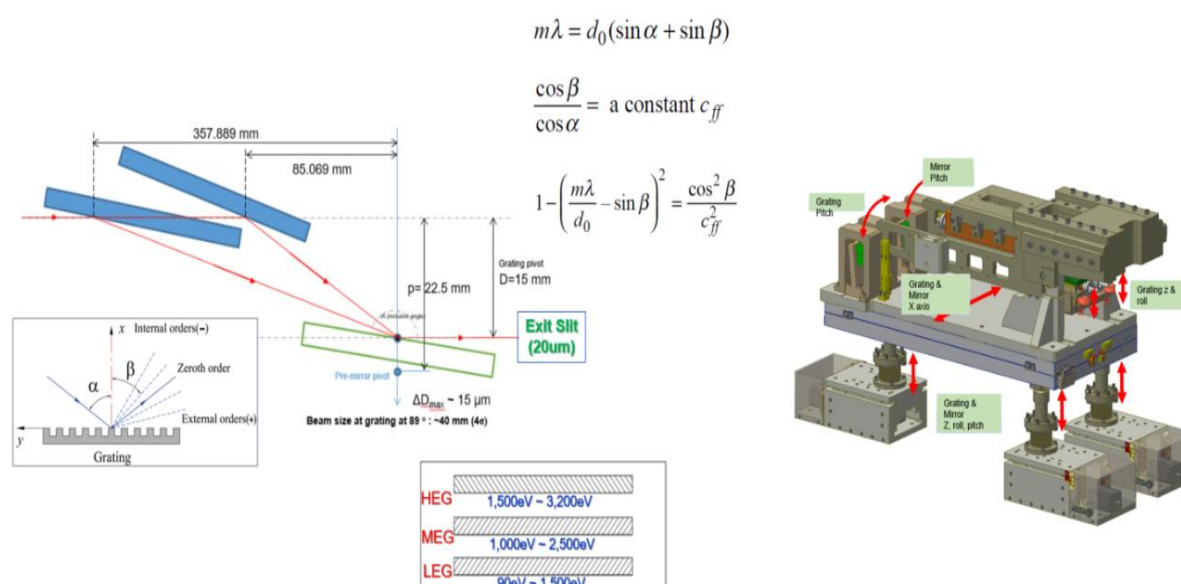
At the mirror position, the beam size is 0.766 mm (H) $\times$ 0.879 mm (V) FWHM, and the beam footprint on the mirror surface is 0.7 mm (width) $\times$ 68 mm (length). The clear aperture of the mirror is 50 mm $\times$ 500 mm, which is sufficient to accept the beam footprint. The surface roughness is specified at 0.3 nm RMS to suppress scattering, and slope error tolerances are 0.5 μrad (tangential) and 5 μrad (sagittal). Alignment tolerances are within 100 μm in translation and 1.2 μrad (pitch) / 3.0 μrad (yaw) in rotation, ensuring precise beam delivery.

- **Monochromator System**

The monochromatic light device is designed as a variable included angle plane grating mirror type. It is driven by the principle that there is a pre-mirror in front of the grating, and the photon beam is incident on the grating at the desired angle by moving the pre-mirror to the horizontal plane and changing the angle at the same time. Therefore, a small change in the angle of the pre-mirror has a large impact on the energy resolution and calibration, so it must have a precision of at least $0.5 \mu\text{m}$ in the vertical direction.

- **M3 Pre-mirror (Plane Mirror)**

The monochromator section of the soft X-ray branch consists of the M3 pre-mirror and a plane grating assembly arranged in a variable included angle configuration, as illustrated in <Figure 3.2.3.12>. The M3 pre-mirror, positioned upstream of the grating, is a plane silicon substrate coated with 60 nm Au to maximize reflectivity in the 90 to 3,200 eV range. It directs and conditions the beam before incidence on the grating, with horizontal translation and pitch adjustment enabling precise control of the included angle. The detailed mechanical and optical specifications of the M3 mirror, including substrate dimensions, coating, cooling method, slope error, and allowable microroughness, are provided in <Table 3.2.3.10>.



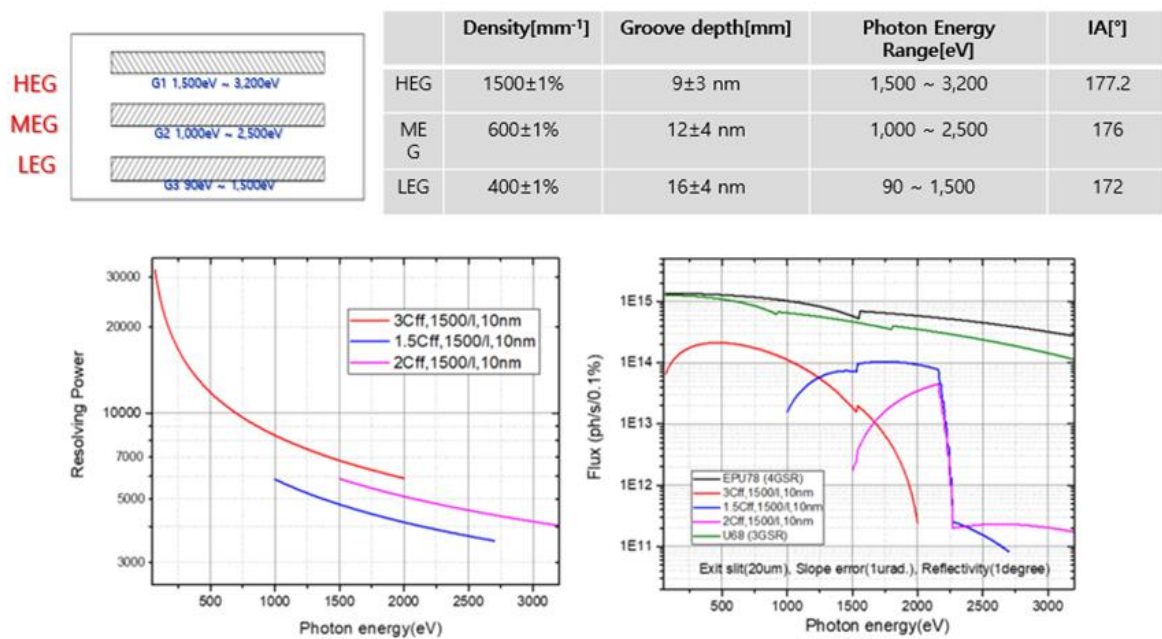
<Figure 3.2.3.12> Monochromator Internal Schematic.

<Table 3.2.3.10> The detailed parameters for M3: Pre-mirror

Type	Plane
Function	Reflection
Tangential radius (meter)	Infinite
Bending resolution	NA
Position	Upward
Sagittal radius	Infinite
Incidence angel	Reference to the required energy
Substrate material	Single crystal silicon (thickness=75 mm)
Clear aperture (mm)	500 (length) , 80 (width)
Thickness (mm)	75
Surface roughness	< 5 Å RMS
Tangential slope error	< 1 μ rad RMS
Sagittal slope error	< 10 μ rad RMS
Coating material	Au
Coating thickness (Å)	Au (600 Å)
Power on Mirror	Reference to the Consideration for Power

○ Grating

Downstream of the M3, the plane grating assembly is installed ~7 m from M2 and covers 90 to 3,200 eV. As shown in <Figure 3.2.3.13>, the grating substrate carries three groove-density regions (G1 to G3) on a flat Si(100) plate; the corresponding groove densities are 400, 600, and 1,500 lines/mm and the groove depths are 16 ± 4 nm, 12 ± 4 nm, and 9 ± 3 nm, respectively. The principal physical specifications substrate, clear aperture ($\approx 200 \times 40$ mm), Au coating, slope error (≤ 0.5 μ rad RMS tangential; ≤ 1.0 μ rad RMS sagittal), and microroughness (≤ 0.5 nm RMS), comparative requirements for the pre-mirror (M3) and grating (clear apertures 500×80 mm and 200×40 mm, Au coatings, power/footprint, cooling, and allowable slope errors) are listed in <Table 3.2.3.11>. The grating mechanism tolerances for pitch/roll/translation e.g., pitch-scan motor resolution ≤ 0.02 μ rad, encoder resolution ≤ 0.03 μ rad, total precision ≤ 0.24 μ rad over 0.5 to 5°; y-axis stability ≤ 2.0 μ m with ≤ 0.05 μ m motor resolution are defined in <Table 3.2.3.12>, ensuring energy calibration stability and alignment reproducibility. Based on these references, we will fabricate/procure gratings with specifications closely matching the present design.



<Figure 3.2.3.13> Grating's groove depth, width and photon energy.

<Table 3.2.3.11> Specification for Grating

Model	Plane Grating ID26		
Material	Mono - silicon (100)		
Dimensions	200 x 52 x 20		
Optical surface	180 x 10 (3 areas)		
Surface figure	Flat		
Slope error	≤0.5 uras RMS tangential, ≤1.0 urad RMS sagittal		
Micro roughness	≤0.5nmRMS		
	HEG	MEG	LEG
Groove density [lines/mm]	1500	600	400
Groove depth [nm]	9	12	16
Photon Energy Range[eV]	1,500 to 3,200	1,000 to 2,500	90 to 1,500
IA[°]	177.2	176	172

<Table 3.2.3.12> Specification on Grating mechanism

Rotation or axis	Stability	Motor resolution	Encoder resolution	Precision	Range	Remark
Pitch scan axis	$\leq 1.0 \mu\text{rad}$ / 20 minits	$\leq 0.02 \mu\text{rad}$	$\leq 0.03 \mu\text{rad}$	$\leq 0.24 \mu\text{rad}$	0.5 to 5.0 deg.	
Pitch alignment axis	$\leq 2.0 \mu\text{rad}$ / 20 minits	$\leq 0.48 \mu\text{rad}$	$\leq 0.24 \mu\text{rad}$	$\leq 2.42 \mu\text{rad}$	$\geq \pm 1.5$ deg.	
Roll alignment axis	$\leq 4.0 \mu\text{rad}$ / 20 minits	$\leq 0.48 \mu\text{rad}$	$\leq 0.24 \mu\text{rad}$	$\leq 2.42 \mu\text{rad}$	$\geq \pm 1.5$ deg.	
y alignment axis	$\leq 2.0 \mu\text{m}$ / 30 minits	$\leq 0.05 \mu\text{m}$	$\leq 0.1 \mu\text{m}$	$\leq 1.0 \mu\text{m}$	$\geq \pm 9.0$ mm	
fine scan PZT axis		≤ 0.3 nm	≤ 0.6 nm	≤ 5.0 nm	$\geq 30.0 \mu\text{m}$	
x transverse position	$\leq 2.0 \mu\text{m}$ / 30 minits	$\leq 0.01 \mu\text{m}$	$\leq 0.05 \mu\text{m}$	$\leq 1.0 \mu\text{m}$	$\geq \pm 35.0$ mm	mirror and grating are applied common
Zeroth order blocking motions		$\leq 0.1 \mu\text{m}$	$\leq 1.0 \mu\text{m}$	$\leq 3.0 \mu\text{m}$	$\geq \pm 7.0$ mm	
Additional specification	1. While varying the pitch angle, the grating pitch axis must either remain stationary or it must vary monotonically and reproducibly, vertically and longitudinally. The variation in the position can be no longer than $5 \mu\text{m}/\mu\text{rad}$, and while at that angle the position must not vary by more than the required stability. 2. When in use, the grating must be positioned so that the grating pitch rotation axis lies on the plane of the grating optical surface to within $10 \mu\text{m}$. 3. When in use, the grating must be positioned so that the grooves are parallel to the grating pitch axis to within $500 \mu\text{rad}$.					

Rotation or axis	Stability	Motor resolution	Encoder resolution	Precision	Range	Remark
Pitch scan axis	$\leq 1.0 \mu\text{rad}$ / 20 minits	$\leq 0.02 \mu\text{rad}$	$\leq 0.03 \mu\text{rad}$	$\leq 0.24 \mu\text{rad}$	0.5 to 5.0 deg.	
Pitch alignment axis	$\leq 2.0 \mu\text{rad}$ / 20 minits	$\leq 0.48 \mu\text{rad}$	$\leq 0.24 \mu\text{rad}$	$\leq 2.42 \mu\text{rad}$	$\geq \pm 1.5$ deg.	
Roll alignment axis	$\leq 4.0 \mu\text{rad}$ / 20 minits	$\leq 0.48 \mu\text{rad}$	$\leq 0.24 \mu\text{rad}$	$\leq 2.42 \mu\text{rad}$	$\geq \pm 1.5$ deg.	
y alignment axis	$\leq 2.0 \mu\text{m}$ / 30 minits	$\leq 0.05 \mu\text{m}$	$\leq 0.1 \mu\text{m}$	$\leq 1.0 \mu\text{m}$	$\geq \pm 9.0$ mm	
Fine scan PZT axis		≤ 0.3 nm	≤ 0.6 nm	≤ 5.0 nm	$\geq 30.0 \mu\text{m}$	
x transverse position	$\leq 2.0 \mu\text{m}$ / 30 minits	$\leq 0.01 \mu\text{m}$	$\leq 0.05 \mu\text{m}$	$\leq 1.0 \mu\text{m}$	$\geq \pm 35.0$ mm	mirror and grating are applied common
Additional specification	Roll and yaw angles must not vary from the nominal values by more than the stability limit for all longitudinal positions of the premirror.					

Based on the performance targets and the specifications summarized in the above tables, the grating will be fabricated and procured in a configuration closely matching the present design parameter.

○ M4 Focusing mirror (Toroidal Mirror)

The M4 mirrors, which collect the beams from the monochromators into the exit slits, are located at 40 meters from the source point.

Since the light dispersed from the grating is diffuse, it is followed by a mirror that needs to focus the diffuse light. Since the angular spread of light from the grating is large, the footprint of the focusing mirror has a large value. In addition, since the ratio of the distance from the light source to the focusing mirror to the distance from the focusing mirror to the exit slit is

large, the aberration (coma) at the exit slit caused by the focusing mirror becomes very large, which greatly affects the energy resolution and throughput.

This mirror is a toroidal mirror, which is used to focus and deliver the light source to the exit slit in the vertical/horizontal direction (y-axis). The radius of curvature in the vertical direction is 44 cm and 31.38 cm ($\pm 1\%$), and the radius of curvature in the horizontal direction is 320 cm and 400 cm ($\pm 6\%$) for the M4-1 & M4-2 mirrors, respectively.

The angle of incidence of the light entering the mirrors is 2° for M3-1 and 1.5° for M3-2, considering the reflectivity. The coating material of the mirrors is Au.

The radius of curvature was obtained using (Equation 3.2.3.5) for a toroidal mirror.

$$\frac{1}{r} + \frac{1}{r'_t} = \frac{2}{\rho_t \cos \theta} \equiv \frac{1}{f_t}, \quad \frac{1}{r} + \frac{1}{r'_s} : \frac{2 \cos \theta}{p_s} \equiv \frac{1}{f_s} \quad (\text{Eq. 3.2.3.5})$$

Where r'_t , r'_s is the distance from the mirror to infinity and the entrance slit, respectively, and ρ_t , p_s is the radius of curvature in the tangential and sagittal directions, respectively. In this case, spherical aberrations can be neglected compared to the size of the light focus. The allowable slope error is $5.9 \mu\text{rad}$ in the tangential direction and $15 \mu\text{rad}$ in the sagittal direction, which becomes smaller at higher energies. To find the acceptable slope error, the value of $1/2$ sigma of the image size in the entrance slit or sample is used as a reference. With this definition of slope error, the total size of the image in the slit and sample has a value of 1.12 sigma.

The micro alignment must be accurate to within $1 \mu\text{m}$, a value of $1/10$ sigma in the vertical direction. In the longitudinal direction, this is less critical and requires a precision within $5 \mu\text{m}$. In the transverse direction, it should be within $20 \mu\text{m}$. Roll and yaw are relatively unimportant, but pitch is very important. Pitch should be accurate to within $0.25 \mu\text{rad}$.

Finally, the positions, specifications, and optical functions of all components in the Soft HT-XPS/XAS branch, including the TFM, are summarized in <Table 3.2.3.13> to guide alignment, manufacturing tolerances, and performance verification.

<Table 3.2.3.13> Major Component list for Branch 2 Soft X-ray XPS/XAS

(m)	Component	Description
26	Movable mask	4-way slit, UHV, Water cooling
31	M 2 (V-Colimating Mirror)	
34	White beam slit	4-way slit, UHV, Water cooling
35	White beam Screen Monitor	Diamond window Fluorescent metal screen, current signal output
38	M3 and PGM	
39	H/V Screen monitor	Fluorescent metal screen, current signal output
40	M 4-1, M4-2 (H/V Focusing Mirror)	
41	H/V Screen monitor	Fluorescent metal screen, current signal output
46	Wire-Flux & Current Monitor	W-Wire ??
49	Mono Beam Slit	4-way slit, UHV
49	Mono Beam Screen	YAG window Fluorescent metal screen, current signal output
51.5	Exit Slit	4-way slit, UHV
52	H/V Screen Monitor	Fluorescent metal screen, current signal output
53	Gas-cell	N ₂ , O ₂ , Ar, Kr, Xe
61	Mono beam screen	YAG window Fluorescent metal screen, current signal output
62	Photon Shutter	
63	Sample Position	

- Integrated Layout and Broad Energy Utilization

The ID26 Soft X-ray NanoProbe beamline adopts a dual-branch optical layout that integrates the tender and soft X-ray branches within a single shielding structure. To prevent potential beam path overlap and to enhance optical alignment stability between the two branches, the optical hutch up to the Double Crystal Monochromator (DCM) is shared. Specifically, the beamline utilizes a common optical path from the vertical collimating mirror (M1C) through to the DCM, after which the branches diverge. The tender branch delivers high-energy photons via a toroidal focusing mirror (M5), while the soft branch employs a plane grating monochromator (PGM) followed by a dual-mirror refocusing system (M4-1, M4-2) optimized for low-energy X-rays.

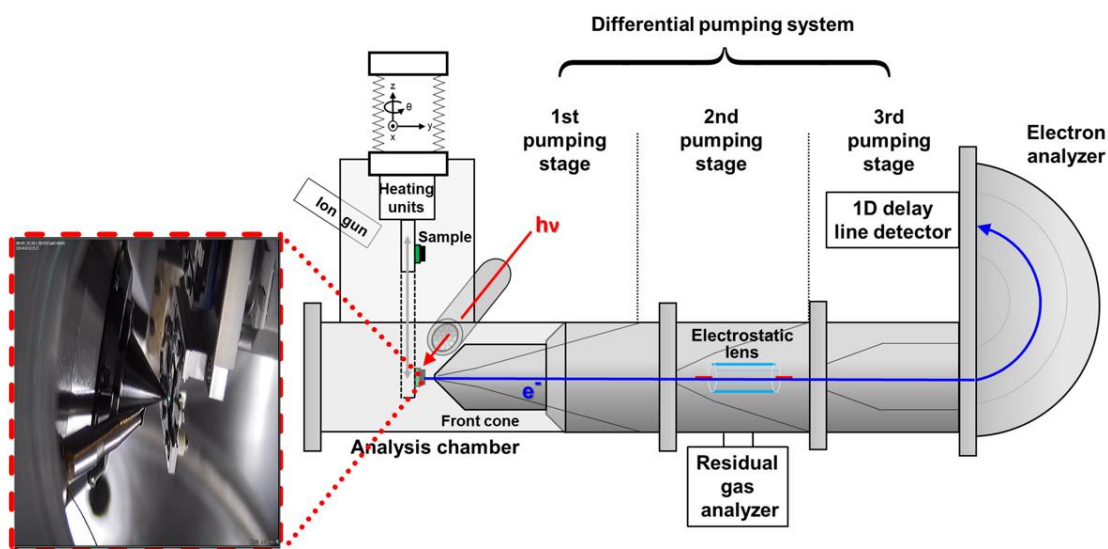
Notably, the M4-2 mirror is engineered to extend the operational range of the soft X-ray energies (0.1 to 3 keV) into the tender branch, allowing users to perform rapid and flexible measurements in the soft energy regime without switching beamlines. This integrated optical scheme minimizes interference between beam paths while supporting full-spectrum operation with high flexibility and precision.

D. End-Station Application

The end-station of the ID26 Soft X-ray NanoProbe beamline is designed as a dual-branch platform in which both branches are fundamentally based on X-ray Photoelectron Spectroscopy (XPS) and X-ray Absorption Spectroscopy (XAS).

<Figure 3.2.3.14> with Branch 1 dedicated to Tender AP-XPS/XAS experiments in the 2 to 5 keV range and Branch 2 optimized for Soft HT-XPS/XAS measurements in the 0.1 to 3 keV region, allowing the beamline to flexibly accommodate a wide variety of surface and interface-sensitive investigations under both ambient pressure and ultra-high vacuum conditions while maintaining high spectral resolution, spatial precision, and operational efficiency.

(1) Branch 1- Tender-APXPS/XAS Beamline



<Figure 3.2.3.14> Conceptual schematic of Ambient Pressure X-ray Photoelectron Spectroscopy (AP-XPS) using differential pumping.

The conceptual design of Ambient Pressure X-ray Photoelectron Spectroscopy (AP-XPS) is illustrated in the schematic shown <Figure 3.2.3.17>, where a conically focused X-ray beam enters a spectroscopy chamber maintained at pressures up to ~ 20 Torr. A differentially pumped electrostatic lens system collects photoelectrons emitted from the sample and transmits them to a hemispherical analyzer operating under ultra-high vacuum ($\sim 10^{-8}$ Torr). A small aperture situated only a few hundred micrometers from the sample surface enables efficient

photoelectron transmission while suppressing gas flow, and multiple differential pumping stages equipped with electrostatic lenses further reduce gas pressure and maintain energy resolution.

Building upon this original principle, the Branch 1 Tender AP-XPS/XAS Beamline is specifically designed to operate in the tender X-ray energy range of 2 to 5 keV, integrating both AP-XPS and X-ray Absorption Spectroscopy (XAS) capabilities within a single, high-performance experimental platform. The AP-XPS system allows real-time analysis of chemical states and electronic structures at near-ambient pressures, overcoming the limitations of conventional UHV-XPS by bridging the “pressure gap” between vacuum-based fundamental studies and practical operating environments. Through multiple stages of differential pumping and carefully designed aperture geometry, the analyzer remains under UHV conditions while the sample is exposed to controlled gas environments, enabling robust surface and interface characterization under realistic catalytic or electrochemical conditions.

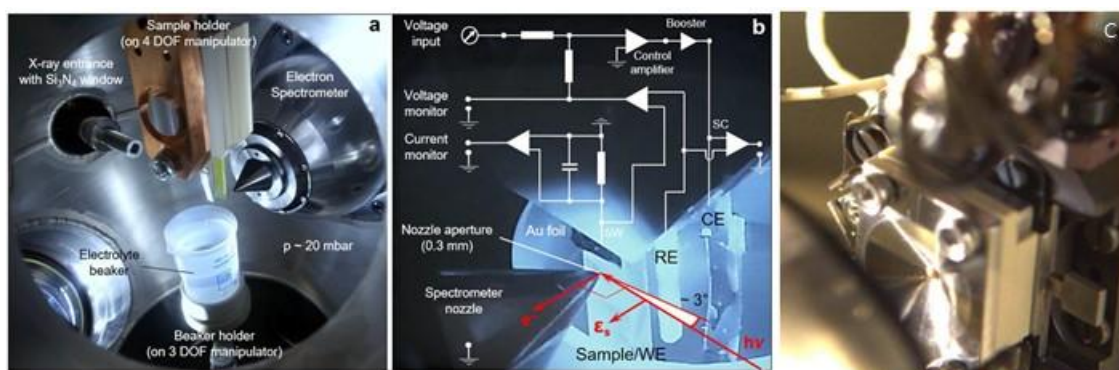
XAS, on the other hand, complements AP-XPS by probing the unoccupied electronic states of specific elements, revealing oxidation states, coordination geometry, and local bonding configurations. In the tender X-ray regime, the increased photoelectron kinetic energy translates to a significantly deeper probing depth on the order of 10 to 20 nm thus making it possible to investigate buried interfaces such as solid–electrolyte boundaries and multilayer architectures. Together, these two spectroscopic techniques offer powerful, element-specific insight into dynamic processes including surface redox reactions, adsorption/desorption behavior, and interface charge transfer under real-world conditions.

This beamline is also equipped with a high-pressure reaction chamber that supports temperature control and gas flow modulation, allowing for detailed operando studies of catalytic mechanisms, energy conversion materials, and electrochemical reactions such as the oxygen evolution reaction (OER). In electrochemical environments, the use of a three-electrode setup with electrolyte film stabilization techniques like “dip-and-pull” allows real-time tracking of potential-induced oxidation state changes at the electrode-electrolyte interface.

In this method, a working electrode (WE) is withdrawn from an electrolyte bath to form a stable, nanometer-scale liquid film on its surface. As shown in <Figure 3.2.3.15 (a)>, the end-station will integrate a multi-axis manipulator with a custom sample holder, an electrolyte beaker, and the electron spectrometer's entrance nozzle inside the analysis chamber.

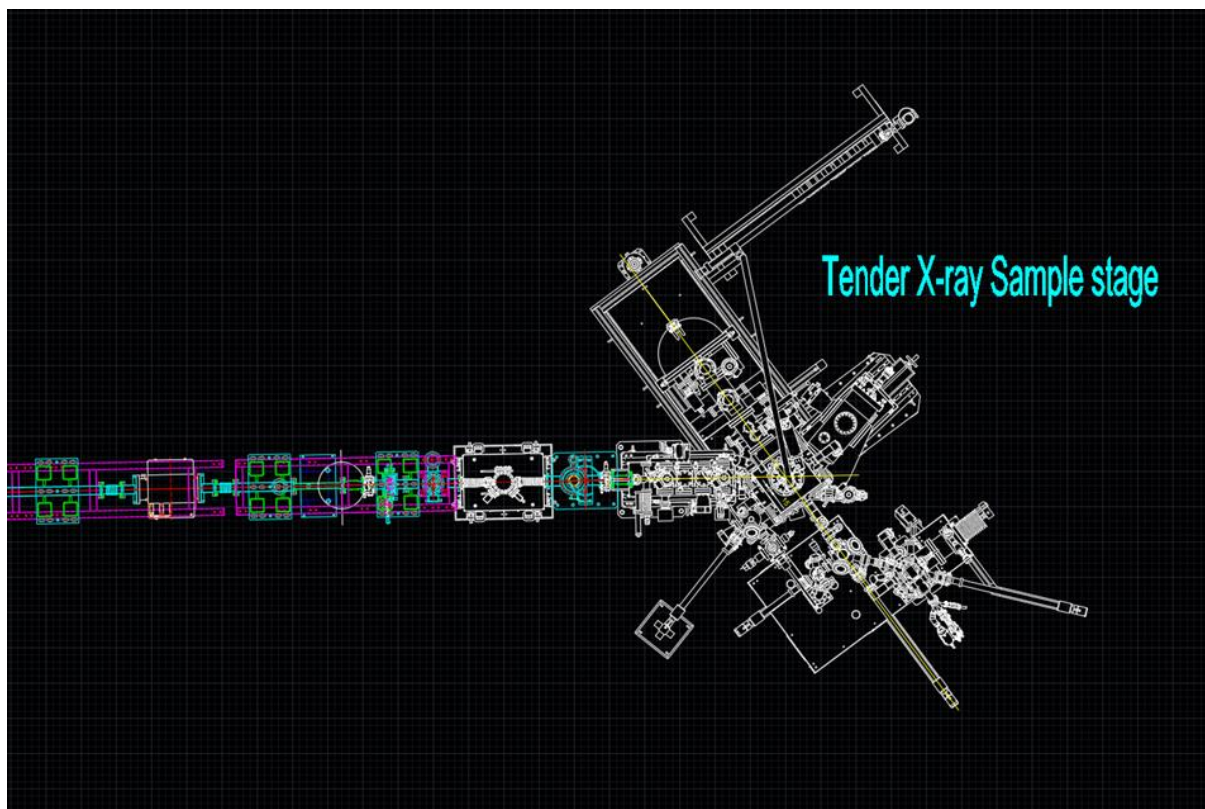
The electrochemical setup, depicted in <Figure 3.2.3.15 (b)>, connects the working (WE), counter (CE), and reference (RE) electrodes to an external potentiostat, enabling in situ electrochemical measurements. After the thin film is formed, the WE is positioned at the intersection of the X-ray beam and the spectrometer's focal point for real-time analysis with full potential control. This capability allows for the molecular-level investigation of dynamic phenomena, such as chemical changes on an electrode surface during battery cycling, degradation in photoanodes for solar water splitting, and the initial stages of corrosion.

As an alternative to this thin-film approach, a liquid cell<Figure 3.2.3.15 (c)> can also be utilized, which isolates the liquid sample from the high vacuum using an electron-transparent membrane. This method allows for the analysis of the sample while fully immersed in a bulk liquid environment, providing the advantage of minimizing the effects of electrolyte vapor pressure or dissolved gases.



<Figure 3.2.3.15> (a) Photograph of the interior of the Dip-and-Pull module analysis chamber, showing the sample holder, X-ray entrance window, electrolyte beaker, and electron spectrometer nozzle. (b) Schematic of the (AP)Tender XPS/XAS measurement geometry and the associated electrochemical circuit diagram.(c) showing the Liquid cell in chamber.

The end-station for Branch 1 is designed and will be constructed according to the layout shown in <Figure 3.2.3.16>, which illustrates the complete assembly of the tender X-ray sample stage and associated vacuum, detection, and manipulation systems.



<Figure 3.2.3.16> Layout of the Branch 1 Tender AP-XPS/XAS end-station sample stage and associated systems.

(2) Branch 2 – Soft HT-XPS/XAS Beamline for High Throughput experiments

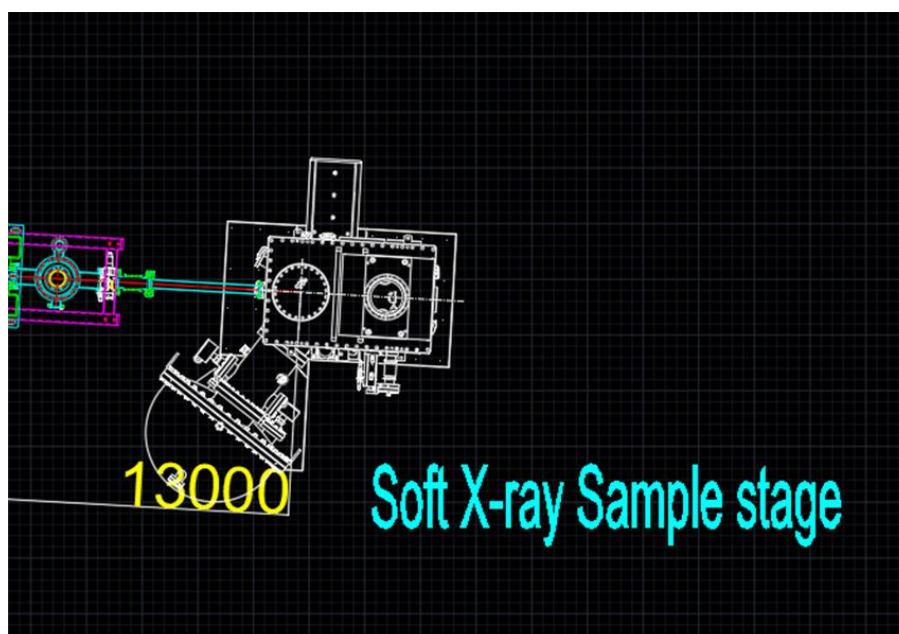
High Throughput X-ray Photoelectron Spectroscopy (HT-XPS) and X-ray Absorption Spectroscopy (HT-XAS) are advanced analytical techniques designed for rapid, automated, and systematic characterization of large numbers of samples or experimental conditions, making them particularly advantageous for synchrotron beamline applications in materials discovery, combinatorial chemistry, and operando studies where experimental throughput is critical. HT-XPS operates on the same fundamental principles as conventional XPS, which probes the elemental composition and chemical states of materials by analyzing the binding energies of photoemitted electrons, but extends its functionality through automation and multiplexing. Automated sample handling systems, high-speed scanning modes, and parallel data acquisition schemes enable efficient analysis of tens to hundreds of samples sequentially or simultaneously within a short time frame, thereby facilitating large-scale compositional screening and correlation studies between material structure and performance.

Likewise, HT-XAS integrates automated sample positioning, fast monochromator scanning,

and multi-sample holders to perform high-throughput X-ray absorption measurements. HT-XAS reveals detailed information on the local chemical and electronic environment of the absorbing atoms. When implemented on high-flux synchrotron beamlines, HT-XAS further supports time-resolved and operando studies under in situ conditions, tracking real-time changes in oxidation state, coordination, and chemical bonding during catalytic reactions or electrochemical cycling. Both HT-XPS and HT-XAS are characterized by their high-speed automated scanning capability, batch-sample measurement, integrated data processing pipelines, and user-friendly software environments, making them ideal for high-efficiency experimentation.

Given its designation as an industry-priority beamline, Branch 2 is specifically designed to accommodate the needs of industrial users and high-throughput research programs, where large numbers of samples must be processed quickly and reproducibly under consistent experimental conditions. This beamline will prioritize operational stability, user accessibility, and rapid data turnaround to support applications in materials qualification, process monitoring, and combinatorial screening.

Branch 2 will be constructed according to a design layout similar to that shown in <Figure 3.2.3.17>.



<Figure 3.2.3.17> Layout of the Branch 2 Soft HT-XPS/XAS end-station sample stage.

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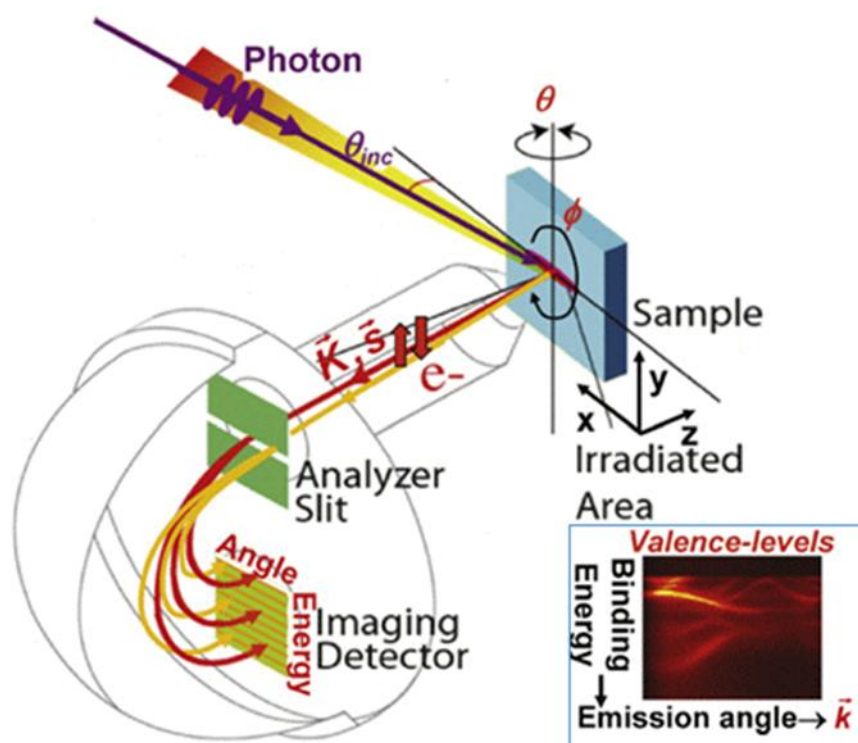
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3.2.4 ID25 NanoARPES Beamline

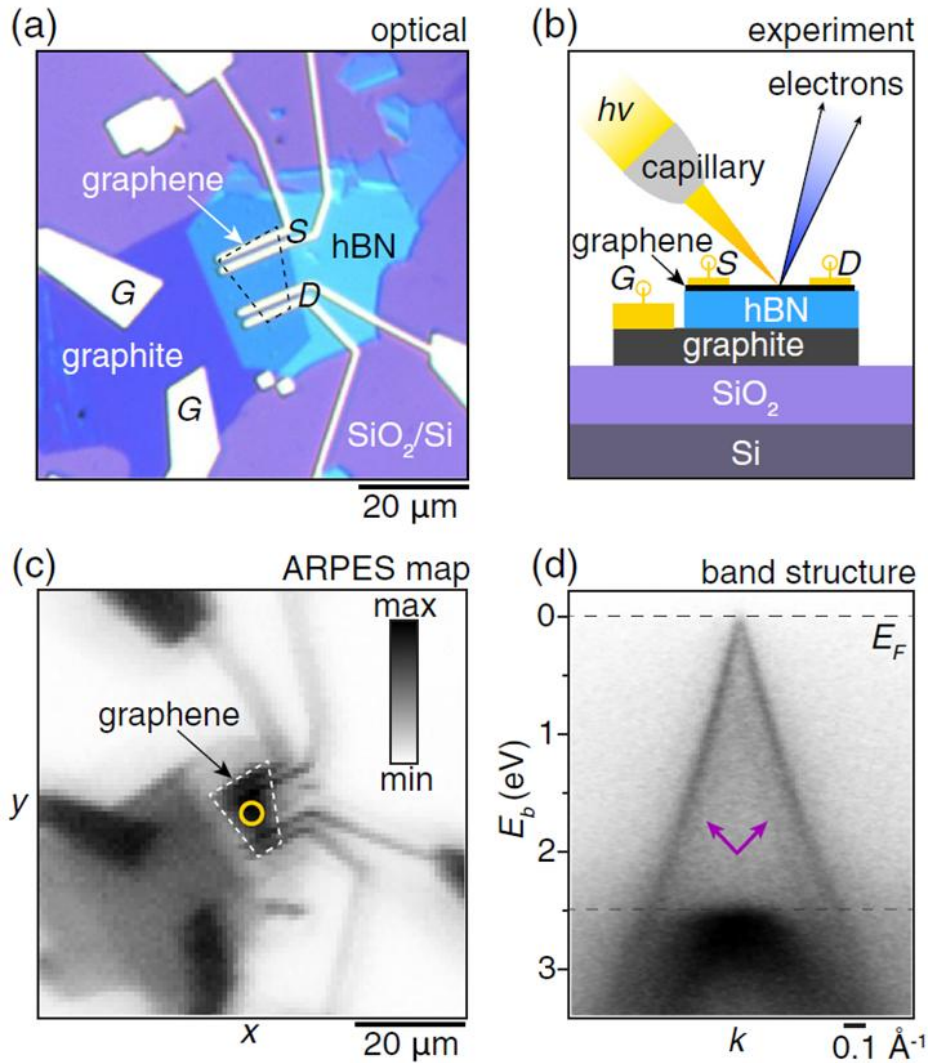
A. Introduction

The rapid evolution of materials science, particularly in the realm of two-dimensional (2D) quantum materials and nanoscale devices, has created an urgent demand for experimental techniques capable of probing electronic structures with both high energy and spatial resolution. Traditional Angle-Resolved Photoemission Spectroscopy (ARPES) has played a pivotal role in mapping band structures. However, its effectiveness diminishes when dealing with samples exhibiting spatial inhomogeneity or limited lateral dimensions. To address these challenges, the development of nanoARPES, combining the power of ARPES with sub-micron spatial resolution, has emerged as a transformative approach. The fourth-generation synchrotron environment, characterized by exceptional brightness and coherence, offers the ideal platform to realize such advanced beamlines.



<Figure 3.2.4.1> Schematic diagram for a traditional ARPES measurement.

The ID25 beamline at the fourth-generation synchrotron facility has been specifically designed to meet these scientific demands. Centered on the implementation of nanoARPES, the beamline employs a variable-line-spacing plane grating monochromator (VLSPGM) and delivers soft X-rays in the range of 50 to 2,000 eV. To accommodate diverse experimental needs, the beamline is divided into two branches: a nanoARPES branch utilizing capillary mirrors or zone plates for sub-micron focusing, and a complementary microARPES branch using a Kirkpatrick–Baez (KB) mirror system for experiments requiring longer working distances. Together, the dual-branch configuration supports a wide range of research scenarios from high-resolution studies of exfoliated 2D flakes and moiré superlattices to more conventional ARPES measurements on bulk-like samples.



<Figure 3.2.4.2> An example of nanoARPES experiment, (a) optical image of nanoscale gating device, (b) schematic cross-section of the device, (c) real space map of the ARPES data, (d) ARPES data.

This section presents the design of the ID25 nanoARPES beamline, including its optical configuration, mechanical integration, beam delivery performance, and experimental systems. The document builds upon prior conceptual designs and simulation results, and it defines the technical specifications necessary to proceed with procurement, construction, and commissioning phases. The content is organized to provide both a scientific rationale and an engineering roadmap, serving as a reference for external reviewers.

B. Scientific Objective

Recent developments in condensed matter physics have highlighted the importance of spatially heterogeneous and dimensionally confined systems, such as exfoliated van der Waals materials, twisted bilayers, domain walls, and nanoengineered heterostructures. In these systems, electronic properties often vary dramatically with local thickness, lattice symmetry, moiré potential, or external stimuli such as gating and strain. Probing such systems requires not only high energy and momentum resolution, but also spatial resolution well below the micrometer scale, capabilities that go beyond the reach of conventional ARPES.

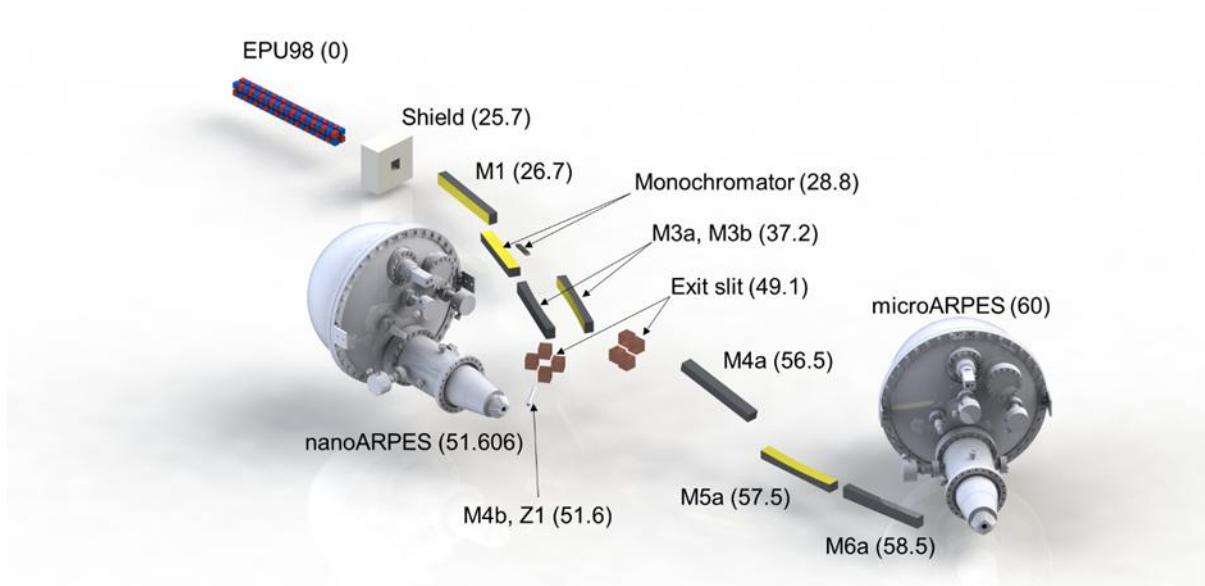
The ID25 nanoARPES beamline is designed to meet these scientific demands by providing ARPES with sub-micron spatial resolution. Using state-of-the-art focusing optics and a high-brightness soft X-ray source, the beamline enables users to map electronic band structures with spatial precision across sample domains, engineered interfaces, or inhomogeneous devices. Moreover, the beamline architecture supports in-operando measurements, allowing the study of electric field-induced band shifts, strain-dependent topological transitions, and other phenomena that require local and dynamic electronic structure characterization.

3.2.4.3 Beamline Insertion Devices (IDs) : [Refer]

3.2.4.4 Beamline Front End: [Refer]

C. Beamline Layout

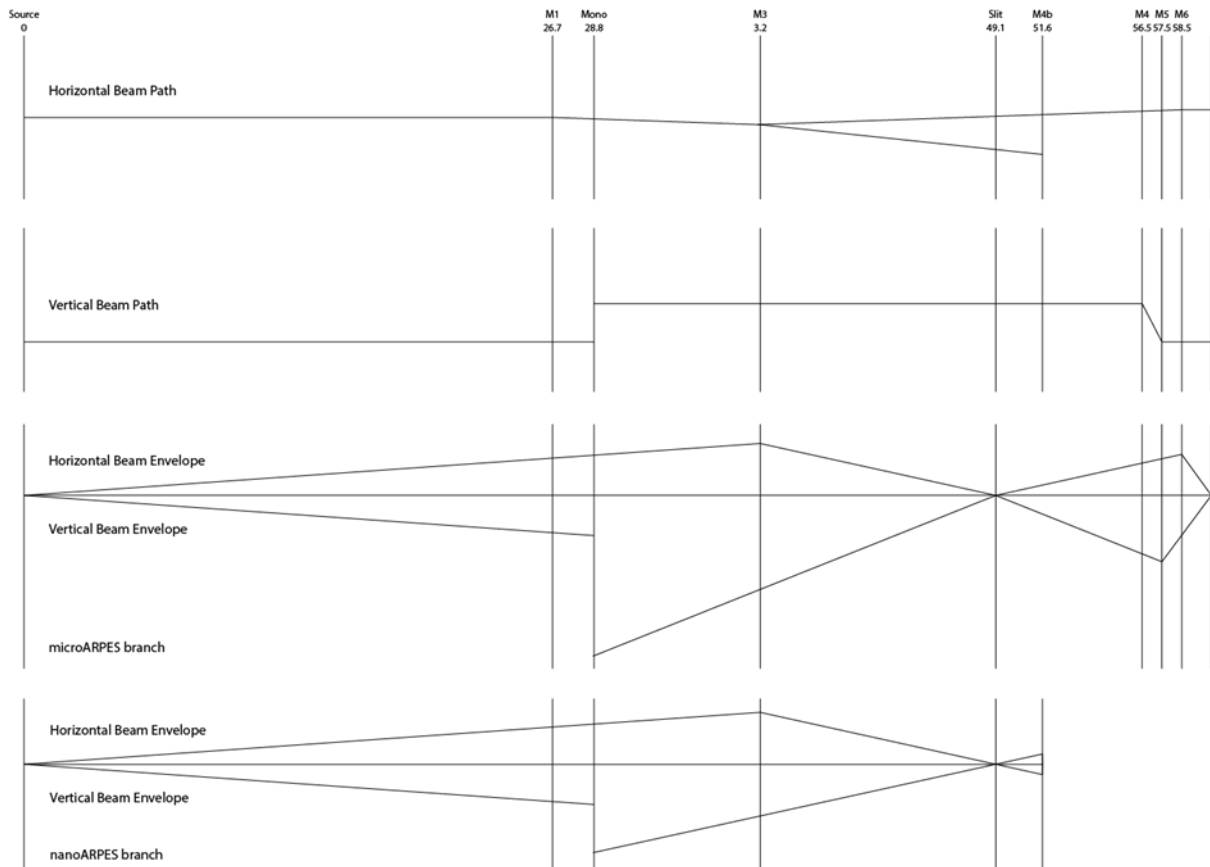
(1) Beamline Overview and Beamline Goal



<Figure 3.2.4.3> Schematic overview of the nanoARPES beamline, including microARPES and nanoARPES branches.

Both branches share upstream components, including a high-brightness undulator (EPU98) and a VLSPGM monochromator. These shared components are used for beam transport and energy selection, but each branch is independently optimized based on distinct optical configurations and operational parameters. Beam separation is achieved using a switching mirror mechanism (M3a, M3b) that provides $\pm 4^\circ$ angular deflection. <Figure 3.2.4.3>

Each branch was designed with a different fixed-focus constant (C_{ff}), selected to best match the optical strategy and focusing requirements of the downstream optics. The nanoARPES branch was designed based on a $C_{ff} = 2.2$ configuration, where vertical and horizontal divergences are nearly identical. This symmetry is favorable for capillary mirrors that rely on axisymmetric acceptance, enabling high-efficiency nanofocusing with minimal beam loss. In contrast, the microARPES branch was designed using a $C_{ff} = 4.0$ configuration. This results in an asymmetric divergence ratio, which allows vertical and horizontal focusing mirrors to be laced at different distances. Consequently, the microARPES branch employs a classical KB mirror system with a working distance of approximately 1.5 meters. This configuration is more versatile for conventional ARPES experiments.



<Figure 3.2.4.4> Beam path and envelope diagrams for the nanoARPES beamline, including nanoARPES and microARPES branches. The C_{ff} values for the beam envelope diagrams on microARPES and nanoARPES are 4.0, and 2.2 respectively.

(2) Beamline Floor Plan

The ID25 beamline extends from the undulator source at 0 m to the experimental hall boundary at 80 m, with a fixed radiation shielding wall positioned at 25.7 m. Upstream optical elements, comprising the water-cooled first mirror (M1), the VLSPGM monochromator, and the focusing mirror (M3a, M3b), are aligned along a shared axis before the beam is separated into two branches to Exit Slits located at 49.1 m. The nanoARPES branch follows a compact layout, terminating at approximately 51.6 m, while the microARPES branch extends farther downstream with additional focusing mirrors placed at 57.5 m (VFM) and 58.5 m (HFM), leading to its endstation at 60.0 m. The two branches are angularly separated by $\pm 4^\circ$, resulting in an 8° divergence that enables clear spatial distinction between the optical paths.

<Table 3.2.4.1> List of optics used for nanoARPES beamline

Element	Position [m]	Notes
Source	0	EPU98
Shielding Wall	25.7	Fixed radiation shielding structure
M1	26.7	Plane, water-cooled, heat load mirror
VLSPGM	28.8	Variable-line-spacing plane grating monochromator coupled with a plane premirror
M3a (M3b)	37.2	Switching, Horizontal focusing mirror for microARPES (nanoARPES)
Exit Slit	49.1	Exit Slits for microARPES (nanoARPES)
M4b	51.6	Capillary mirror for nanoARPES
nanoARPES Endstation	51.606	
M4a	56.5	Plane mirror for deflection downward
M5a	57.5	Vertical focusing mirror (2.5 m upstream of endstation)
M6a	58.5	Horizontal focusing mirror (1.5 m upstream)
microARPES Endstation	60.0	

The microARPES endstation is deliberately placed at 60 m, significantly upstream of the typical 70 m position adopted by other beamlines, to secure a 20 m segment between the endstation and the experimental hall boundary. This space is reserved for a user-accessible experimental hutch and an integrated sample preparation area. The preparation area includes a glove box connected to a load-lock system, which allows samples to be transferred under inert or vacuum conditions. A dedicated transfer mechanism links this preparation zone to the microARPES endstation, ensuring contamination-free delivery of sensitive samples into the ultra-high-vacuum measurement chamber. This spatial arrangement enhances operational flexibility and enables a streamlined, vacuum-compatible workflow that supports advanced material research under clean and controlled conditions.

D. Optics Overview

(1) Optical Simulation

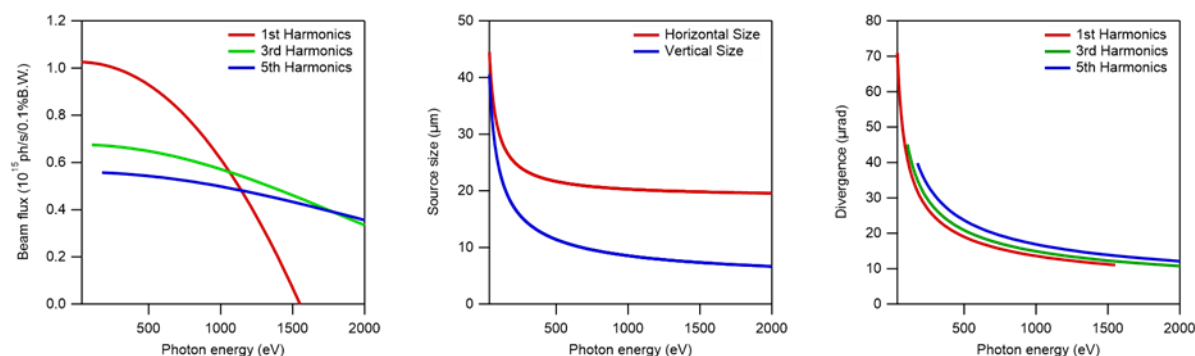
Ray-tracing simulations were performed using SHADOW4 within the OASYS platform to evaluate and optimize the optical performance of both branches of the beamline. The primary objective was to maximize photon flux at the sample while maintaining spatial resolution targets specific to each branch. Simulations were conducted at 100 eV, a representative photon energy within the soft X-ray regime where flux and focusing conditions are most critical. The nanoARPES branch was simulated with a $C_{ff} = 2.2$, chosen to produce a symmetric horizontal and vertical divergence. The microARPES branch was simulated under $C_{ff} = 4.0$, which introduces divergence asymmetry suitable for separated focusing optics.

For the nanoARPES branch, beam propagation from the VLSPGM through the horizontal focusing mirror (M3b) to the capillary mirror was analyzed. To ensure that the beam footprint fits within this annular region, the distance from Exit Slit to the capillary was set to 2.5 m. This geometry enables full utilization of the capillary's functional area while minimizing geometric clipping. Simulations confirmed that the beam was focused to below $1\ \mu\text{m}$ in both axes at the sample plane, satisfying the spatial resolution requirement for nanoARPES experiments targeting small, inhomogeneous samples.

In the microARPES branch, the asymmetric divergence resulting from the $C_{ff} = 4.0$ configuration allowed the vertical and horizontal focusing mirrors to be placed independently. The vertical focusing mirror (VFM) was positioned 2.5 m upstream of the endstation, and the horizontal focusing mirror (HFM) at 1.5 m. These distances were informed by minimizing diffraction limited beam spot size and mechanical design constraints. The 1.5 m space downstream of the HFM also accommodates an in-vacuum camera, enabling visual confirmation of beam placement on the sample. The resulting beam spot size at 100 eV was approximately $10\ \mu\text{m}$ in both directions, meeting the specifications for general ARPES measurements and ensuring compatibility with auxiliary equipment.

(2) Detailed Optical Layout

The ID25 beamline is driven by an elliptically polarized undulator (EPU98) located at 0 m, providing soft X-rays with tunable polarization across the photon energy range of 35 to 2,000 eV. The undulator serves as the primary source for both the nanoARPES and microARPES branches.



<Figure 3.2.4.5> Undulator characteristics including beam flux, directional sizes and divergences of EPU98 for Korea-4GSR, calculated with SPECTRA

SPECTRA simulations were performed to evaluate the source properties over the full operating energy range. The resulting energy-dependent profiles of photon flux, source size, and source divergence will be presented in <Figure 3.2.4.5> These values were used as input parameters for downstream ray-tracing simulations and optical design optimization.

At a representative photon energy of 100 eV, the following source characteristics were obtained:

- Photon Flux: 1.02×10^{15} photons/s/0.1%BW
- Source Size (FWHM): $30.3 \mu\text{m}$ (H) $\times$ $24.1 \mu\text{m}$ (V)
- Source Divergence (FWHM): $41.8 \mu\text{rad}$ (H) $\times$ $41.7 \mu\text{rad}$ (V)

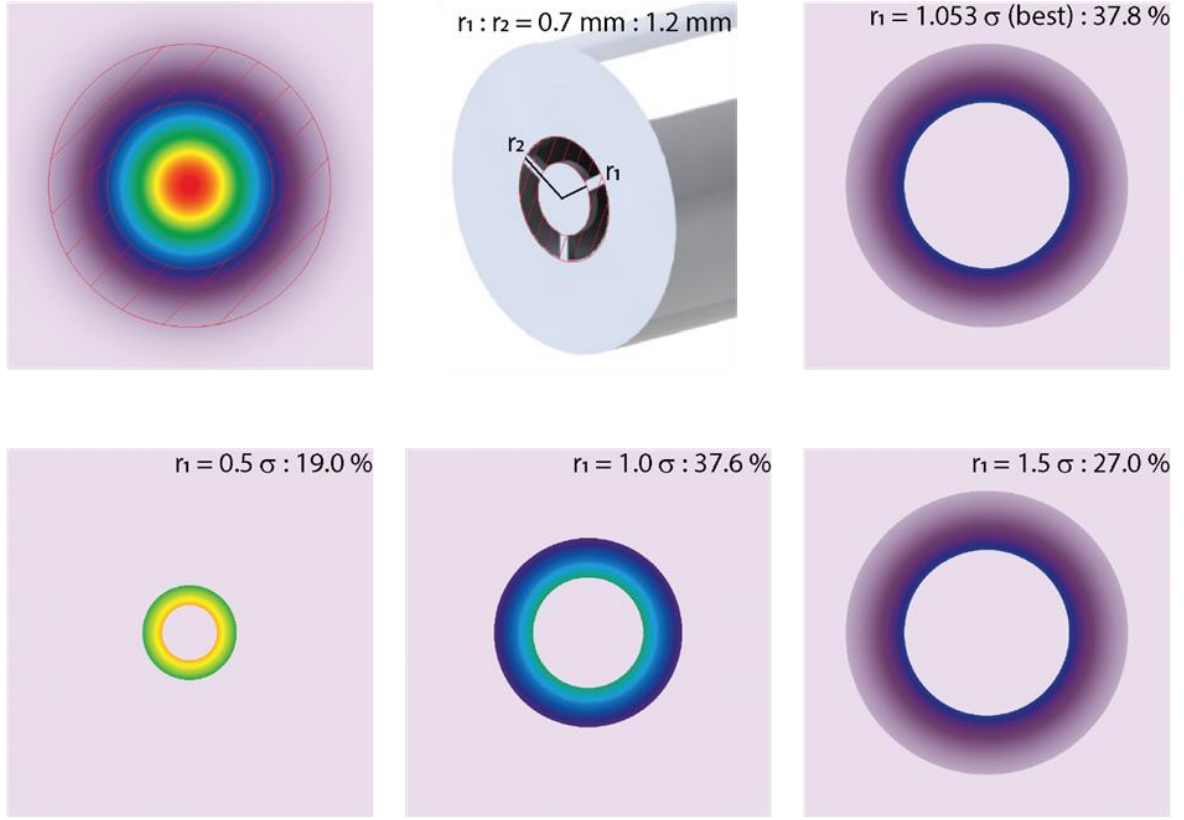
These values define the initial conditions of the beam entering the optical system and were used to guide the design of both the monochromator and the focusing optics. The compact source size and angular spread allow efficient beam transport and focusing over long beamline distances.

<Table 3.2.3.2> Detailed list of the optical components used for nanoARPES beamline

Optics	M1	M2	Grating	M3a (M3b)
Type	Plane	Plane	Plane VLS	Elliptic cylinder (tangential)
p-q	-	-	28.8 to 20.3	37.2 to 11.9
Location (m)	26.7	28.8 to δ	28.8	37.2
Grazing angle (deg)	1	2.9 to 12.9	4 to 8	2
Clear Aperture (mm x mm)	230 x 5	250 x 5	135 x 5	160 x 7
Coating	Au	Au	Au	Au
Note	Heat load, H-deflecting	premirror	V-focusing	H-focusing, Switching
Optics	M4b	M4a	M5a	M6a
Type	Capillary	Plane	Elliptic cylinder (tangential)	Elliptic cylinder (tangential)
p-q	2.5 to 0.006	-	7.4 to 2.5	8.4 to 1.5
Location (m)	51.6	56.5	57.5	58.5
Grazing angle (deg)	90	1.15	1.15	0.7
Clear Aperture (mm x mm)	1.2 x 1.2	360 x 4	360 x 5	360 x 9
Coating	Au / Pt	Au	Au	Au
Note	Focusing	V-Deflecting	V-focusing	H-focusing

Before describing the details of the VLSPGM monochromator, we summarize the key optical components used in the ID25 beamline. These include all major mirrors installed upstream and downstream of the monochromator, along with their surface coatings, nominal grazing incidence angles, and effective optical lengths. A complete list of these mirror specifications is provided in the table below.

The VLSPGM monochromator is positioned at 28.8 m, and its location was selected to satisfy two essential design constraints: (1) minimizing physical interference between upstream and downstream optics, and (2) ensuring optimal beam divergence at the exit slit to maximize throughput at the nanoARPES capillary mirror. To achieve this, the upstream optical layout was optimized such that the divergence profile at the capillary matches its spatial acceptance, which is defined by a 0.7 mm central stop and a 1.2 mm outer aperture.



<Figure 3.2.4.6> Illustration of the entrance aperture of the capillary mirror from SIGRAY, and the throughput of the beam depending on the illumination shape at the entrance aperture. The best throughput is about 38 % if the central stop matches with the 1.053σ of the gaussian distribution.

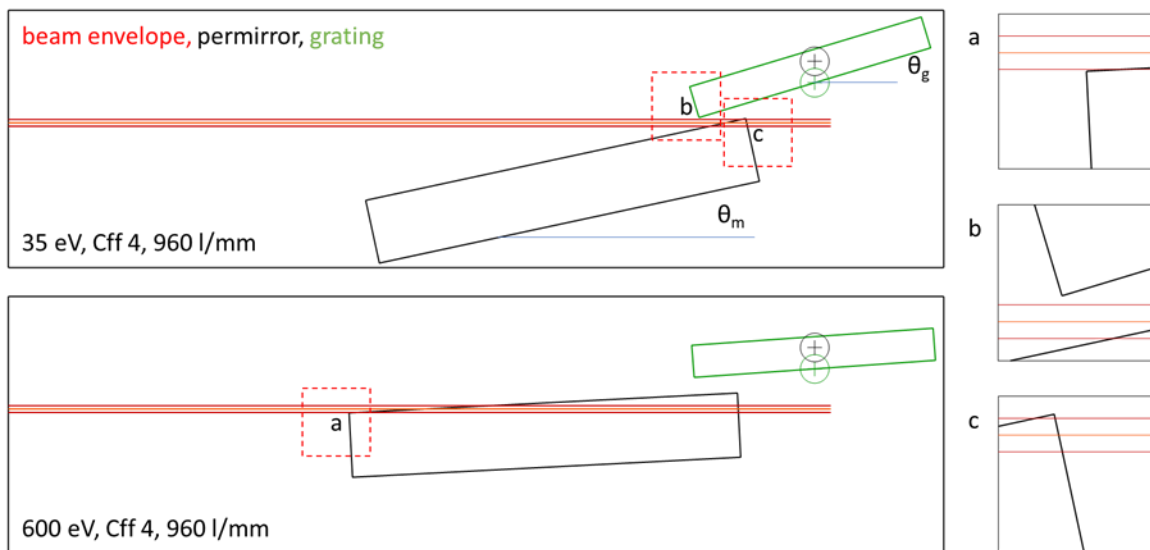
The VLSPGM adopts the SX-700 geometry, in which the rotation axis of the premirror (defined by the angle θ_m) is fixed, and the grating angle (θ_g) is varied to scan the photon energy while preserving the C_{ff} . To maintain a beam offset of 25 mm between the premirror and the grating, and to prevent the incoming beam from being clipped by the edge of the grating at high angles, the maximum allowable grating angle (θ_g) was set to 17.76° . For the beam reflected by the premirror to avoid clipping at the grating even at the lowest incidence angles, the minimum value of θ_m must support this geometry. Calculations show that to accommodate the required α under each configuration, θ_m must be no smaller than approximately 2.9° for $C_{ff} = 2.2$.

Conversely, when the grating is operated at its maximum angle of 17.76° , the corresponding upper limit of θ_m is determined to be 12.84° under the $C_{ff} = 2.2$ condition. These boundary

angles define the mechanical and optical constraints of the premirror, particularly its optical aperture, which was consequently set to approximately 250 mm to avoid beam loss at extreme.

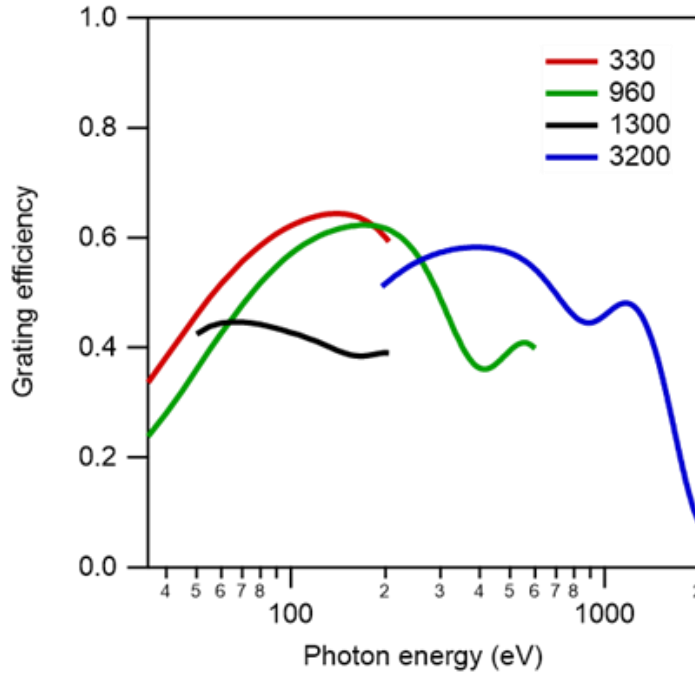
To establish the rotation center of the premirror, three representative θ_m values; 2.9° , 12.9° , and their midpoint at 7.9° were selected. For each angle, the premirror was oriented such that the reflected beam is directed to the center of the grating. The locus of these three mirror positions defines a common circle, and the center of this circle was adopted as the fixed rotation center for the premirror. The resulting coordinates are $x = -0.0605$ mm and $y = 13.2764$ mm.

To validate this geometry, especially under the most extreme optical conditions, ray-path diagrams were generated for a grating with 960 lines/mm at photon energies of 35 eV and 600 eV. These diagrams show that the beam path avoids physical interference with both the front and rear edges of the premirror optical aperture and the grating itself. Key points labeled a, b, and c in the figures illustrate the foremost edge of the mirror aperture, the beam-grating interaction zone, and the rear edge of the mirror aperture, respectively—confirming unobstructed beam propagation across the designed energy range.



<Figure 3.2.4.7> Detailed dimensions of the premirror and the grating in mm. Optical apertures are colored by red. Illustration of the two extreme conditions: (top box) lowest energy case with maximal angles of θ_m and θ_g . The insets (b) and (c) confirm that the beam envelope of 0.15 mrad is not clipped nor missed by either of the grating and the rear edge of the premirror. (bottom box) Highest energy case with minimal angles of θ_m and θ_g . The inset (a) confirms that the beam envelope is not clipped by the front edge of the premirror.

Based on these constraints, the groove densities of the gratings were selected to cover the entire operational energy range (35 to 2,000 eV). The configuration includes: (1) Three gratings optimized for $C_{ff}=2.2$ operation: 330, 960, and 3,200 lines/mm, for high-flux modes. (2) One grating optimized for high-resolution operation at $C_{ff}=4.0$: 1,300 lines/mm.



<Figure 3.2.4.4> Grating efficiencies calculated by GSolver.

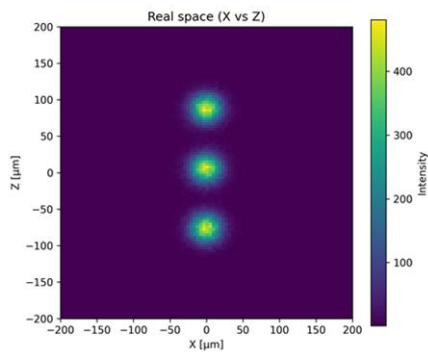
The groove depths and duty ratios for each grating were optimized using GSolver to maximize diffraction efficiency within the angular and energy constraints described above. The efficiencies for each grating as a function of energy are illustrated in <Figure 3.2.4.8> Ray-tracing results demonstrating resolving power under $RP = 10,000$ conditions are summarized in <Figure 3.2.4.9> for each grating configuration.

Grating specifications, including groove density, C_{ff} value, and typical energy ranges, are presented in the table below.

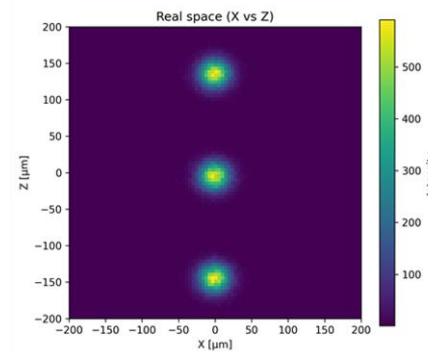
<Table 3.2.4.3> List of detailed parameters for the gratings

Groove Density (l/mm)	Energy Range (eV)	C_{ff}	Mode	Duty cycle (%)	Depth (nm)	E/dE with 100 μ m Exit Slit at 100 (500) eV
330	35 to 205	2.2	High throughput	37	56	7,000
960	35 to 600	2.2	Intermediate energy range	40	30	13,000
3,200	110 to 2,000	2.2	Extended energy range	41	11	(10,000)
1,300	40 to 205	4.0	High resolution	25	46	16,000

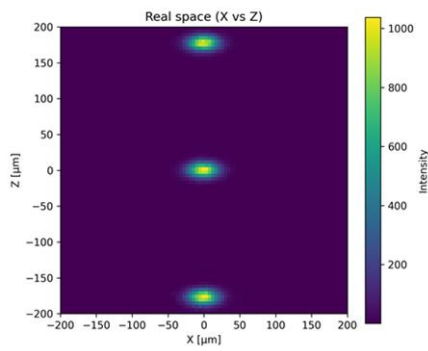
Groove Density (l/mm) {optimized energy}	G0 (l/m)	G1 (l/m ²)	G2 (l/m ³)	G3 (l/m ⁴)
330 {100 eV}	330,000	46,801	2,693	210
960 {100 eV}	960,000	135,340	7,705	593
3,200 {500 eV}	3,200,000	349,525	23,760	1,626
1,300 {100 eV}	1,300,000	141,334	9,520	643



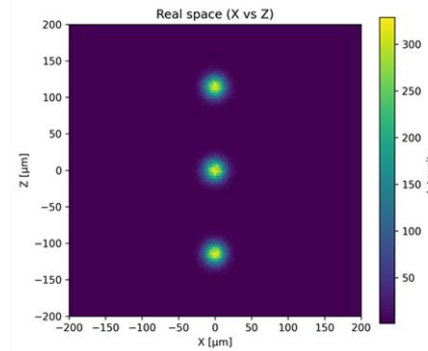
330 l/mm 100 eV



960 l/mm 100 eV



1300 l/mm ($C_{ff} = 4$)

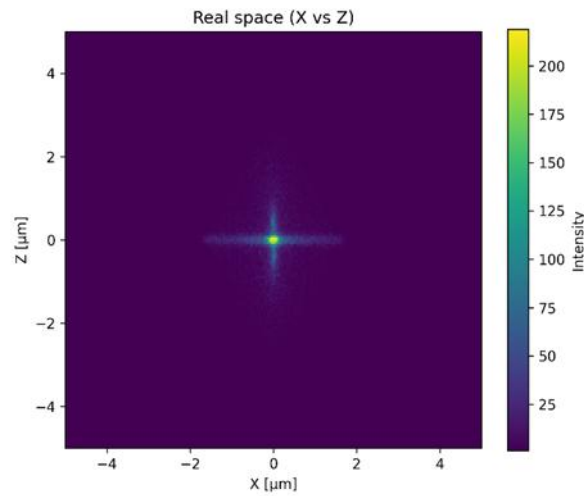


3200 l/mm (500 eV)

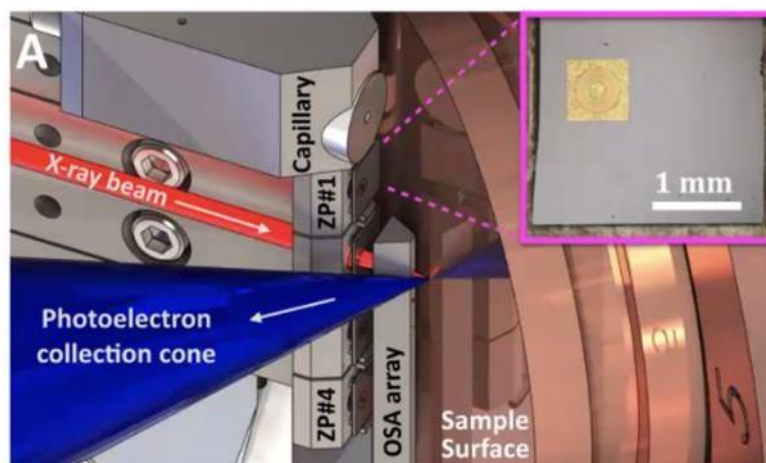
<Figure 3.2.4.9> Ray tracing result at the exit slit, with energy of 100 (500) eV and 100 (500) $\pm$ 0.01 (0.05) eV, resolving power = 10,000. The intensity is shown in arbitrary units.

The nanoARPES branch follows a compact optical path, optimized for axisymmetric focusing. Due to mechanical constraints from the nanoARPES endstation, the distance from Exit Slit to the capillary mirror was fixed at 2.5 m in order to avoid physical interference. This spatial constraint was treated as a design input, and the upstream optical elements (particularly the VLSPGM and M3b) were positioned accordingly to match the beam divergence with the spatial aperture of the capillary mirror. The capillary mirror, located at 51.6 m, features a 0.7 mm central stop and a 1.2 mm outer aperture. At 100 eV and $C_{ff} = 2.2$, the beam footprint was shown to match this annular aperture maximizing the throughput, and ray-tracing simulations confirmed sub-micron focusing at the sample position. The nanoARPES endstation is located 6 mm downstream of the capillary mirror, with a minimal beamline footprint that enables high-resolution measurements on small or inhomogeneous samples.

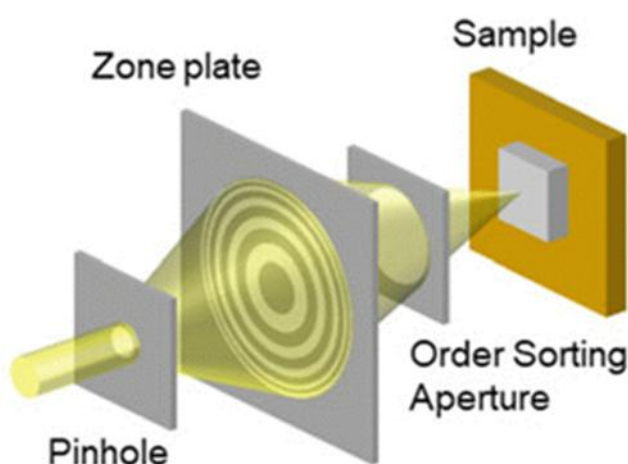
The Nano-ARPES experimental apparatus is designed to be equipped with multiple zone-plates separated by the energy band of the photon beam as shown in the <Figure 3.2.4.11> below and to use one capillary mirror.



<Figure 3.2.4.10> Ray tracing result of nanoARPES endstation with capillary mirror. The FWHM is expected to be ~200 nm in the ideal case. The intensity is shown in arbitrary units.



<Figure 3.2.4.11> Optics stage of MAESTRO beamline at the Advanced Light Source.
Conceptually the same configuration for the 4GSR nanoARPES beamline.



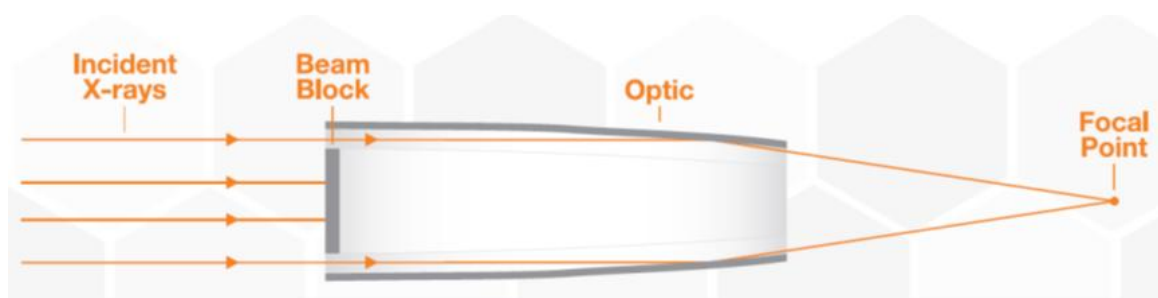
<Figure 3.2.4.12> Fresnel Zone Plate with order sorting aperture.

A zone plate is a device used to focus light or other objects that exhibit wave properties. Unlike lenses or curved mirrors, which are common optical devices, zone plates use diffraction instead of refraction or reflection and are based on the analysis of French physicist Augustin-Jean Fresnel and are sometimes called Fresnel zone plates in his honor. The focusing ability of zone plates is an extension of the Arago spot phenomenon, which is caused by the diffraction of an opaque disk. The zone plate is made of concentric structures known as Fresnel zones that alternate between opaque and transparent, and photon beams that reach the zone plate are diffracted around the opaque zones. Because diffraction is utilized, it is necessary to block photon beams of other orders than the required order, which requires a pin-hole at the incident

side and an order sorting aperture (OSA) at the emission side.

When using an FZP, the structure of the device that controls the FZP must be sized and installed so that it does not interfere with the vertical direction of the photoelectrons emitted from the sample surface. When using FZPs for focusing, design them to have a size of $100 \times 100 \text{ nm}^2$ or less in the sample. Since the number of FZPs varies depending on the energy band of the photon beam used in the experiment, the structure and focal length of the FZPs vary depending on the energy band of the photon beam used in the experiment, a stage that can adjust the distance between the FZPs and the OSA should be installed to position the sample in the focusing position of the photon beam.

(2) Capillary Mirror focusing optics

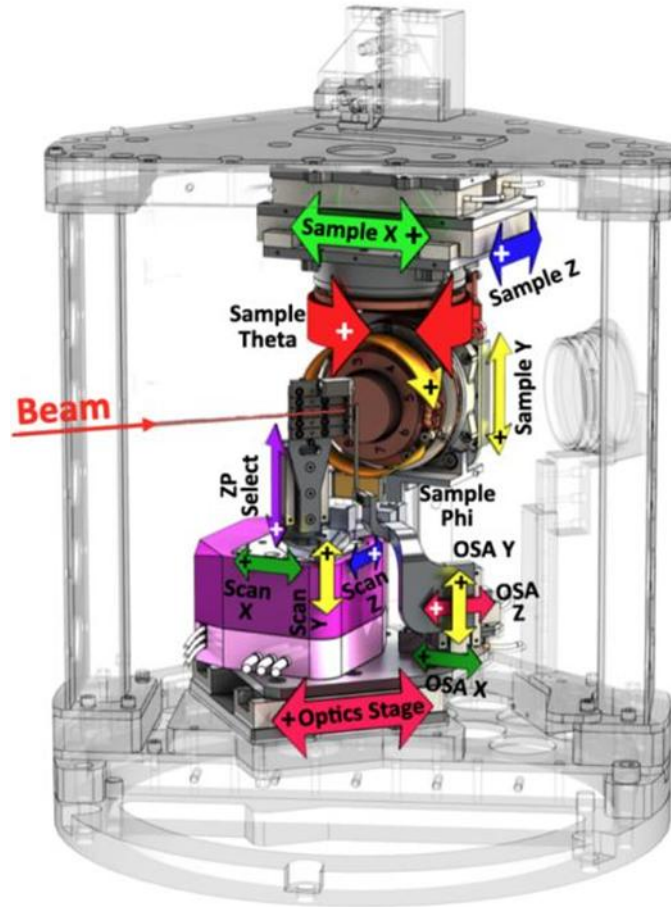


<Figure 3.2.4.13> The cross-section of a capillary mirror, including central beam stop to block the unfocused portion of the beam.

The capillary mirror to be introduced into the nanoARPES experimental apparatus should be a single bounce type capillary mirror with a beam blocking block in the center so that the photon beam entering the capillary does not pass through the capillary and directly reach the sample, and only the photon beam reflected and collected inside the capillary reaches the sample. The final focused photon beam size of the capillary mirror should be set to 200 nm or less. The reflective surface inside the mirror should be coated with gold (Au) as with other mirrors to minimize the degradation of reflectivity in the energy region of the photon beam used.

It is installed inside the UHV chamber of the nanoARPES experimental apparatus to regulate the focused optics to produce the final nm-sized photon beam, to position the sample, and to

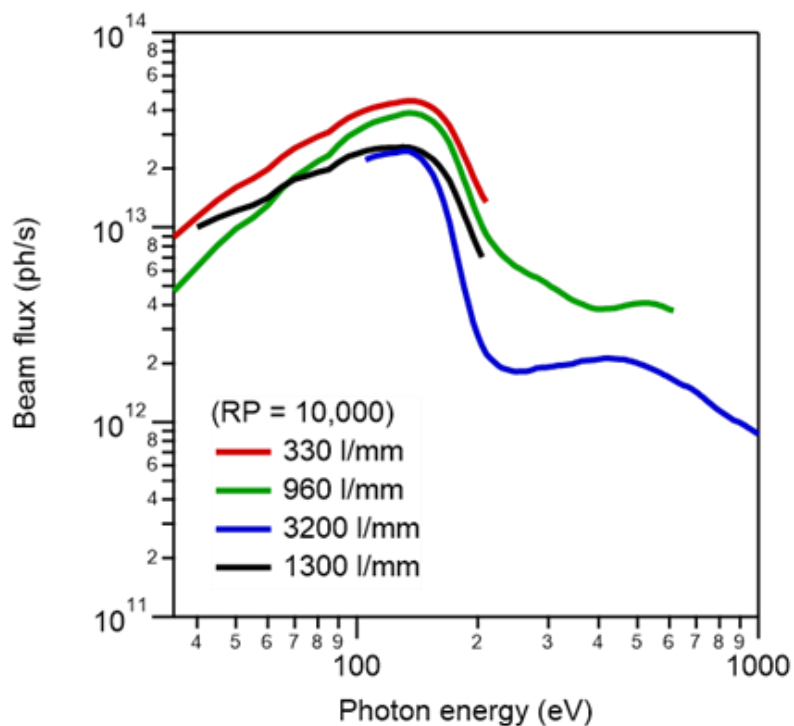
provide cooling and connection. All components inside the experimental apparatus for ARPES spectroscopy experiments must be made of non-magnetic materials to prevent the emission angle of the photoelectrons from being distorted by the magnetic field, and must be built using actuators with nm-scale resolution. The material of the sample positioning device (manipulator), to which the sample holder with the sample is attached, should be made of a material that is non-magnetic and capable of operating at ultra-low temperatures.



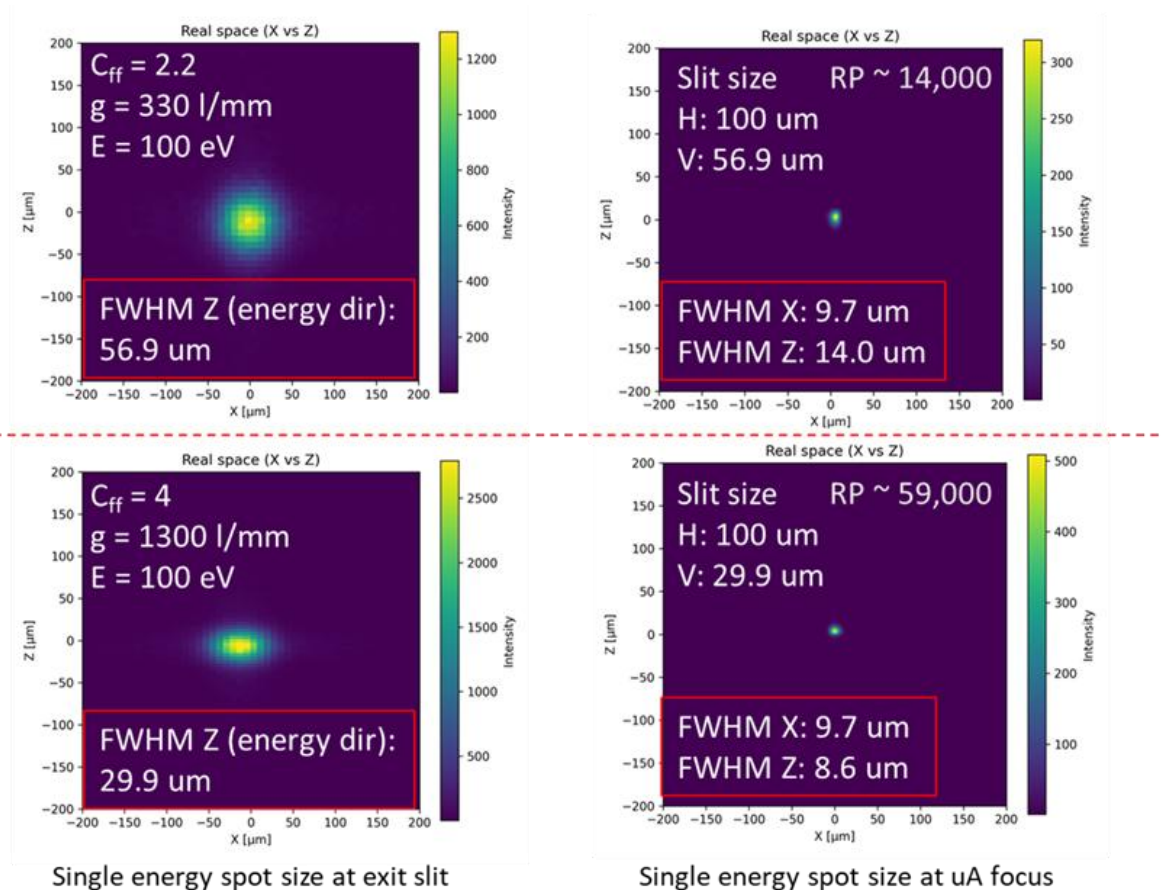
<Figure 3.2.4.14> nanoARPES sample stage at the MAESTRO.

The microARPES branch supports a more conventional optical layout using a KB mirror pair. The divergence asymmetry from the $C_{ff} = 4.0$ configuration allows the vertical and horizontal focusing mirrors to be placed independently. The vertical focusing mirror (VFM) is located 2.5 m upstream of the sample (at 57.5 m), while the horizontal mirror (HFM) is placed 1.5 m upstream (at 58.5 m). These distances were selected to avoid mechanical interference, both between the mirrors themselves and between the HFM and the microARPES endstation.

The 1.5 m space downstream of the HFM also accommodates a camera system, which allows users to visually confirm beam positioning on the sample surface during alignment and measurement. The endstation is located at 60 m, and the 20 m stretch from 60 m to 80 m is reserved for user infrastructure. This includes a user hutch, glove box, loadlock chamber, and vacuum transfer system. The layout accommodates flexible experimental workflows while preserving the optical and mechanical integrity of the beamline.



<Figure 3.2.4.15> Calculated beam flux at the microARPES endstation with reflectivity of mirrors, 0.15 mrad of acceptance, and the grating efficiencies.



<Figure 3.2.4.16> Beam spot size at the exit slit and at the microARPES endstation. The magnification along the energy dispersive (vertical) direction from the slit to the microARPES focus is about $4\times$. The intensity is shown in arbitrary units.

3.2.4.6.3 Heat Load Considerations: [Refer]

3.2.4.6.4 Beam Delivery Specifications

3.2.4.6.5 Beam Specifications and Optics Specifications

3.2.4.7 Exp. system overview

3.2.4.7.1 Scientific Scope

3.2.4.7.2 Exp. system I

3.2.4.7.3 Exp. system II

3.2.5 ID04 CoXRD Beamline

A. Introduction

The performance of a material is fundamentally governed by the type of constituent atoms, the nature of interatomic bonding, and their periodic arrangement within the crystal lattice. These aspects have been extensively studied over the past century. In parallel, crystallographic defects have been shown to drastically alter material properties. For instance, the inhibition of dislocation motion can significantly enhance mechanical strength. Consequently, a deep understanding of structural disorder is essential for advancing material functionality. Historically, techniques based on incoherent X-rays—such as diffuse scattering—have been employed to study disorder within periodic systems. However, such methods inherently rely on long-range periodicity and are limited in their ability to resolve local, non-periodic disorder over extended sample volumes. The advent of coherent X-ray beams has opened a new frontier in this domain. Even without spatial symmetry, coherent X-rays can probe local structural heterogeneities because of their great spatial coherence. Among the emerging techniques, Bragg Coherent X-ray Diffraction Imaging (BCDI) stands out as one of the most advanced and widely utilized approaches.[1-5] Notably, the enhanced coherence provided by fourth-generation synchrotron sources—currently under development and upgrade worldwide—has significantly increased the resolution and sensitivity of BCDI, making it a particularly promising tool for nanoscale materials characterization.

The CoXRD beamline at the Korean 4th Generation Synchrotron Radiation Facility (4GSR) is being developed with a primary focus on BCDI to enable quantitative analysis of local disorder in crystalline materials. By leveraging the intrinsic coherence of the source, the beamline is designed to maximize spatial resolution in BCDI reconstructions. A key challenge under investigation is the acquisition of coherent diffraction patterns near the absorption edge of selected elements, which would allow elemental-specific imaging and spatial localization. Additionally, the inherent flexibility of the BCDI setup allows for microbeam X-ray diffraction, enabling investigations of phase transitions in confined systems such as nanowires.[6-8] The beamline is also being configured to support three-dimensional X-ray diffraction (3DXRD) by employing high-energy X-rays (up to 30 keV) combined with azimuthal sample rotation, allowing for grain-resolved mapping of orientation and strain within polycrystalline samples. This 3DXRD capability is seamlessly integrated into the BCDI experimental station, thus

broadening the scientific applications of the beamline. In the second phase of development, the beamline will be further expanded to incorporate Dark-field X-ray Microscopy (DFXM) by installing a Compound Refractive Lens (CRL) stack in the far-field geometry. To accommodate the long working distances required for DFXM—including sufficient sample-to-detector distance and rotation angle flexibility—the hutch length is planned to be approximately 10 meters.

Collectively, the CoXRD beamline aims to provide a comprehensive platform for multiscale defect characterization in materials: probing local lattice distortions via BCDI, grain orientation and strain mapping via 3DXRD, and site-specific defect structures via DFXM. Through this integrated approach, the beamline will play a key role in advancing our understanding of the interplay between disorder and functionality in advanced materials

B. Beamline Requirements for the Insertion Devices

An in-vacuum undulator with a period of 22 mm and a length of 3 m will be installed on the ID03 coherent X-ray diffraction beamline. It will generate a highly coherent flux and provide a continuous energy range of 5 to 30 keV(5 to 16 mm gap). With a minimum gap of 5 mm, the undulator achieves a maximum deflection parameter(K) of 2.315. Under a storage ring current of 400 mA, it generates a maximum radiation power of 15.165 kW.

<Table 3.2.5.1>. ID03 Coherent X-ray Diffraction Beamline Source Parameters

Beamline	Undulator	Period (mm)	Length (m)	Max. Power (kW)	Max. K value
Coherent X-ray Diffraction	In-vacuum	22	3	15.165 (400 mA)	2.315 (5 mm gap)

C. Beamline Requirements for the Front End

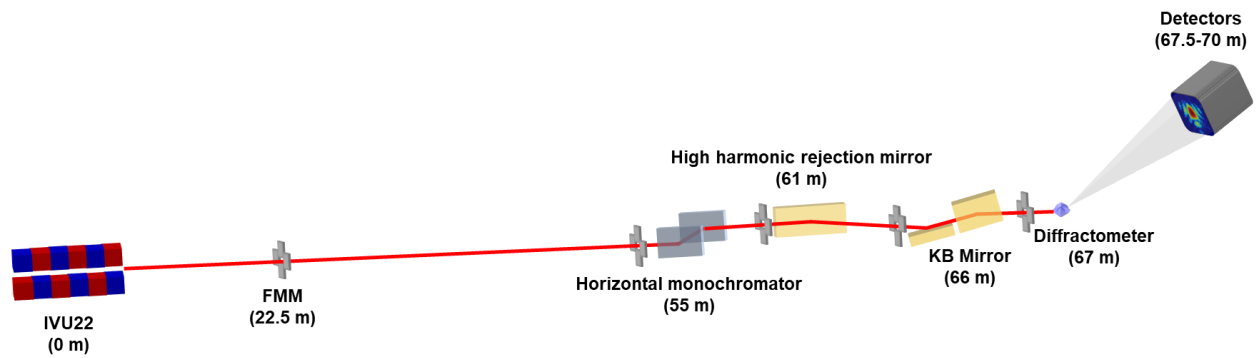
The front end(FE) of this beamline is designed for all optical component under the following conditions. (Reference the 4GSR beamline FE section)

- Structural stress due to heat load should not exceed the yield strength.
- The temperature rise due to heat load should not exceed the softening temperature of the materials.
- The LCW temperature of the wall should not exceed the boiling point of water.

The maximum power from the IVU22 is 15.165 kW, which is gradually attenuated throughout the FE. Approximately 0.872 kW is absorbed by the first fixed mask, which has an opening angle of 0.6 mrad. An additional power is further attenuated by second fixed mask located downstream which has an opening angle of 0.46 mrad. Near the end of the FE, before the photon shutter, a front-end movable mask adjusts the beam to approximately its FWHM. As a result, the power delivered to the PTL is reduced to approximately 130 W.

D. Beamline Layout

(1) Beamline overview



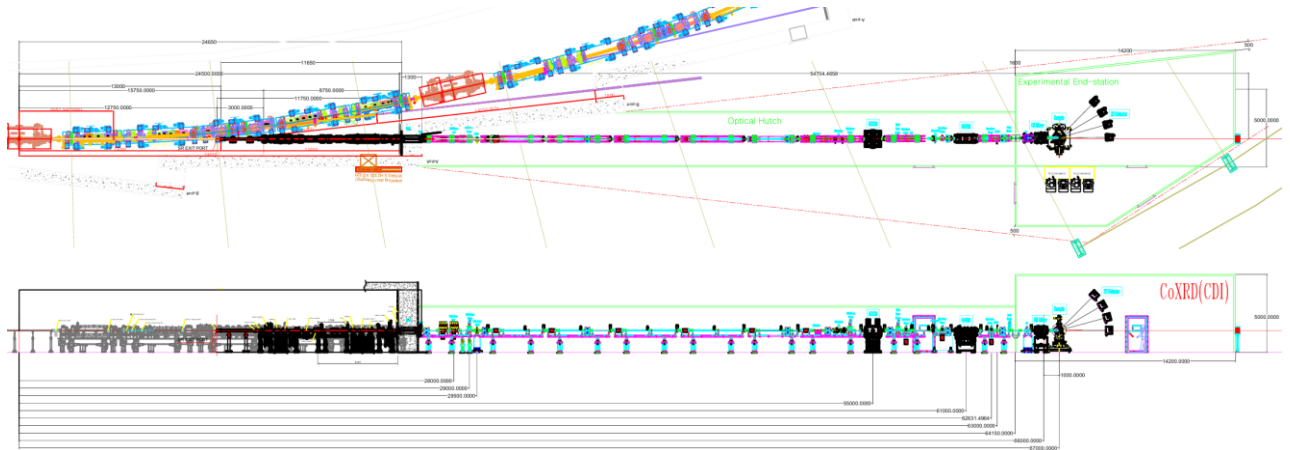
<Figure 3.2.5.1> Coherent X-ray Diffraction Beamline layout schematic.

The layout of this beamline is designed to minimize optics to preserve wavefront as much as possible from thermal load, vibration, and other factors. So, the main optics are horizontal monochromator(HDCM), high harmonic rejection mirror(HHRM), KB mirror and these are positioned close to the experimental hutch: the HDCM at 55 m, the HHRM at 61 m, and the KB mirror at 66 m. And the KB mirror has long focal length of 1 m, providing sufficient space to accommodate various in-situ and operando experiments. Consequently, the sample position, defined as the rotation center of the diffractometer, is set at 67 m. The current design is provisional and may be revised in response to ongoing discussions and future technical requirements.

(2) Beamline floor plan

Several diagnostic instruments and major optical components not shown in <Figure 3.2.5.1>, are listed in <Table 3.2.5.2>. The table provides the specifications and distances of each components. As shown in <Figure 3.2.5.2>, the white beam attenuator, screen and PBPM are

located downstream of the shielding wall, enabling diagnostics of the beam after FE. At the end of the optical hutch, the beam position monitor(BPM) is installed to monitor the position of the beam incident on the experimental hutch. In addition, there are slits and diagnostic devices located in front and behind each main optics. Currently, the optical and experimental hutches share one side, but future separation is possible to address vibration and air-conditioning.

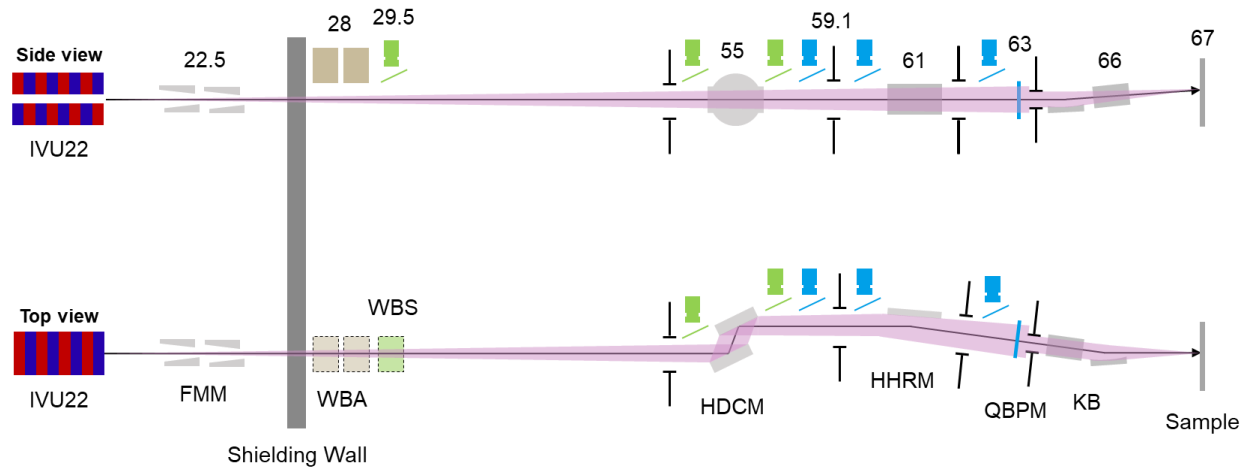


<Table 3.2.5.2 > Coherent X-ray Diffraction Beamline Component Table

Distance (m)	Component	Description
22.5	Movable mask	4-way slit, UHV, Water cooling
28	White beam attenuator	CVD Diamond : 0.2 mm, 0.3 mm, 0.5 mm 2 set, Water cooling
29	White beam screen	Diamond window, Fluorescent metal screen, current signal output
29.5	White beam PBPM	4-Blade-type
52.9	White beam slits	4-way slit, UHV, Water cooling
53.6	White beam screen	Diamond window Fluorescent metal screen, current signal output
55	HDCM	Si (111)/Si(311), fixed exit
56.7	White beam screen	Diamond window Fluorescent metal screen, current signal output
57.1	Mono beam screen	YAG window Fluorescent metal screen, current signal output
59.1	Mono beam slits	4-way slit, UHV
59.5	Mono beam screen	YAG window Fluorescent metal screen, current signal output
61	High harmonics rejection mirror	2-stripe coating (Pt, Rh)
62	Mono beam slits	4-way slit, UHV
62.6	Mono beam screen	YAG window Fluorescent metal screen, current signal output
63	Beam position monitor	UHV QBPM, Ti foil : 500 nm / Ni foil : 500 nm
65.3	Slits	4-way slit, UHV
66	KB mirror	2-stripe coating (Pt, Rh), Vertical/Horizontal focusing, Pair
	Be window	Double-side polished, 127-um-thick
	Slits	4-way slit, HV
	Attenuator	8-channel (Al, Mn + block)
67	Kappa diffractometer	LM-guide or Air-bearing base plate

E. Optics Overview

(1) Optical layout

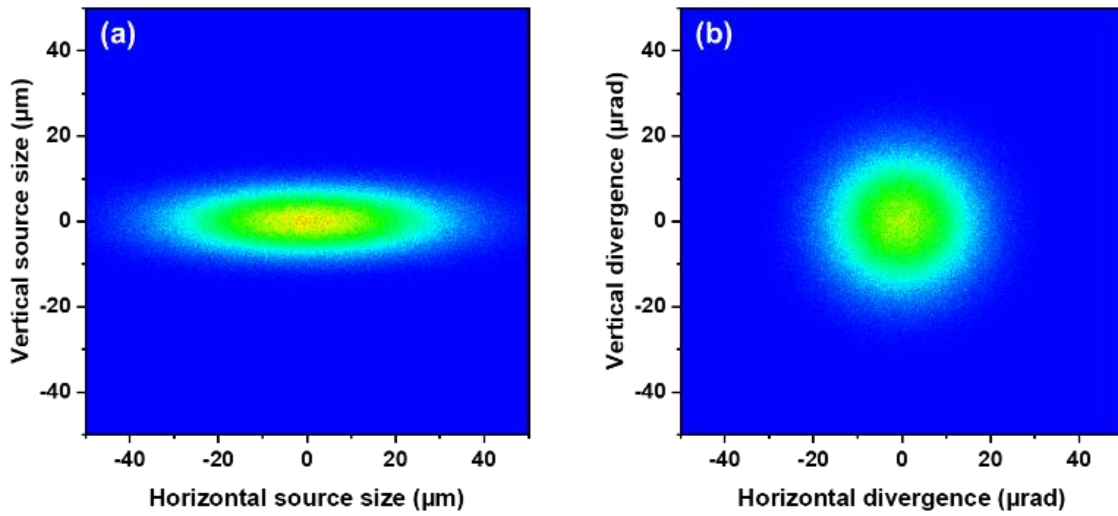


<Figure 3.2.5.3> Optical layout of Coherent X-ray Diffraction beamline. HDCM is horizontal deflection double crystal monochromator. HHRM is horizontal deflection high harmonics rejection mirror, and incidence angle is fixed at 2.5 mrad. Focusing optics is only KB mirror, there have fixed curvature FMM: Front-end Movable Mask, WBA: White Beam Attenuator, WBS: White Beam Screen, QBPM: Quadrant Beam Position Monitor.

<Figure 3.2.5.3> shows the optical layout of the coherent X-ray diffraction beamline. The specifications of the optical components must be defined to preserve the wavefront along the beam path to the sample. In order to achieve this, each optical element must be designed with a slope error of less than $0.1 \mu\text{rad}$ and the surface roughness below 0.1 nm . In addition, all slits will be manufactured with super-polished slit blades to have a roughness of less than 25 nm RMS to minimize parasitic scattering. Horizontal deflection optics are employed to minimize vibration effects, and the minimum window design ensures UHV conditions are maintained up to the KB mirror.

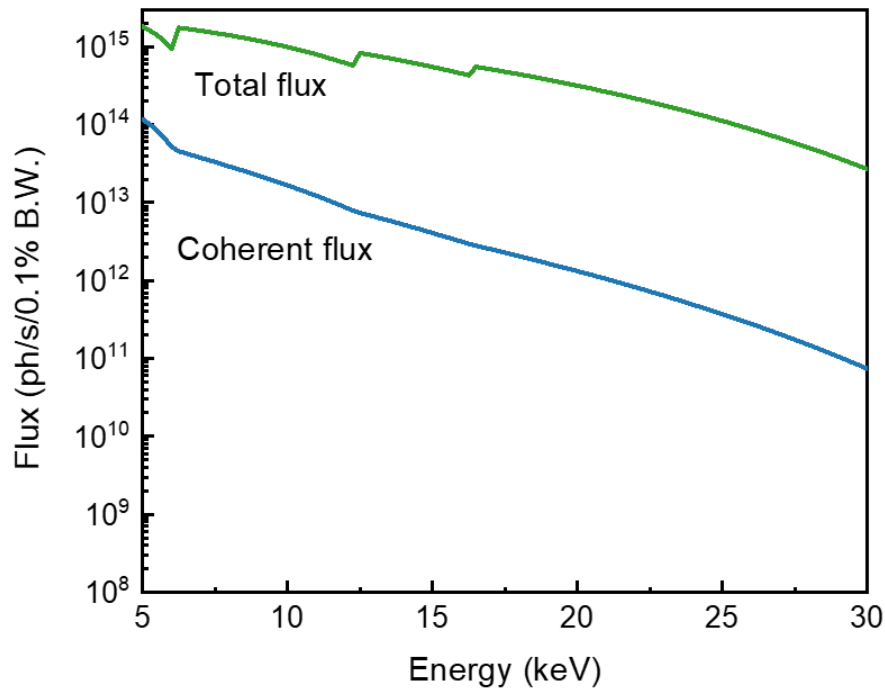
(2) Optics Simulation and beam properties

The simulation results were obtained using ShadowOui and XOPPY within the OASYS environment, along with SPECTRA. And the focal spot size using KB mirror is calculated based on the results of Hybrid simulation. All values are reported as FWHM.



<Figure 3.2.5.4> (a) IVU22 source size, (b) divergence at 6 keV (ideal).

As shown in <Figure 3.2.5.4.(a)>, the source size is approximately vertically 10 μm and horizontally 40 μm at 6 keV, and remains nearly constant over the entire energy range (5 to 30 keV). And the divergence is about 22 μrad both, as shown in <Figure 3.2.6.4.(b)>. As the beam propagates downstream, the vertical and horizontal beam size become increasingly similar.



<Figure 3.2.5.5> IVU22 source total flux and coherent flux at 5 to 30 keV (0.1% B.W.).

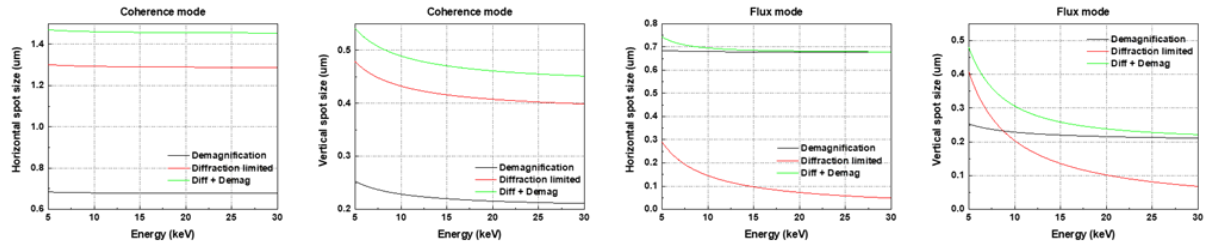
<Figure 3.2.5.5> shows the profiles of the total flux and coherent flux generated by the IVU22, including contributions up to the 7th harmonics. The values are from the source and are calculated assuming the 0.1% bandwidth. Around 5 keV, the coherent flux accounts for approximately 6% of the total flux, and this fraction decreases as the energy increases. At 30 keV, the coherent flux is reduced to about 0.27% at 30 keV.(Undulator phase error not considered.)

<Table 3.2.5.3> Flux of coherence mode and flux mode at the sample(idea)

	6 keV (3rd)	15 keV (5th)	30 keV (7th)
Coherence mode(ph/s)	3.54 x 10 ¹²	1.67 x 10 ¹¹	1.73 x 10 ⁹
Flux mode (ph/s)	2.55 x 10 ¹³	6.26 x 10 ¹²	2.2 x 10 ¹¹

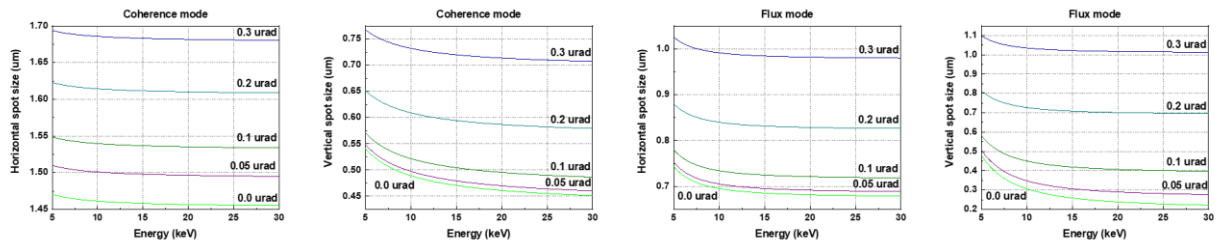
The beamline provides two operational modes: coherence mode and flux mode. The distinction between these modes lies in the degree of coherence, which is adjusted by the slit located in front of the KB mirror. In coherence mode, the slit is configured to deliver a fully coherent beam to the sample. In flux mode, the slit is opened to the maximum aperture size accepted by the KB mirror, which is 750 μm , in order to maximize the photon flux. The corresponding flux values at 6, 15, and 30 keV for both modes are shown in<Table 3.2.5.3>.

The focal spot size at the sample is calculated using a HYBRID method. This approach considers the effects of source demagnification, the diffraction-limited focus, and the slope error of the KB mirrors. The source demagnification is defined by the geometric reduction of the source size according to the distance ration from the source to the KB mirror and from the KB mirror to the sample. The diffraction-limited focus represents the smallest possible beam size achievable, constrained by the wavelength and the numerical aperture. And slope error, originating from imperfections during mirror manufacturing, leads to deviations from the ideal mirror surface. These deviations cause wavefront distortions that result in broadening of the focal spot size.



<Figure 3.2.5.6> Calculated focal spot size in coherence mode and flux mode using HYBRID method.

The source demagnification effect is the same in both modes, because it depends only on the source size and the distance between the source, the KB mirror, and the sample. On the other hand, the diffraction-limited spot size is determined by the slit located upstream of the KB mirror. This is because the source size and the focal length are the same in both modes, but the numerical aperture is different. In the coherence mode, the coherence length varies with energy, so the numerical aperture varies, which changes the effective aperture size of the beam incident on the mirror. However, in the flux mode, the aperture size is fixed. As shown in <Figure 3.2.5.6>, the diffraction-limited effect dominates over demagnification in coherence mode due to the smaller aperture size compared to flux mode. On the other hand, in flux mode, the horizontal spot size is more influenced by demagnification, while the dominant factor for the vertical spot size is reversed with energy.



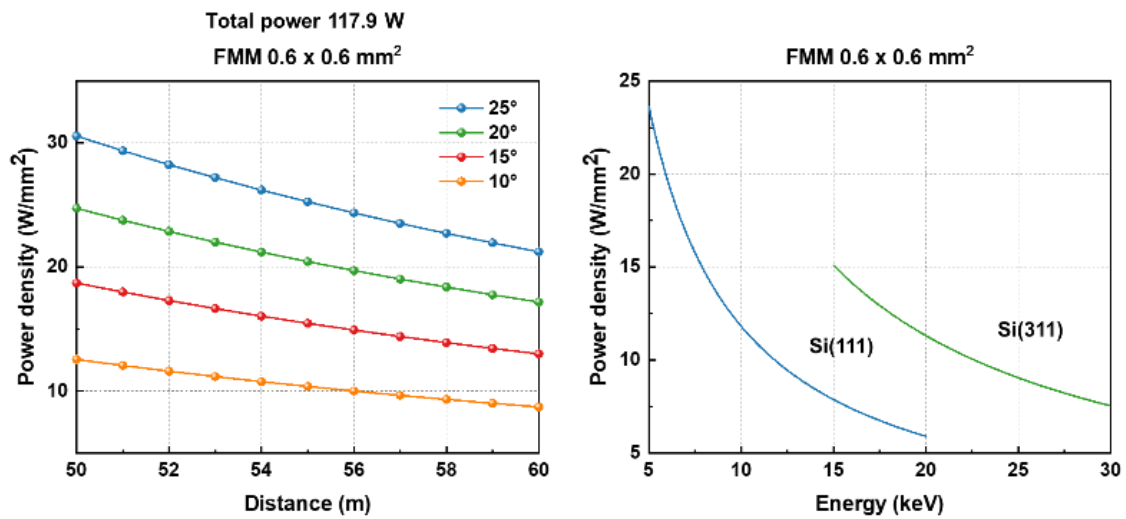
<Figure 3.2.5.7> Effect of slope error on focal spot size in coherence mode and flux mode.

In addition to the effects of demagnification and diffraction-limited focus, the influence of the mirror slope error is considered. The resulting focal spot size, including all contributions, is shown in <Figure 3.2.5.7>. The slope error is an inherent characteristic of all mirrors, and minimizing it is essential to reduce spot broadening. As the mirror length increases, the slope error tends to increase. The KB mirror is 300 mm length, and according to the specification from JTEC, the slope error is maintained below $0.1 \mu rad$. In coherence mode, the horizontal

spot size approximately $1.55\ \mu\text{m}$, and the vertical size is around 500 nm. In flux mode, the beam can be focused down to approximately 700 nm horizontally and to the 400 nm range vertically.

(3) Heat Load Consideration

This section discusses the heat load on the HDCM, as it is the first optics in the beamline and absorbs most of the heat load.



<Figure 3.2.5.8> Calculated power density on the HDCM with FMM opening of $0.6 \times 0.6\ \text{mm}^2$.

The incidence power on the HDCM is defined by the opening size at the FMM. Since the $0.6 \times 0.6\ \text{mm}^2$ opening is typically used during operation, the total power is approximately 117.9 W. The power density absorbed by the DCM varies depending on the Bragg angle, meaning that at low energy or when the DCM is positioned closer to the source(upstream), the beam footprint on the DCM becomes smaller, leading to higher power density. <Figure 3.2.5.8, (left)> shows the calculated power density as a function of distance from the source. In this beamline, the DCM is placed as far downstream as possible to reduce the power density. <Figure 3.2.5.8, (right)> presents the power density absorbed by the DCM as a function of energy at the fixed distance of 55 m. Currently available monochromator from overseas manufactures are designed to withstand up to three times the power density shown <Figure 3.2.5.8>, so significant thermal load issues are not expected. However, a small slope error may arise due to thermal bump, and the detailed thermal analysis will be conducted.

(4) Optics specification and tolerance

<Table 3.2.5.4> Specifications of the Coherent X-ray Diffraction beamline optical components

	HDCM	HHRM	KB (VFM)	KB (HFM)
Distance	55 m	61 m	65.6 m	66 m
Incident Angle	3 to 45 degree	2.5 mrad	2.5 mrad	2.5 mrad
Direction	Horizontal (Hall 25 mm offset)	Horizontal (Hall)	Vertical (Up)	Horizontal (Ring)
Shape	Plane	Plane	Elliptical	Elliptical
Image distance	-	-	1.4 m	1 m
Coating materials	-	Si, Rh, Pt (50 nm)	Si, Rh, Pt (50 nm)	Si, Rh, Pt (50 nm)
Mirror size (L x W x T, mm³)	1 st : 50 x 20 x 40 2 nd : 60 x 20 x 40	800 x 50 x 50	300 x 50 x 50	300 x 50 x 50
Slope error (μrad, RMS)	< 1	< 0.1	< 0.1	< 0.1
Roughness (nm, RMS)	< 0.5	< 0.2	< 0.2	< 0.2

The specifications of the crystals and mirrors of main optics are summarized in <Table 3.2.5.4>. The HDCM incorporates both Silicon 111 and 311 crystals to cover the energy range from 5 to 30 keV. Considering the heat load, the crystals are designed with a side-cooling mechanism, resulting in a thickness of 40 mm. The HHRM deflects the beam horizontally toward the experimental hall, and its surface shape is flat. The mirror is coated with Si, Rh, and Pt. With an incidence angle of 2.5 mrad, it can cover energy up to 30 keV. Similarly, the KB mirrors also adopt the same incidence angle; however, the mirrors are 300 mm length and fabricated with an elliptical surface. All mirrors are designed with a slope error of less than 0.1 μ rad and surface roughness below 0.2 nm.

<Table 3.2.5.5> Vertical and horizontal beam offset at each optical component

	IVU22	HDCM	HHRM	QBPM	VFM	HFM	Diffractionmeter	Detector	
Distance (m)	0	55	61	63	65.6	66	67	67.5	70
Vertical (mm)	1,400	1,400	1,400	1,400	1,400	1,402	1407	1,409.5	1,422
Horizontal (mm)	0	0	-25	-10	-2	0	0	0	0
Remark	-	Offset 25 mm	Hall 2.5 mrad	-	Up 2.5 mrad	Ring 2.5 mrad	-	-	-

<Table 3.2.5.5> summarizes the beam offset at each optical component position. The undulator beam generates at a height of 1400 mm, and its horizontal offset is set to 0 as the reference point. The coordinate system is defined such that, with respect to the beam propagation direction, the ring direction is negative and the experimental hall is positive; upward is positive and downward is negative. The fixed horizontal offset is introduced at the HDCM toward the hall direction. Subsequently, the HHRM reflects the beam toward the hall direction with an incidence angle of 2.5 mrad.

As a result, the actual reflection angle becomes 5 mrad, leading to a horizontal offset of -10 mm at the QBPM. The beam is then reflected again by the HFM toward the ring, also with an angle of incidence of 2.5 mrad, restoring the horizontal beam offset to 0 mm at the sample position. In the vertical direction, there is one upward reflection from the VFM, which moves the beam height at the sample from the floor to 1,407 mm. At the detector position, the beam can reach a maximum height of 22 mm. Based on the beam path offset described in <Table 3.2.5.4>, the translation range of each optical component must be considered. In addition, in the event that a different focusing optic is used in place of the KB mirror in the future, the manipulator will be designed to allow for the KB mirror to be by-passed.

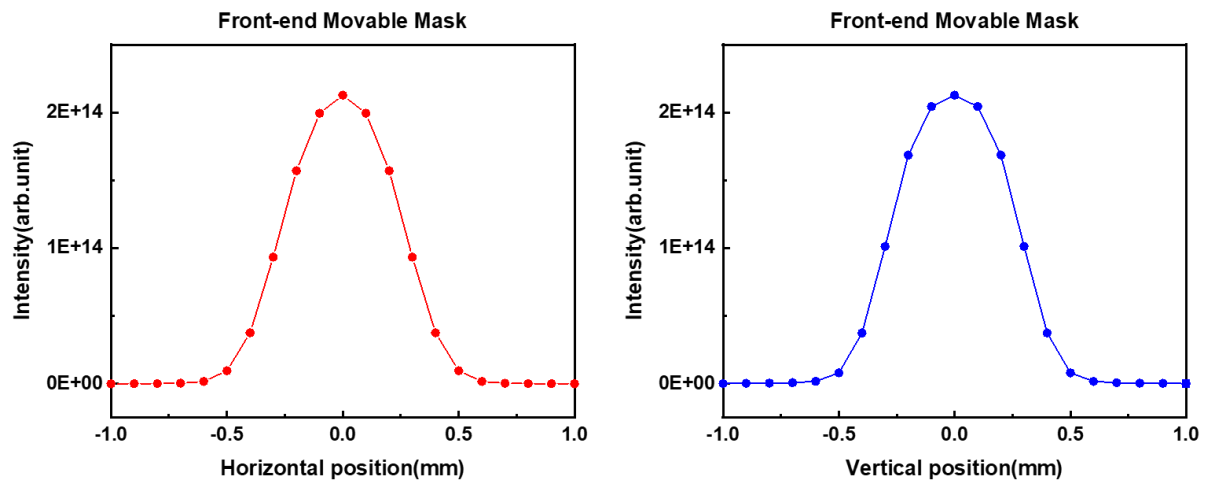
(5) Optics alignment

- Beamline alignment is performed sequentially from upstream to downstream.

The slits located in the optical hutch are opened sufficiently around 5 mm to avoid interfering with the beam. The first process is the movable mask alignment located in the front-end, which is initially opened to $0.2 \times 0.2 \text{ mm}^2$. The scan is then scanned in the vertical and horizontal directions the mask $\pm 1 \text{ mm}$. The intensity is monitored using the QBPM positioned at the end

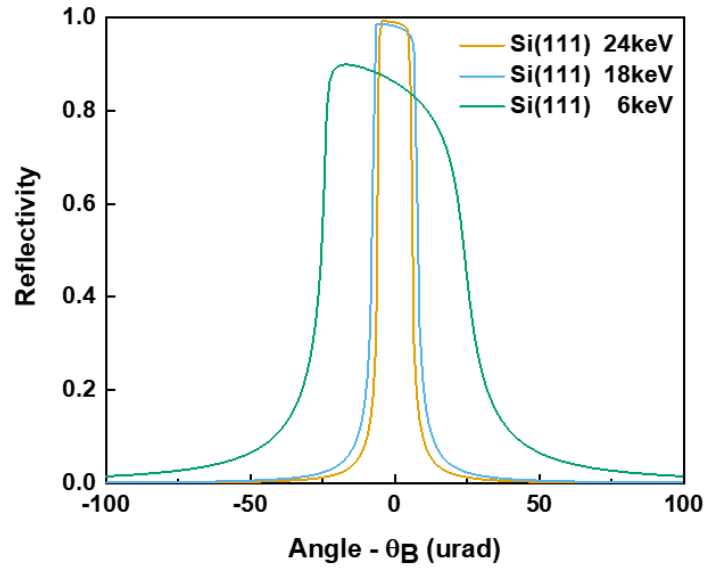
of the optical hutch. The scan results in the beam profile, as shown in <Figure 3.2.5.9>. The movable mask is aligned to the center position of this profile. Then, based on the FWHM of the profile, the opening of the mask is adjusted accordingly—typically to 0.5 or 0.6 mm, depending on the photon energy.

Next, the white beam slit located upstream of the HDCM is opened to $0.5 \times 0.5 \text{ mm}^2$, similar to the movable mask, and scanned $\pm 2 \text{ mm}$. The vertical and horizontal slit positions are then aligned to the center of the beam profile. The slit is opened to approximately twice the FWHM of the profile in each direction. As a result, only the beam with parasitic scattering removed by the movable mask is incident on the HDCM.



<Figure 3.2.5.9> Front End Movable Mask alignment beam profile.

DCM alignment involves two procedures: one is calibrating the Bragg angle variable by scanning the absorption edge of the reference foil near the target energy, and the other is detuning the high order harmonics generated by the silicon crystal. Energy calibration is performed by the reference foil and scanning the energy to obtain the absorption spectrum. The difference between the measured and ideal absorption edge is used to correct the Bragg angle. This can be done by using the foil located at the QBPM. Alternatively, the reference foil set can be installed upstream of the QBPM and inserted only during the calibration process. The final design of the calibration system will be determined after testing at PLS-II.



<Figure 3.2.5.10> Darwin width curve at 6 keV and its high-order harmonics.

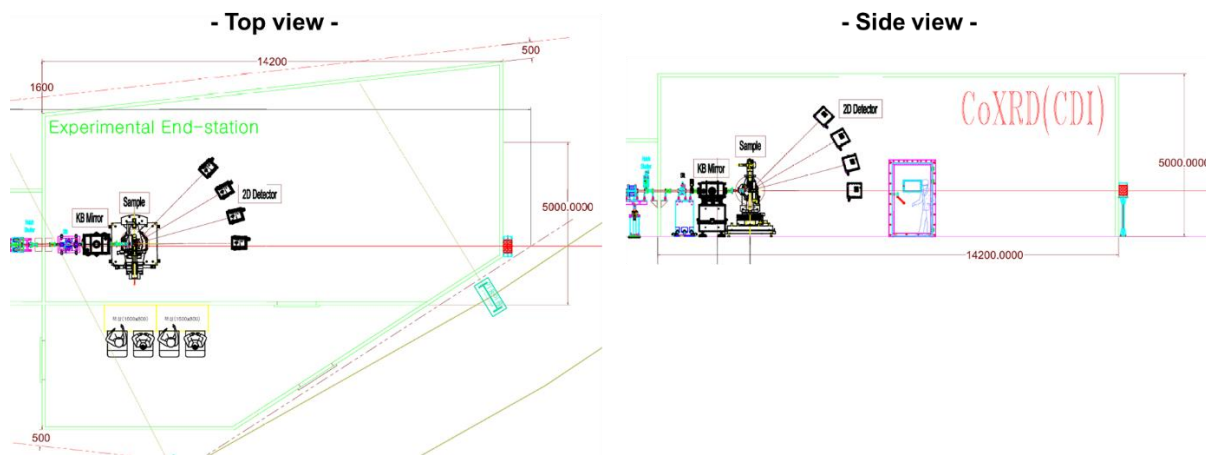
DCM detuning is the method used to suppress high-order harmonics generated from the silicon crystals. As shown in <Figure 3.2.5.10>, the Darwin width decreases with increasing energy, which can be exploited to attenuate high-order harmonics. The procedure involves adjusting the pitch of the second DCM crystal while monitoring I_0 at the QBPM. The intensity is typically reduced to 70–80% of the maximum to effectively suppress harmonics. However, at lower energy, where the difference in Darwin width between the fundamental and harmonic reflections is relatively small. So, detuning may need to be increased up to 50% for sufficient suppression. Downstream of the DCM, several slits are placed to remove parasitic scattering of the mono beam. These slits are scanned with a small opening and then opened to about twice the FWHM.

The HHRM operates with a fixed incidence angle, so alignment is not required; only the coating material needs to be switched depending on the energy range. The slit located in front of the KB mirror determines the degree of coherence of the beam incident on the KB mirrors. In coherence mode, the slit opening is defined based on the transverse coherence length at each energy. In flux mode, the slit is fully opened to the maximum aperture size accepted by the mirrors, which is $750\ \mu\text{m}$. This is also aligned by scanning its center position of the beam, using the QBPM placed in front of the sample to measure I_0 . Finally, the rotation center of the diffractometer is aligned using a knife-edge or alignment pin. If an experiment requires a larger

beam size, the pitch motion of the KB mirror can be adjusted to defocus the beam at the rotation center of the diffractometer.

F. Instrument Overview

(1) Experimental floor and hutch design



<Figure 3.2.5.11> Experimental hutch drawing of Coherent X-ray Diffraction Beamline.

Beam stability directly affects data quality; therefore, temperature and humidity control are critical factors. Since the KB mirror, which serves as the focusing optics, is located inside the experimental hutch, thermal drift and vibrations of the mirror surface, mirror chamber, or supporting girder may cause shifts in the focused beam position at the sample. Therefore, the system is designed to maintain thermal stability within ± 0.1 K (long term, 1 to 2 days) and ± 0.05 K (short term, 1 to 2 hours).

Currently, to minimize temperature and vibration fluctuations caused by air inflow, plans are underway to separate the space housing the KB mirror chamber from the diffractometer at the sample position. Additionally, to prevent ingress of outside air during access and to maintain stable temperature and humidity inside the hutch, an independent air curtain area will be installed at the hutch entrance, enabling a double-door system for controlled access. The current design is provisional and may be revised in response to ongoing discussions and future technical requirements.

(2) Experimental method

○ Bragg Coherent Diffraction Imaging (BCDI)

BCDI enables three-dimensional imaging of lattice strain and structural defects in single-crystalline particles ranging from tens of nanometers to several micrometers in size. In a typical experiment, isolated crystalline particles are sparsely deposited onto a flat substrate. A high-precision micro- or nano-positioning stage is used to locate individual particles that produce coherent diffraction signals. An auxiliary optical microscope aligned perpendicular to the sample surface assists in determining the approximate spatial distribution of particles and pre-aligning the focal plane. Automated routines—including half-cut scanning strategies—are implemented through custom-coded control software. Experimental parameters such as the sample-to-detector distance and detector pixel size are carefully optimized to achieve a high oversampling ratio, which is critical for resolving interference fringes (streaks) in the diffraction pattern arising from finite particle dimensions. A detector with a large active area provides a wider reciprocal space coverage, facilitating the capture of extended diffraction features and multiple Bragg peaks.

BCDI measurements can also be performed under resonant conditions, where the X-ray energy is tuned across the absorption edge of a specific element. This allows element-specific imaging by acquiring datasets below, at, and above the absorption edge, thereby enabling spatial mapping of selected atomic species. A full 3D reciprocal space dataset is collected via omega rocking scans, and real-space reconstruction is carried out using phase retrieval algorithms. To streamline user access, the entire data acquisition and analysis workflow is automated via integrated software pipelines, and future development aims to incorporate machine learning-based reconstruction algorithms for enhanced robustness and speed.

○ Microbeam X-ray Diffraction (μ XRD)

The μ XRD technique adopts the same optical and geometric principles as BCDI, but emphasizes control over the beam size to suit various sample requirements. In particular, when measuring nanostructures such as nanowires, μ XRD can be performed in multimodal mode, simultaneously acquiring X-ray diffraction, X-ray fluorescence (XRF), and X-ray absorption near-edge structure (XANES) data from a specific location on the sample. This provides comprehensive structural and chemical information from the same spatial region, enabling detailed in-situ or operando investigations of localized phenomena.

○ **Three-Dimensional X-ray Diffraction (3DXRD)**

3DXRD is implemented using high-energy X-rays (upto 30 keV) to penetrate polycrystalline samples and resolve the orientation and strain state of individual grains. The sample is mounted on an azimuthal rotation stage, and diffraction patterns are recorded at various angles to reconstruct a full 3D reciprocal space volume. A fixed-area detector is positioned at a distance of approximately 40 to 50 cm from the sample, providing sufficient angular resolution. In the case of 3DXRD, the beam size defines the field of view and is typically set in the range of a few to several tens of micrometers, depending on the grain size and spatial resolution requirements. Computational methods are then applied to reconstruct the real-space distribution of crystallographic domains, enabling grain-resolved imaging of microstructure in materials such as stainless steel and other engineering alloys.

○ **Dark-field X-ray Microscopy (DFXM)**

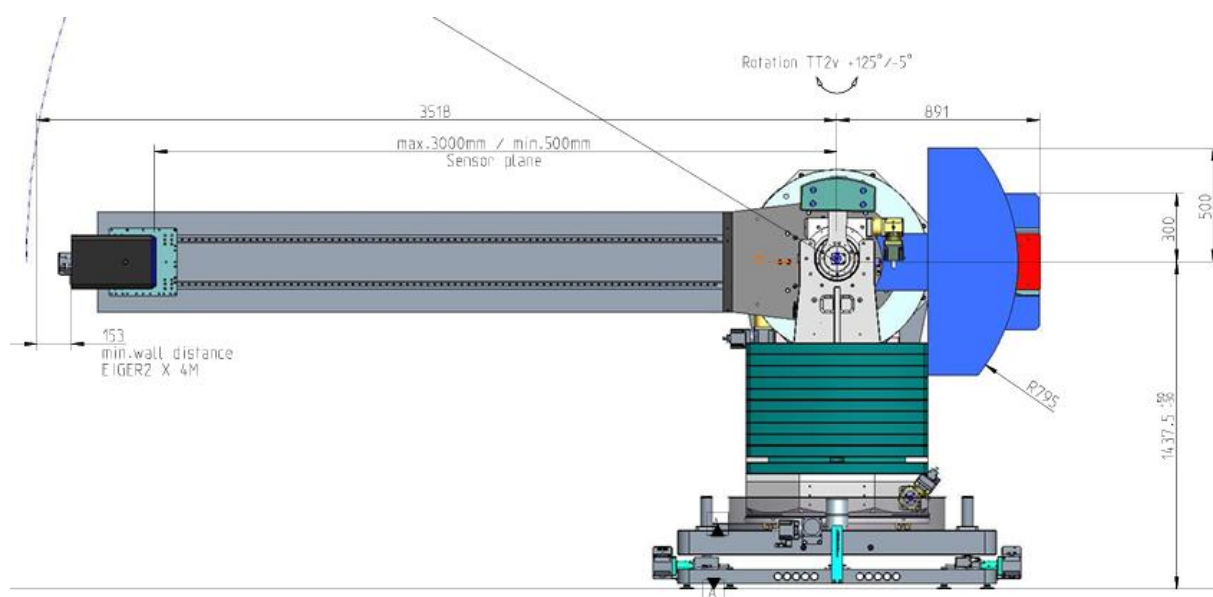
DFXM is a lens-based Bragg imaging technique that converts coherent diffraction signals collected in the far-field into real-space images by inserting a stacked compound refractive lens (CRL) at the diffraction condition corresponding to a selected Q vector. The technique requires an extended optical path length between the CRL and detector to achieve high spatial resolution. The beamline hutch is therefore designed to support sample-to-detector distances exceeding 10 meters, and the detection geometry is configured to accommodate 2θ angles from approximately 10° to 50° . Because DFXM forms images based on Bragg peak intensities, it exhibits high sensitivity to local lattice distortions and defects, making it an ideal tool for studying materials with complex defect structures. The method is particularly powerful for probing strain fields, dislocation networks, and domain boundaries in functional crystalline systems.

(3) Diffractometer

The diffractometer is a customized combination of a 6-circle and Kappa goniometer, optimized for a wide range of *in-situ/operando* X-ray diffraction experiments. This diffractometer is particularly well-suited for diffraction-based studies, as it enables precise measurement of both specular and off-specular diffraction geometries, thereby providing enhanced versatility for probing a wide range of crystallographic planes and structural features.

To accommodate various sample environments, the goniometer is designed with a maximum load capacity of 20 kg, allowing for the integration of advanced stages and environmental chambers—including nano-positioning stages, heating and cooling units, and battery test cells.

The detector arm will support automated translation of an image detector over a range of 0.5 to 3 meters, enabling flexible acquisition geometries for matching proper oversampling ratio and angle-resolved measurements and 3D-XRD geometry. The experimental hutch is dimensioned to permit a two-theta angular range exceeding 90° in the out-of-plane direction and up to $\pm 45^\circ$ in the in-plane direction, ensuring comprehensive reciprocal space coverage for advanced diffraction and imaging applications.



<Figure 3.2.5.12> Design of the 6-circle diffractometer with Kappa goniometer.

(4) Detector

The detection system will incorporate two two-dimensional detectors—EIGER2 X 4M and LAMBDA 250k—as well as a silicon drift detector to enable multi-modal data acquisition. The EIGER2 X 4M detector, featuring a pixel size of $75 \mu\text{m}$ and a matrix of $2,068 \times 2,162$ pixels, provides a sufficiently large active area to fully capture the diffraction patterns typically observed in Bragg Coherent Diffraction Imaging (BCDI) experiments. The flexibility in the sample-to-detector distance, ranging from approximately 0.5 to 3 meters, allows for tuning of the oversampling ratio, and—when considered together with the pixel size—supports measurements of crystalline particles ranging from $\sim 100 \text{ nm}$ to several micrometers in size.

The LAMBDA 250k detector, with its 55 μm pixel size, offers a higher oversampling ratio compared to larger-pixel detectors, making it particularly advantageous for coherent diffraction imaging.

Furthermore, its high frame rate capabilities render it well-suited for investigating fast structural dynamics. The beamline is thus designed to support time-resolved X-ray diffraction experiments, enabling the study of ultrafast processes in crystalline materials. The SDD will be employed for XRF, GIXRF, GIXRF-XANES and also it will be particularly suitable for mapping the spatial distribution of elements during Bragg ptychography. Given that the final construction and commissioning of the beamline is still underway, it is important to note that the choice of detector remains subject to change. As the procurement will occur closer to the completion date, there is a strong possibility of selecting detectors that reflect the highest performance available at the time.

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3.2.6 ID03 CoSAXS Beamline

A. Introduction

COSAXS (Coherent Small-Angle X-ray Scattering) beamline is aiming to provide the dynamic measurement techniques using a hard X-ray speckle. A higher spatial coherence fractions and photon flux enhanced by the implementation of a multi-bend achromat lattice on the storage ring will help users to collect sufficient speckle contrast on the detector with a sufficient photon flux. X-ray Photon Correlation Spectroscopy (XPCS) will be one of the main activities planned at the COSAXS beamline, but also Small-Angle X-ray Scattering (SAXS) and Wide-Angle X-ray Scattering (WAXS) together with grazing incidence techniques can be foreseen taking advantage of the high flux of the 4th generation synchrotron radiation source.

The primary photon energy range of COSAXS beamline will be 8 to 12 keV, which offers sufficient coherent flux for the speckle-based experiments, Photon energies up to 30 keV will be available upon the user request, enabling measurements condensed matter systems that requires deeper penetration depth and/or higher wavevector for atomic scale investigations. To support this, two coating materials, e.g., Rhodium (Rh) and Platinum (Pt), will be applied to the High Heat Load Mirror (HHLM) to suppress high harmonic energies generated by the in-vacuum undulator. The focusing scheme using two CRL (Compound Refractive Lens) transfocators for varying X-ray beam size on the sample. This tunable beam size enables to improves speckle contrast and signal to noise ratio (*SNR*) while optimizing the X-ray dose delivered to the sample during XPCS measurement.

A sample hexapod with high precision and freedom of movement helps overcome limitations in sample mounting strategies. It allows for a wide range of sample environments and supports the integration of various sample chamber designs, whether for user experiments or in-house development projects. This flexibility enables diverse in-situ and operando experiments, including XPCS, time-resolved, and real-time SAXS and WAXS measurements. The scattered signal will travel through a vacuum flight tube and reach a two-dimensional area X-ray detector located up to 8 meters downstream from the sample. During measurements, the sample to detector distance can be varied between 3 and 8 meters to optimize experimental conditions. The flight tube length will be adjustable accordingly while maintaining vacuum conditions. The COSAXS beamline will also support wide angle scattering geometries by swinging the detector and flight tube system up to 30 degrees in the horizontal direction. An additional

detector stage positioned 1 meter downstream of the sample will be available for scattering angles greater than 30 degrees or for simultaneous SAXS and WAXS measurements.

The mission of the COSAXS beamline is to serve as a dedicated platform for coherent X-ray scattering experiments, with a particular focus on dynamic studies using techniques such as X-ray Photon Correlation Spectroscopy. At the same time, it will provide comprehensive support for a broad spectrum of conventional X-ray scattering methods, including SAXS and WAXS, both in transmission and grazing incidence geometries. To meet the increasingly diverse and challenging experimental demands from academic and applied research communities, the beamline must maintain a high level of adaptability in both optical configuration and operational conditions. This includes the ability to finely tune beam properties ensuring compatibility with a wide variety of experimental setups. Moreover, the experimental infrastructure is designed to accommodate different specialized sample environments, allowing seamless integration of user defined or in-house developed chambers, including those for in-situ and operando studies. Such flexibility is essential for enabling advanced measurements under realistic sample conditions, ultimately supporting a wide range of scientific programs from soft matter physics to complex materials research.

B. Scientific Objective

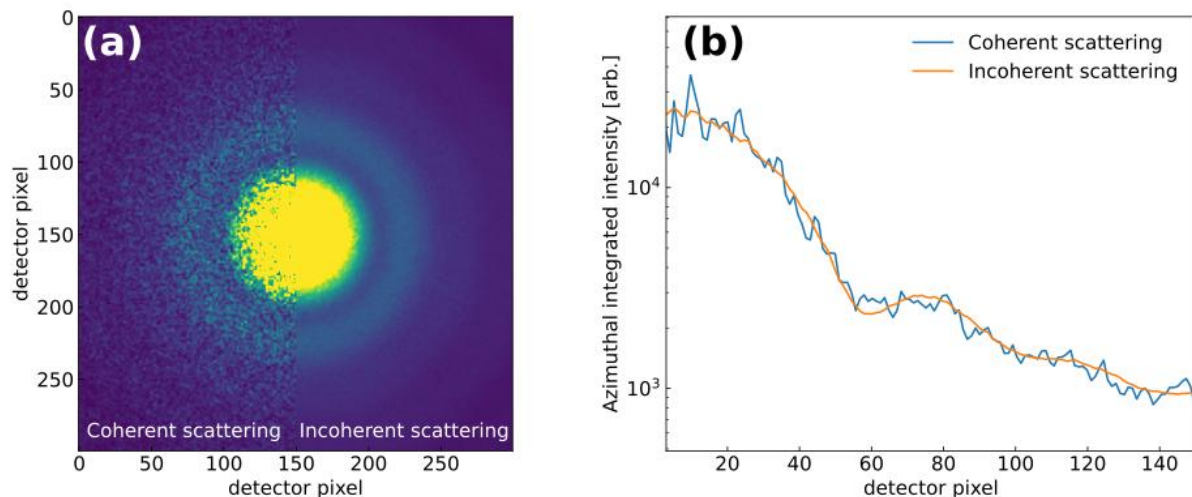
This beamline is dedicated to enabling comprehensive investigations of nanoscale structure and dynamics in soft condensed matter, complex fluids, biological assemblies, and other non-crystalline systems. Leveraging the high brightness and transverse coherence of a 4GSR, the primary experimental techniques will include SAXS and XPCS, with additional capabilities extending into grazing incidence geometries and wide-angle scattering as well. SAXS will provide access to static structural information across a broad range of length scales, enabling precise characterization of hierarchical architectures, mesoscopic domains, and self-assembled nanostructures. In parallel, XPCS will enable quantitative analysis of dynamic processes under equilibrium and non-equilibrium conditions, as well as in systems exhibiting spatial or temporal heterogeneity. Two-time correlation functions (TTCF) will be employed to capture the full temporal evolution of the system, providing insight into aging, intermittency, and non-stationary behavior that cannot be accessed through conventional time averaged approaches. To further expand the scientific reach, GI- SAXS and XPCS will be actively utilized to probe

interfacial and surface phenomena. These measurements will be conducted under in-situ and operando conditions, enabling time-resolved observation of structural and dynamical transformations in thin films, membranes, and confined environments. The beamline will be optimized to routinely achieve millisecond scale time resolution for XPCS, with dedicated efforts aimed at pushing the frontier toward the microsecond regime. In response to emerging scientific demands, speckle based experiments in the wide-angle scattering domain will also be explored, enabling the investigation of faster dynamics and short range order in dense or partially ordered systems. By integrating high coherent flux, advanced detection capabilities, and versatile sample environments, the beamline will serve as a unique platform for addressing fundamental and applied research challenges across soft matter physics, materials science, and biophysics.

(1) X-ray photon correlation spectroscopy

X ray Photon Correlation Spectroscopy (XPCS) is a powerful and well-established technique for investigating the dynamics of complex disordered systems in condensed matter. It has been successfully applied to a wide range of materials, including colloids (*Dierker et al., 1995; Grübel & Zontone, 2004; Jo et al., 2021*), polymers (*Frenzel et al., 2019; Lehmkuhler et al., 2018*), capillary waves (*Gutt et al., 2003*), metallic glasses (*Evenson et al., 2015; Ruta et al., 2012a*), molecular glasses (*Chushkin et al., 2012*), and water (*Perakis et al., 2017, 2018*).

XPCS evolved from the well-established visible light Photon Correlation Spectroscopy (PCS) technique (*Cipelletti & Weitz, 1999; Dorfmueller, 1992; Provencher, 1979*), in which a coherent laser beam serves as the light source. The advent of high brilliance 3rd generation synchrotron radiation facilities enabled PCS to be extended to X-ray wavelengths, thereby expanding the accessible scattering vector range from approximately $10^{-3} \text{ \AA}^{-1}$ to several $\text{\AA}^{-1}$. Because the wavelength of the probe beam determines spatial resolution, using X-rays as the probe is essential for studying atomic scale dynamics (*Leitner et al., 2009*).



<Figure 3.2.6.1> Coherent and incoherent scattering simulation result. (a) The 2D image of scattering from coherent (left) and incoherent (right) scattering, respectively. (b) The azimuthally integrated intensity profiles.

In XPCS, a disordered sample is illuminated with a coherent X ray beam, producing a grainy interference pattern, commonly referred to as a “speckle” pattern (*Sutton et al., 1991*), in the far field. A high resolution 2D area detector records these speckles, which encode detailed information about the spatial arrangement of scatterers in the sample. If the arrangement evolves over time, the speckle pattern changes accordingly. By acquiring a time series of speckle images, temporal intensity fluctuations can be analyzed through the intensity–intensity autocorrelation function to extract quantitative information on the dynamics of the system.

<Figure 3.2.6.1> (a) presents simulated two-dimensional detector images for coherent (left) and incoherent (right) scattering. In the coherent case, a well-defined speckle interference pattern is observed, while the incoherent case exhibits a featureless and smoothly varying scattering distribution due to the absence of mutual phase relationships among the scattered waves. <Figure 3.2.6.1> (b) shows the corresponding azimuthally integrated intensity profiles. The incoherent scattering yields a typical Small-Angle X-ray scattering (SAXS) profile that represents the ensemble averaged structure of the sample. In contrast, the coherent scattering profile displays numerous pronounced intensity modulations superimposed on the SAXS profile. These modulations arise from the discrete speckle maxima and minima in the coherent scattering image, which directly encode the instantaneous spatial configuration of the scattering entities and are a hallmark of the interference of coherently scattered X-rays.

The first experimental demonstration of XPCS was reported in 1995 (*Brauer et al., 1995*). Since then, dedicated XPCS beamlines have been established at facilities such as the European Synchrotron Radiation Facility (ESRF) in France (*Grübel et al., 1994*) and the Advanced Photon Source (APS) in the USA (*Sandy et al., 1999*). A second generation of XPCS beamlines, offering higher coherent flux and more versatile scattering geometries, was later constructed at PETRA III and NSLS II. XPCS has also become a key driver in the development of X ray free electron laser (XFEL) science, with dedicated instruments such as X ray Correlation Spectroscopy (XCS) at LCLS (*Alonso-Mori et al., 2015*) and the Materials Imaging and Dynamics (MID) instrument at the European XFEL (*Madsen et al., 2021*). The impact and growth of XPCS have been quantitatively analyzed by (*Lehmkuhler et al., 2021*), who surveyed the number of publications per year and their research topics. A bibliometric search in SCOPUS and Web of Science for “X-ray Photon Correlation Spectroscopy” and its alternative terms, “X-ray Intensity Fluctuation Spectroscopy” (XIFS) and “X ray Speckle Visibility Spectroscopy” (XSVS), restricted to titles, keywords, and abstracts, revealed a steady linear increase in publications since the late 1990s, reaching more than 40 papers in 2020. The actual number is likely higher, as the search criteria may exclude relevant works.

The temporal correlation in XPCS is quantified through the normalized intensity autocorrelation function $g(q, t)$. For an ergodic system, g_2 can be expressed in terms of the ensemble averaged temporal correlation function of the scattered field (*Ferreira et al., 2020*; *Siegert, 1943*):

$$g(q, \tau) = \frac{\langle I(q, t)I(q, t + \tau) \rangle}{\langle I(q) \rangle^2} = 1 + \beta(q)\exp(-2\Gamma(q)\tau)$$

Here β and τ are speckle contrast and delay time, respectively. $I(q, t)$ is the intensity at the wavevector q and time t . The momentum transfer q is defined by the X-ray wavelength λ and the scattering angle 2θ according to $q = \frac{4\pi}{\lambda}\sin\theta$. The β is determined by the experimental setup and configuration which will be described in the Beamline Goal chapter. For a system of Brownian colloidal nanoparticles dispersed in a solvent, the relaxation rate $\Gamma(q)$ is related to the free particle diffusion coefficient $D_0 = \Gamma(q)/q^2$. The Stokes-Einstein relation, expressed as $D_0 = \frac{k_b T}{6\pi R\eta}$, where R, η, k_b , and T are particle radius, solvent

viscosity, Boltzmann constant, and absolute temperature of the system, respectively, provides the thermodynamic properties of the measured system. In concentrated suspensions, interparticle interactions slow down the dynamics, and the effective diffusion coefficient becomes q dependent:

$$D(q) = \frac{D_0 H(q)}{S(q)}$$

Where $S(q)$ is the static structure factor and $H(q)$ is the hydrodynamic function that accounts for hydrodynamic interactions, electrostatic repulsion, and solvent flow perturbations induced by particle motion (*Grübel et al., 2000; Riese et al., 2000*).

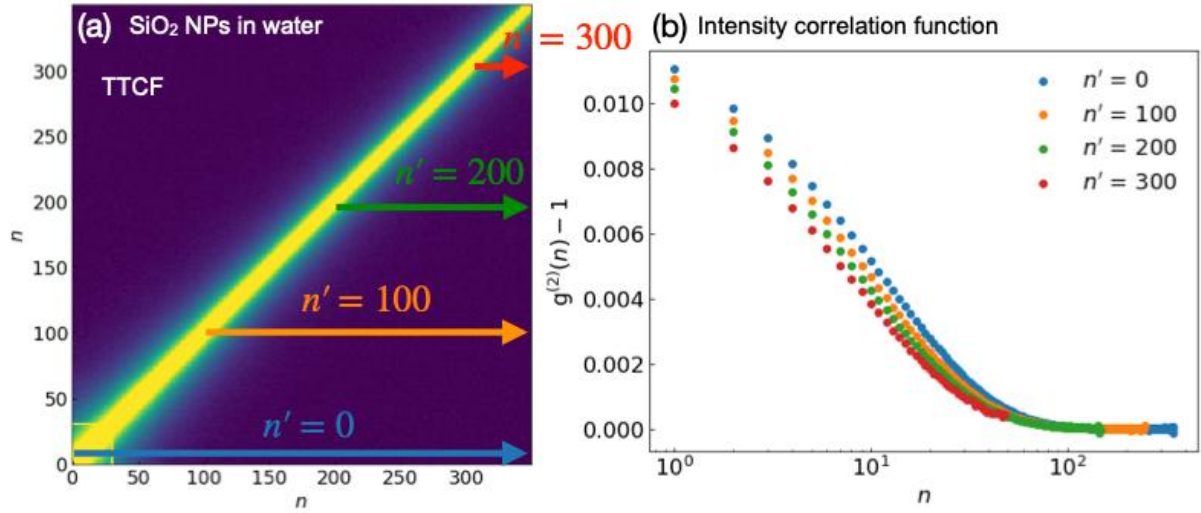
When the sample dynamics evolve during the measurement, the g_2 function may fail to capture the true dynamics due to averaging over time. In such cases, the two time correlation function (TTCF) is employed (*Madsen et al., 2010*):

$$C(q, t_1, t_2) = \frac{\langle I(q, t_1) I(q, t_2) \rangle}{\langle I(q, t_1) \rangle \langle I(q, t_2) \rangle}$$

The TTCF measures correlations between intensities at times t_1 and t_2 , averaged over all detector pixels corresponding to the same q , without time averaging. It is symmetric with respect to $t_1=t_2$, i.e., $C(q, t_1, t_2)=C(q, t_2, t_1)$. The conventional $g_2(q, \tau)$ functions is also extracted by averaging the TTCF over t_1 :

$$g_2(q, \tau) = \langle C(q, t_1, \tau) \rangle_{t_1} \text{ with } \tau = t_2 - t_1$$

<Figure 3.2.6.2> shows an example of XPCS results obtained at the Materials Imaging and Dynamics (MID) instrument of the European XFEL. The width of the diagonal in the TTCF reflects the sample diffusivity: narrower widths correspond to shorter correlation times. The extracted g_2 functions for various values of n' , the number of X-ray pulses included in the analysis, are shown in <Figure 3.2.6.2> (b). Increasing the number of pulses results in faster decorrelation, which is attributed to X-ray induced heating (*Dallari et al., 2024; Lehmkuhler et al., 2018*).



<Figure 3.2.6.2> XPCS result measured from European XFEL. (a) Two-time correlation function, and (b) extracted intensity correlation function for various number of X-ray pulses took into the calculation.

X-ray speckle-based techniques, including XPCS, provide a powerful means to investigate the dynamics of soft matter systems over a broad range of length and time scales, spanning from the atomic to the molecular scale and from several hours down to the sub millisecond regime. Owing to their versatility, these methods have found widespread application across diverse areas of condensed matter and materials science. Recent advances in high brilliance X-ray sources, such as state-of-the-art storage rings and XFELs, combined with the development of fast, low noise two-dimensional area detectors, have substantially extended the accessible dynamical window toward faster processes, thereby expanding the scientific reach of XPCS. Consequently, the technique is now employed to study an exceptionally wide spectrum of systems, including proteins (*Anthuparambil et al., 2023*), polymers (*Dallari et al., 2024*), biological environments (*Otto et al., 2022*), amorphous ice (*Ladd-Parada et al., 2022a*), bulk metallic glasses (*Frey et al., 2025*), charge density wave materials (*Campi et al., 2022*), and energy related materials (*Steinrück et al., 2020*). With its unique capability to probe nanoscale and mesoscale dynamics with high statistical precision, XPCS is poised to play an increasingly critical role in advancing our understanding of complex and functional materials.

(2) Small-Angle X-ray Scattering

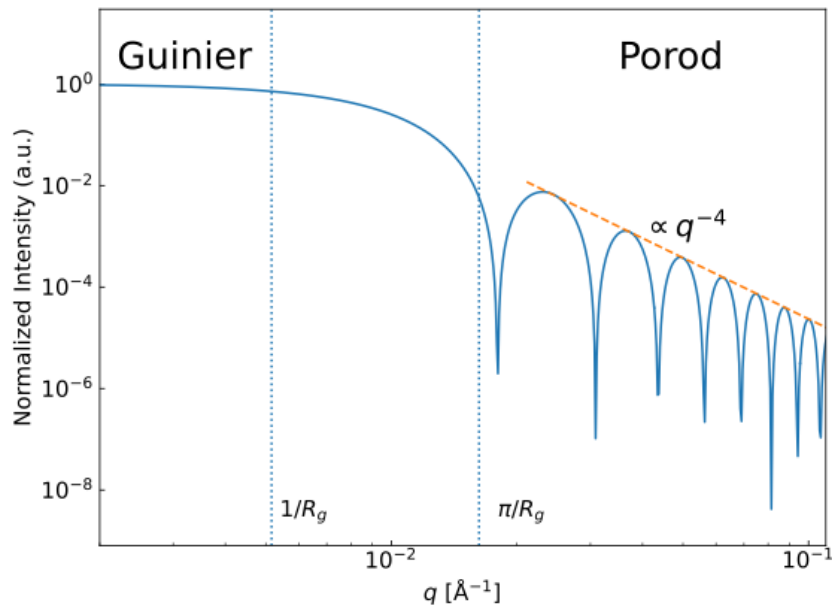
Small-Angle X-ray Scattering (SAXS) is one of the most fundamental and historically established techniques in X-ray scattering science (*Li et al., 2016*). Originating in the pioneering work of André Guinier in the 1930s and published in 1950s (*Guinier & Fournet, 1955*), SAXS has become a standard method for characterizing nanostructures in materials, with applications spanning soft matter (*Likos, 2006*), biology (*Schneidman-Duhovny et al., 2013*), and condensed matter physics (*Wang et al., 2003*). Its enduring relevance comes from the ability to non-destructively probe structures from a few nanometers to hundreds of nanometers with high statistical accuracy. In SAXS, a collimated or focused monochromatic X-ray beam is directed at the sample, and the scattered intensity is recorded at small scattering angles, typically corresponding to momentum transfer q in the range of $0.001 \text{ \AA}^{-1}$ – to $1 \text{ \AA}^{-1}$, which in real space corresponds to structural length scales of approximately 600 nm to 0.6 nm. The scattering pattern contains information on electron density fluctuations, which can be analyzed to extract parameters such as particle size, shape, internal structure, and spatial correlations.

A fundamental feature of SAXS analysis is the Guinier region, which corresponds to the very small q range where the scattering intensity reflects the overall size of the scattering object rather than its detailed internal structure. In this regime, the intensity can be described by the Guinier approximation (*Hammouda, 2010*):

$$I(q) \approx I(0) \exp\left(-\frac{q^2 R_g^2}{3}\right)$$

Where $I(q)$ is the forward scattering intensity and R_g is the radius of gyration of the particle. This expression is valid for $qR_g \lesssim 1$ provides a straightforward method to determine R_g by plotting $I(q)$ versus q (Guinier plot). The Guinier analysis is widely used in the characterization of proteins, polymers, colloids, and nanoparticles, offering a direct link between the measured scattering and the overall dimensions of the scattering entities. At intermediate q values, the scattering curve reflects information on particle shape, internal structure, and interparticle correlations. In this regime, the slope of the log-log plot of $I(q)$ versus q can often be related to the dimensionality of the scattering object: a slope of approximately -1 corresponds to rod-like structures, -2 to platelike structures, and -4 to compact spheres with smooth surfaces. Slopes between these values may indicate

polydispersity, surface roughness, or hierarchical structures. This region is often analyzed using model fitting or indirect Fourier transformation to reconstruct the pair distance distribution function $P(r)$, which yields insights into real space structural parameters such as maximum particle dimension and shape anisotropy. For systems with hierarchical or multi scale structures, the intermediate region may exhibit multiple structural features corresponding to different characteristic length scales. At high q values, in the so called Porod region, the scattering intensity often follows the Porod law: $I(q) \propto q^{-4}$ which indicates sharp interfaces between regions of different electron density. Deviations from the q^{-4} dependence can be used to infer surface roughness, fractal characteristics, or diffuse interfaces. Analysis of the Porod region is therefore valuable for quantifying surface to volume ratios and interface morphology in systems such as nanoparticles, porous materials, and composite structures. <Figure 3.2.6.3> shows an expected normalized SAXS profile of the simple sphere model.



<Figure 3.2.6.3> Normalized SAXS curves of sphere with the radius of $R = 25$ nm.

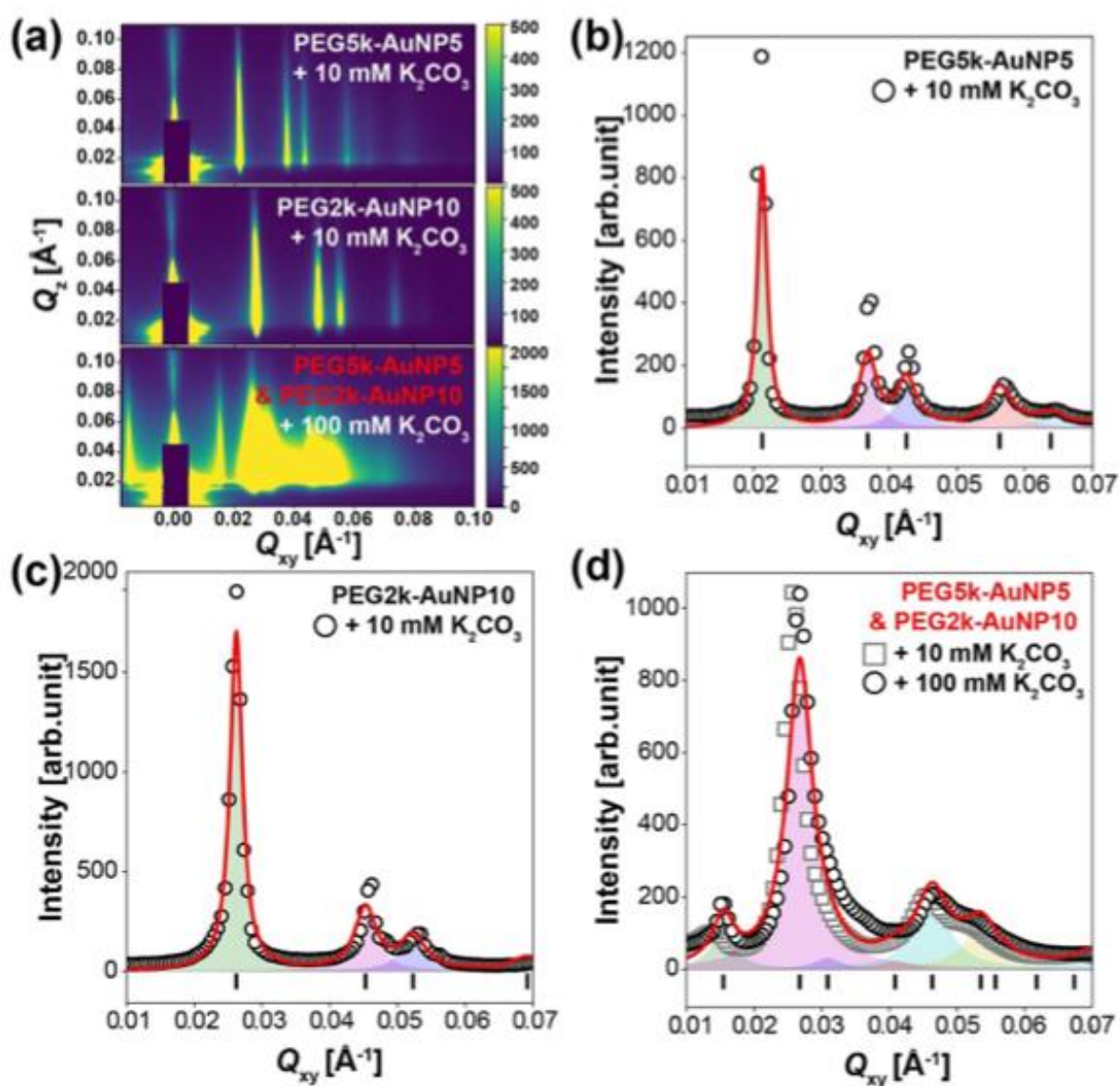
Several important variations of the SAXS technique have been developed to extend its applicability and to address specific research needs. Ultra Small-Angle X-ray Scattering (μ SAXS) extends the measurable q range to values as low as 10^{-4}Å^{-1} or even lower, corresponding to real space length scales up to a few micrometers (*Chu & Hsiao, 2001; Myers et al., 1999*). This is achieved through specialized optical configurations, such as Bonse–Hart

crystal optics (*Chu et al., 1992*), or by employing very long sample to detector distance with optimized collimation. μ SAXS is particularly powerful for probing large scale hierarchical structures, aggregate morphologies, and ultra-low angle scattering from porous or particulate systems.

In recent years, μ SAXS has become increasingly important in research on multi-scale materials where microstructural features bridge the gap between the nanoscale and the microscale. Examples include the study of hierarchical biomaterials (e.g., bone and plant cell walls), advanced composites with multi-level reinforcement, geological and cementitious materials, and industrial products with complex pore networks. The growing interest in multi scale characterization, especially in energy materials and environmental science, has made μ SAXS an essential complement to conventional SAXS and Wide-Angle X-ray Scattering (WAXS) in modern synchrotron facilities.

Grazing Incidence Small-Angle X-ray Scattering (GISAXS) adapts SAXS principles to the investigation of surfaces, thin films, and interfacial nanostructures by using an incidence angle close to or below the critical angle for total external reflection (*Levine et al., 1989*). This geometry enhances surface sensitivity while providing simultaneous in plane and out of plane structural information. GISAXS has become a key technique in nanotechnology, thin film physics, and soft matter interface studies.

Recent research trends show GISAXS being widely applied to study in-situ and operando processes such as nanoparticle self-assembly on a surface (*Lin et al., 2005*), ordering of block copolymer thin films (*Lee et al., 2005*), surface pattern formation (*Rebollar et al., 2015*), and the growth kinetics of semiconductor or perovskite films (*Giovanni et al., 2021*). The ability to capture morphological evolution in real time under relevant processing conditions has made GISAXS a powerful tool in both fundamental science and industrial R&D, particularly in photovoltaics, flexible electronics, and functional coatings.



<Figure 3.2.6.4> (a) GISAXS patterns for AuNPs synthesized by different PEG conditions. (b)-(d) Line-cut intensity as a function of Q_{xy} . Reproduced from Ref (Kim *et al.*, (2022)) with permission.

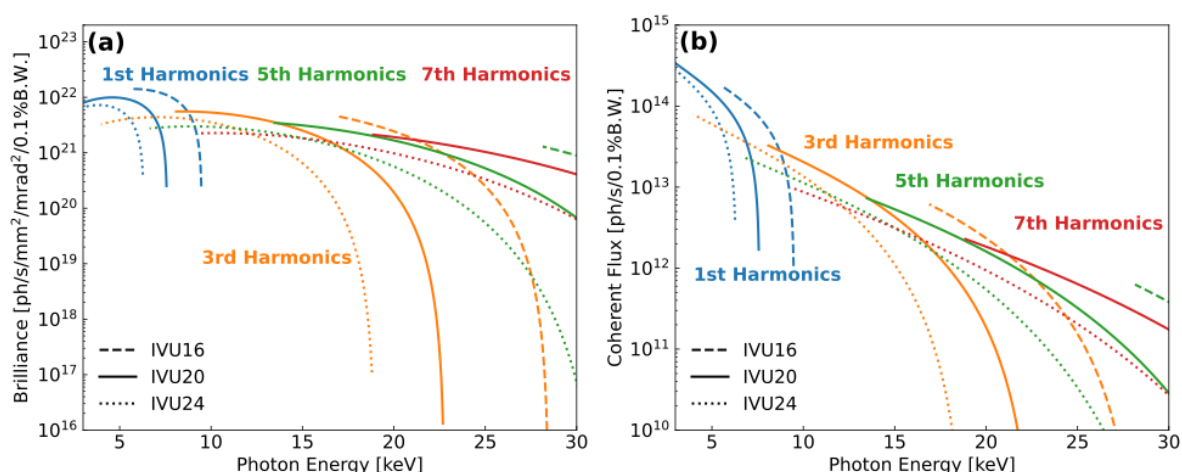
The versatility of SAXS has led to its adoption across a broad range of scientific disciplines. In soft matter research, SAXS is used to study colloidal, polymers, surfactants, liquid crystals, and biomacromolecules such as proteins and nucleic acids. In materials science, it is applied to characterize nanoparticle assemblies, porous materials, hierarchical structures, and composites. In the life sciences, SAXS is an indispensable tool for probing the solution structure of proteins and protein complexes, enabling insights into conformational changes and assembly mechanisms. In energy research, SAXS is used to investigate electrode materials, catalysts,

and membranes under operando conditions.

In the context of the 4th Generation Synchrotron Radiation Facility (4GSR), the implementation of a high performance SAXS capability will significantly strengthen the facility's potential as an international research platform. The combination of the high brilliance and transverse coherence of the 4GSR source with advanced focusing optics and large area pixel detectors will enable high sensitivity measurements of weakly scattering systems, rapid time resolved studies, and simultaneous access to wide and small angle scattering regimes. This will open new opportunities for in situ and operando characterization of structural evolution in complex soft matter, biomaterials, nanomaterials, and energy related systems under realistic operating conditions. By integrating multiple complementary techniques, including XPCS and WAXS at COSAXS beamline, the 4GSR will offer a truly multi-modal experimental platform that delivers unprecedented flexibility and efficiency for nanoscale structural science.

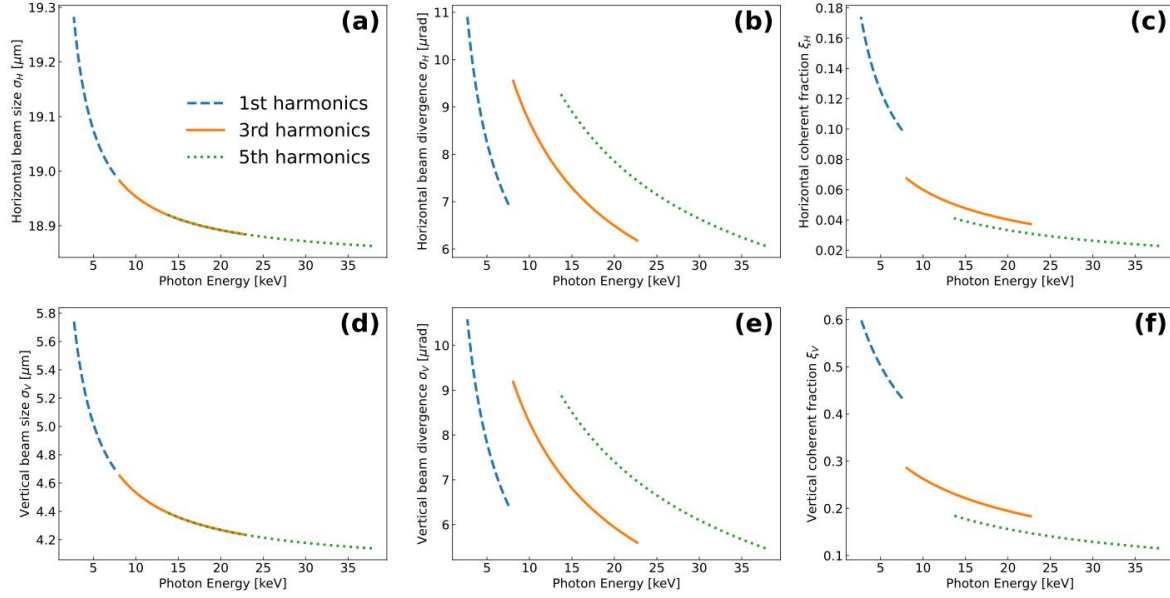
(3) Beamline Insertion Devices (IDs)

An In-Vacuum Undulator (IVU) system will be implemented in the COSAXS beamline to cover the photon range from 8 keV to 30 keV. <Figure 3.2.6.5> shows the X-ray beam parameters calculated by the SPECTRA for various IVU periods λ_u . To deliver the high coherent photon flux around 9 keV, and cover the broad photon energies up to 30 keV, λ_u is chosen to be 20 mm with the total undulator length of 3 m as shown in a solid line in <Figure 3.2.6.5>.



<Figure 3.2.6.5> Estimated X-ray beam parameters for three undulator periods, e.g., λ_u of 16, 20, and 24 mm are represented by dashed, solid, and dotted lines, respectively.

The effective photon beam size σ and angular divergence σ' , taking into account the electron bunch energy dispersion, are shown in <Figure 3.2.6.6>. Around 9 keV, σ_H , σ_V , σ'_H , σ'_V are about 18.95 μm , 4.6 μm , 9.1 μrad , and 8.7 μrad , respectively.



<Figure 3.2.6.6> Photon parameters of IVU20 estimated by SPECTRA.

The coherent fractions in both directions (ξ_H and ξ_V) are 0.063 and 0.274, around 9 keV, and the corresponding the coherence length at the source positions are 1.193 and 1.26 μm , respectively. The detailed undulator parameters are in the <Table 3.2.6.5>.

<Table 3.2.6.6> Undulator parameters

Insertion device, ID		IVU20
Total length	m	3
Number of periods, N		148
Period length, λ_u	mm	20
Magnetic field, B_0	T	1.0211
Maximum K value, K		1.9069
Gap distance	mm	5 to 16
Fundamental photon energy	keV	2.695
G. A. Brilliance	ph/s/mm ² /mrad ² /0.1%B.W.	$\sim 5.5 \times 10^{21}$ @ 9 keV
Coherent Flux	ph/s/0.1%B.W.	$\sim 2.6 \times 10^{13}$ @ 9keV
Source size, σ_H, σ_V	μm	18.95, 4.6
Source divergence, σ'_H, σ'_V	μrad	9.1, 8.7
Total power	kW	12.49
Power density	kW/mrad ²	164.2

(4) Beamline Front-End

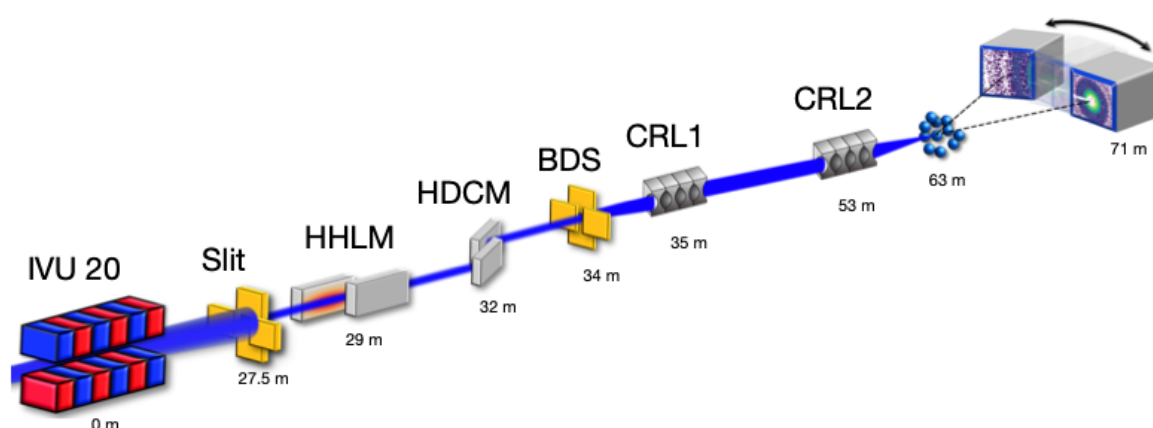
The beamline front end serves as the interface between the storage ring and the beamline optics. It includes critical components such as fixed masks, movable mask, photon shutters, and safety shutters to ensure radiation shielding and machine protection. The front end is designed to handle high thermal loads from the synchrotron radiation and maintain ultra-high vacuum conditions. Precise alignment and aperture control in the front end are essential for preserving beam quality and defining acceptance. For the COSAXS beamline, it is particularly important to preserve the wavefront of the X-ray beam in order to maintain coherence. Therefore, the use of minimal windows and optics, along with optics that have extremely low figure and slope errors, is required to minimize wavefront distortion.

(5) Beamline Layout

○ Beamline Overview and Beamline Goal

The COSAXS beamline is designed as a dedicated platform for coherent X-ray scattering experiments, with a particular emphasis on dynamic studies using techniques such as XPCS. It also supports conventional SAXS experiments, including those performed in grazing incidence geometry. Thanks to the low emittance beam delivered from the undulator and a long sample to detector distance of 8 meters, the beamline will enable access to much lower scattering angles to investigate larger structural domains within samples. This measurement regime is referred to as ultra-SAXS or μ SAXS. To achieve this, high precision slit systems are required to suppress parasitic scattering, which often contaminates the signal near the beam stop.

The ID04, COSAXS beamline will be located in one of the straight sections on the northern part of the storage ring. The total beamline length is 79.2 meters from the insertion device, with a shielding wall positioned at approximately 25 meters, followed by the optics hutch extending to 33.7 meters. Within the optics hutch, key components such as white beam slits, a pair of high heat load mirrors, and a monochromator will be installed. A Beam Defining Slit (BDS) and two Compound Refractive Lens (CRL) transfocators are located at 34 meters, 35 meters, and 53 meters, respectively. In the experimental hutch, which starts at 61 meters and extends 16 meters downstream, the beam positioning monitor, guard slits, sample stage, and detector system will be implemented. A general overview of the beamline layout is shown in <Figure 3.2.6.7>.



<Figure 3.2.6.7> The overview of the layout of COSAXS beamline.

The beamline measurement strategy of XPCS experiment is optimizing speckle contrast β to improve the signal to noise ratio (SNR) described as (Möller *et al.*, 2019)

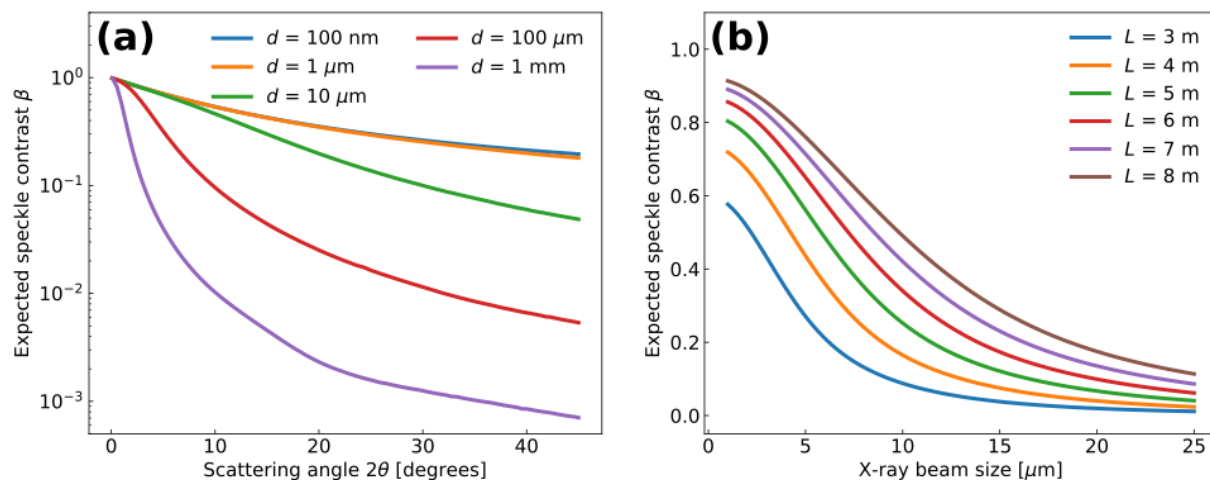
$$SNR = \beta \bar{k} \sqrt{N_f N_p}$$

where $\bar{k}$, N_f , and N_p denote the averaged intensity, number of frames, and number of pixels in a certain region of interest, respectively. The more N_f and N_p , which correspond to longer measurement durations and larger detector areas (or smaller pixel size), improve the SNR . However, their contribution is subject to diminishing returns due to the square root dependence. The averaged scattering intensity $\bar{k}$ [photons/pixel/frame] is determined not only by the coherent photon flux delivered from the undulator, but also by the scattering volume and X-ray scattering cross-section of the system. Typically, materials with high atomic number (Z), such as metallic glasses system, produces strong scattering signals. In contrast, biological sample or protein solutions generate significantly weaker scattering intensity at the detector. The coherent flux, which determines the signal intensity, is already defined by the undulator, while the X-ray scattering cross-section is governed by the sample system and the scientific objective, often selected upon the user request. Therefore, these parameters are essentially fixed and offer little flexibility to be adjusted at the end-station during the experimental setup. Given those constraints, optimizing the speckle contrast β becomes a key priority in the experimental preparation.

The speckle contrast β is governed by the many experimental parameters, i.e., longitudinal coherence length ξ_l , sample thickness d , detector pixel size P , scattering angle θ , sample to detector distance L , and coherent beam size at the sample a . The ξ_l (also called temporal coherence length) is defined by monochromaticity, as expressed by the formular: $\xi_l = \lambda^2/\Delta\lambda$, where λ is the X-ray wavelength. At typical storage ring beamlines, ξ_l is considered about 1 to 2 μm at the photon energy of 10 keV when the Si (111) or Si (311) crystals are used for a monochromator.

In <Figure 3.2.6.8>, we calculate the expected speckle contrast for the case of our beamline configurations (Jo *et al.*, 2021; Mills, 2002). The speckle contrast β can be expressed by $\beta = \beta_{cl}(a, d, \theta, \lambda, \Delta\lambda) \times \beta_{res}(a, L, \lambda)$. The β_{cl} represents the effect of transverse and longitudinal coherence length, and β_{res} corresponds to the finite angular resolution of the experimental

setup.



<Figure 3.2.6.8> Estimated speckle contrast β (a) as a function of scattering angle for various sample thickness and (b) as a function of X-ray beam size for various sample to detector distance.

<Figure 3.2.6.8> (a) shows the estimated β as a function of 2θ for various d with fixed parameters: photon energy $E = 9$ keV, $L = 8$ m, $a = 1$ μm , and $P = 75$ μm , using a Si (111) double crystal monochromator (DCM). The gradual decrease of β at higher θ originates from the optical path length difference along the beam direction, which is influenced by both sample thickness and longitudinal coherence length. The effect becomes more significant when the sample thickness exceeds the longitudinal coherence length which is approximately 1 μm under the given conditions.

As the speckle contrast reaches a sufficiently value in the SAXS regime, within the limits set by the experimental constraints such as ξ_l , a , L , and P , the standard XPCS configuration of COSAXS beamline will adopt a SAXS. While SAXS is the primary setup due to its favorable contrast conditions, the beamline will also explore challenging WAXS XPCS measurement where feasible, in response to user demands and scientific objectives. <Figure 3.2.6.8> (b) shows the expected β as a function of a for various L with fixed parameters: $E = 9$ keV, $2\theta = 0.35$ degrees, $d = 1$ mm, and $P = 75$ μm , using Si (111) DCM as well. The chosen scattering angle corresponds to a wavevector $q = 0.28$ nm^{-1} and the scattering signal appears approximately 5 cm from the beam center on the detector plane when $L = 8$ m.

The target criterion of COSAXS beamline is to optimize the β to approximately 0.2 – 0.3

by adjusting a and L during the beamtime preparation. The beamline will be designed to accommodate diverse user requirements depending on their scientific objectives, such as employing a larger beam size to reduce the X-ray dose on sensitive samples or smaller beam size to access higher q regime with high speckle contrast. In all cases, the beamline must maintain flexibility in tuning a and L to optimize β without causing radiation damage to the sample during XPCS measurements. The significance of β under general experimental conditions is summarized in <Table 3.2.6.2>.

<Table 3.2.6.2> Required acquisition time for $SNR > 5$, when $\bar{k} = 10^{-3}$ photons/pixels/frame, $N_p = 0.1$ M and the detector frame rate $f = 500$ Hz

Contrast β	Needed number of frames N_f	Acquisition time [s]
0.01	2,500,000	5,000
0.1	25,000	50
0.2	6,250	12.5
0.3	2,777	5.55

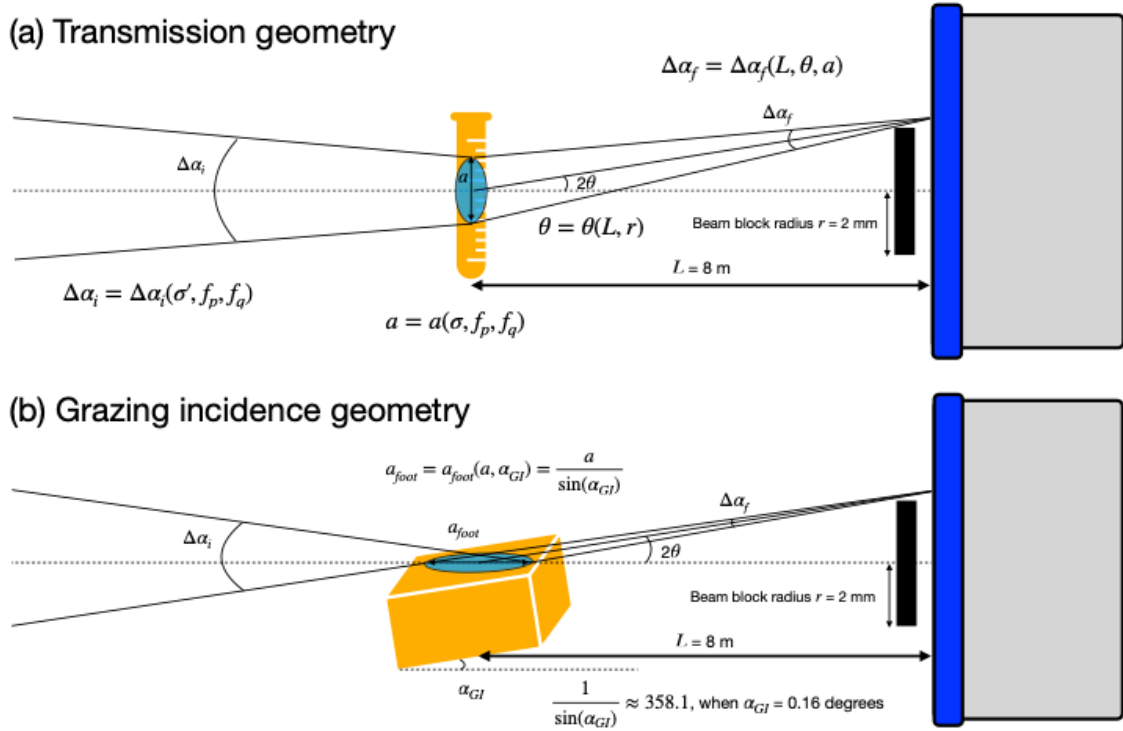
For the ultra-SAXS (μ SAXS) measurement, which is a powerful technique for probing structural features in relatively large sample domains, the resolution in momentum transfer, denoted as Δq , becomes a key factor in determining the minimum reliable scattering vector q that can be extracted from the recorded image data. This is particularly important when analyzing subtle structural features or long-range correlations in soft matter systems, where small-angle scattering carries critical information. The scattering vector q is defined by the well-known relation $q = \frac{4\pi}{\lambda} \sin \theta$, where λ is the X-ray wavelength and 2θ is the scattering angle.

The precision in determining q , or the momentum resolution Δq , is limited by two main experimental parameters: the angular divergence of the scattered beam and the spectral bandwidth of the incident X-ray. These two contributions are combined in quadrature, leading to the expression:

$$\left(\frac{\Delta q}{q}\right)^2 = \left(\frac{\Delta \theta}{\theta}\right)^2 + \left(\frac{\Delta \lambda}{\lambda}\right)^2$$

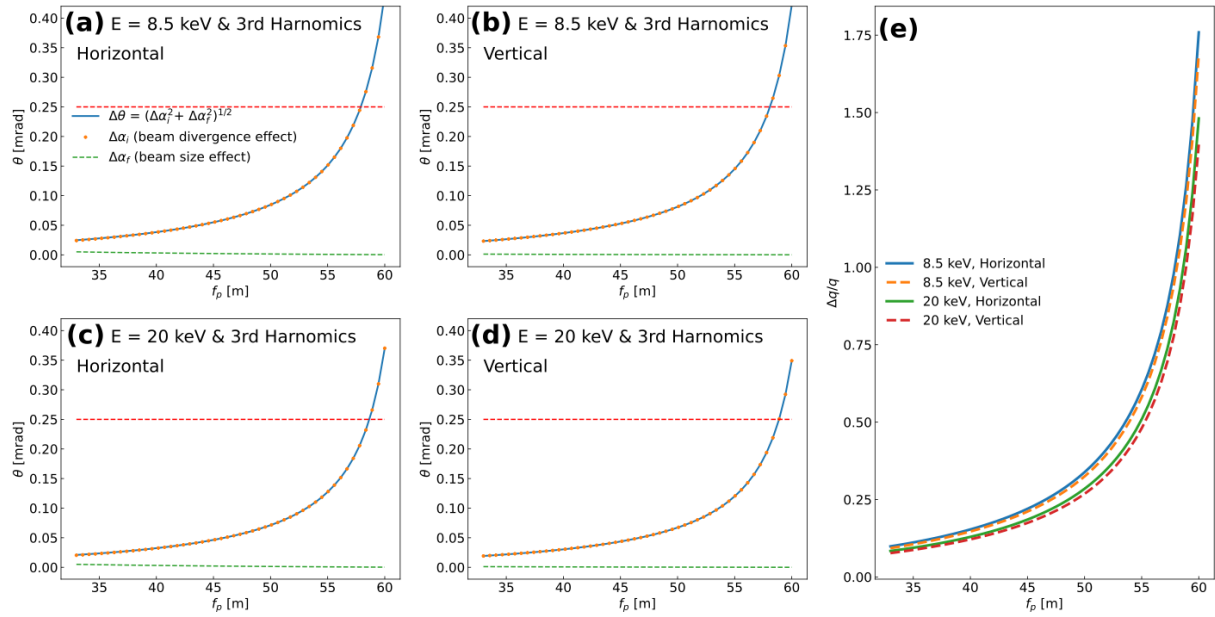
The second term of right-hand side of the equation is governed by the energy bandwidth

from the monochromator. The angular resolution $\Delta\theta$ is also defined as $\Delta\theta = \sqrt{\Delta\alpha_i^2 + \Delta\alpha_f^2}$, where $\Delta\alpha_i$ and $\Delta\alpha_f$ represent the contributions from beam divergence and beam size, respectively.



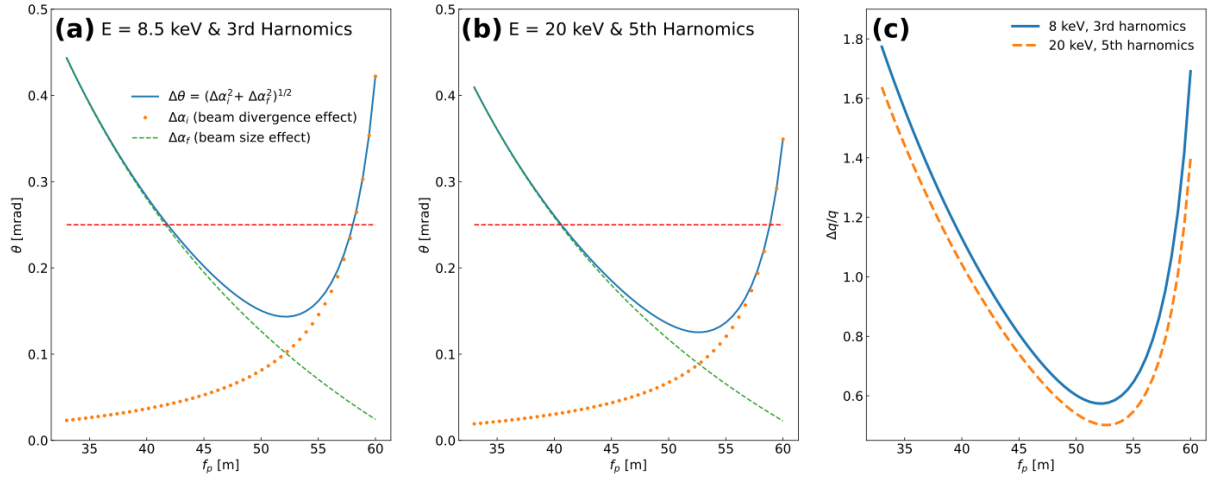
<Figure 3.2.6.9> Schematic of (a) conventional SAXS and (b) Grazing incidence SAXS geometry.

<Figure 3.2.6.9> (a) illustrates the schematics of the angular resolution components in transmission geometry. Since both beam divergence and the beam size are determined by the source parameters (i.e., σ and σ') and the position of the focusing optics (denoted as f_p and f_q , the distance from the source and to the sample, respectively), the resulting angular resolution $\Delta\theta$ and relative momentum resolution $\Delta q/q$ can be calculated analytically. <Figure 3.2.6.10> shows the calculated result for $E = 8.5$ and 20 keV in both the vertical and horizontal directions as a function of f_p . In <Figure 3.2.6.10> (a) through (d), the solid blue lines represent $\Delta\theta$, which increases gradually with longer (shorter) distance from the source (sample). This trend is primarily attributed to the beam divergence contribution α_i , indicated by orange dots in figures. Under the given conditions, the contribution from the beam size $\Delta\alpha_f$ is found to be negligible.



<Figure 3.2.6.10> Angle and wavevector resolutions as a function of position of focusing optics from the source f_p . The red dashed lines in (a)-(d) represent the θ_{min} defined by the beam stop size.

In contrast, under the Grazing Incidence geometry such as in GISAXS, the effective beam size a becomes larger due to the shallow incident angle α_{GI} , as illustrated in <Figure 3.2.6.9> (b). This geometric effect leads to an elongation of the footprint of the beam on the sample surface, which in turn influences the contribution of the beam size α_f in the final resolution. A typical grazing incidence angle of 0.16 degrees increases the effective beam footprint by approximately a factor of 358 compared to that in the transmission scattering geometry. <Figure 3.2.6.11> shows the results obtained using the same approach applied to the GISAXS geometry. In both photon energy cases, i.e., (a) 8.5 keV and (b) 20 keV, the contribution of the beam size effect is clearly pronounced, gradually decreasing as the f_p increasing. This analysis reveals that the optimal position for the focusing optics, where the angular resolution is maximized, is located approximately 53 meters from the source.



<Figure 3.2.6.11> Angle and wavevector resolutions as a function of position of focusing optics from the source f_p in vertical scattering directions.

(6) Optics Overview

The COSAXS beamline is designed to support two primary experiment techniques, e.g., XPCS and μ SAXS. For XPCS measurement, not only the beam size flexibility described earlier, but also preservation of X-ray coherence is essential. This demands high quality X-ray optics with minimal figure error and surface roughness. In addition, thermal distortions caused by the high intensity X-ray beam generated by the fourth-generation synchrotron radiation source can significantly affect the slope error of optical components and should be carefully addressed during the beamline design phase.

As shown in <Figure 3.2.6.10> and <Figure 3.2.6.11>, the optimal positions of the focusing optics differ between μ SAXS and μ GISAXS configurations. To accommodate this, two CRLs translocators (e.g., CRL1 and CRL2, located at 35 m and 53 m from the source, respectively) will be implemented to offer variable beam focusing schemes:

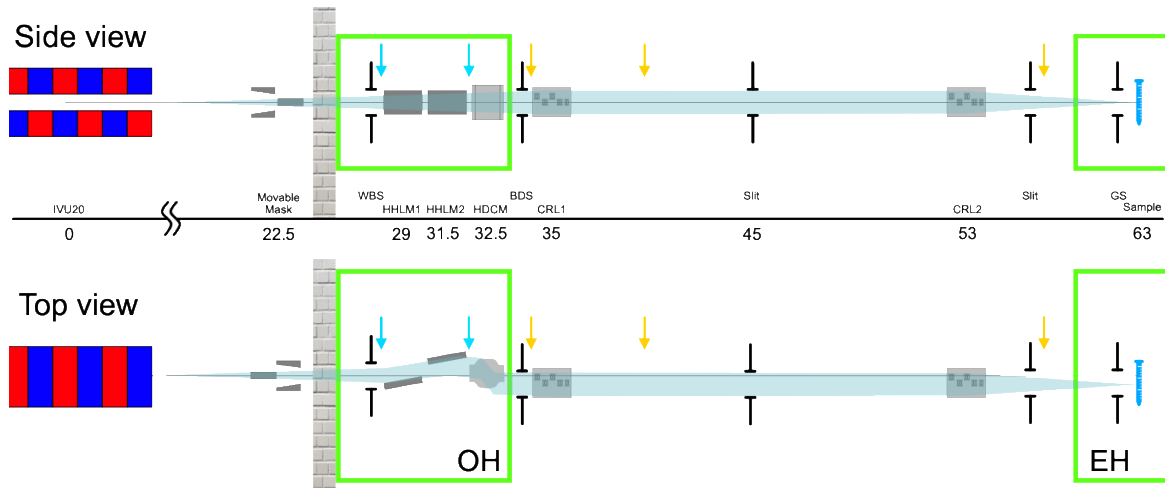
CRL1 only mode: For the conventional μ SAXS. Low divergence beam on the sample.

CRL2 only mode: For the GI- μ SAXS. Optimized position ($f_p = 53$ m) in <Figure 3.2.6.11>.

Combined mode: For XPCS. CRL1 for beam collimation or medium focusing, and CLR2 for tight focusing or varying the beam size on the sample.

Two High Heat Load Mirrors (HHLM) will be positioned upstream of the Double Crystal

Monochromator (DCM) to absorb high harmonic components and the associated beam power. This setup helps suppress thermal distortions on the DCM crystals, ensuring lower slope errors and beam divergence. Total four slits will be implemented downstream of the monochromator until the sample position. The first and last slits are Beam Defining Slits (BDS, 33.7 m) and guard slits (62.8 m) to define the beam shape. The first slit (i.e., BDS, 33.7 m) will slit down the beam to remove the tails of the Gaussian profile for SAXS or select the spatially coherent portion by filtering out incoherent components for speckle-based experiments. The final slit (i.e., guard slit, 20 cm upstream of the sample) will removes any remaining parasitic scattering near the main beam just before it reaches the sample. Two additional slits, located at 40 and 58 meters, can be used optionally to suppress unwanted parasitic scattering originating from upstream optical elements. The beamline optical layout is shown in <Figure 3.2.6.12>.



<Figure 3.2.6.12> The optical layout of COSAXS beamline. The arrows denote the beam positioning monitor (BPM) positions.

○ Optical Simulation

The optical properties of the X-ray beam at the source point of the COSAXS beamline were initially characterized using SPECTRA (Tanaka, 2021; Tanaka & Kitamura, 2001a, 2001b), based on the input parameters of the storage ring and the in-vacuum undulator configuration. The resulting spectral and angular distributions were then validated through ray tracing simulations using the SHADOW4 (del Rio et al., 2025) engine within the OASYS framework (Rebuffi & Rio, 2017b), demonstrating excellent agreement between two different simulation models. Subsequent optical simulations were conducted by constructing a complete beamline

model in OASYS, incorporating all major components such as the high heat load mirrors, double crystal monochromator (DCM), and compound refractive lenses (CRLs). The propagation of rays along the optical path was simulated using SHADOW4, and the spatial coherence properties of the focused beam at the sample position were quantitatively evaluated using the Hybrid Screen and Wofry tools (*Rebuffi & Rio, 2017a*) [TBD]. These tools allowed estimation of the transverse coherence length and beam quality under various focusing conditions. For thermal analysis, the SRW package (*Chubar, 1998; Rakitin et al., 2018*) was employed to calculate the spectral power density of the incident beam on each optical component. In the meantime, XOPPY (*Río & Dejus, 2011*) was used to evaluate the absorbed power and thermal load distributions across the optics. This combined approach enabled a detailed assessment of both wavefront preservation and potential thermally induced distortions, which are particularly critical for ensuring coherence in high-flux X-ray experiments.

○ Detailed Optical Layout

The optical layout of the COSAXS beamline is designed to preserve the coherence of the X-ray beam while allowing high configurability for various scattering techniques.

Key components include white beam slits, a pair of high heat load mirrors, a double crystal monochromator (DCM), beam defining slits, and two CRL transfocators for tunable focusing. Each element has been carefully selected and positioned to minimize wavefront distortion and to accommodate a broad range of experimental geometries.

A complete list of optical components and their specifications is provided in <Table 3.2.6.3>.

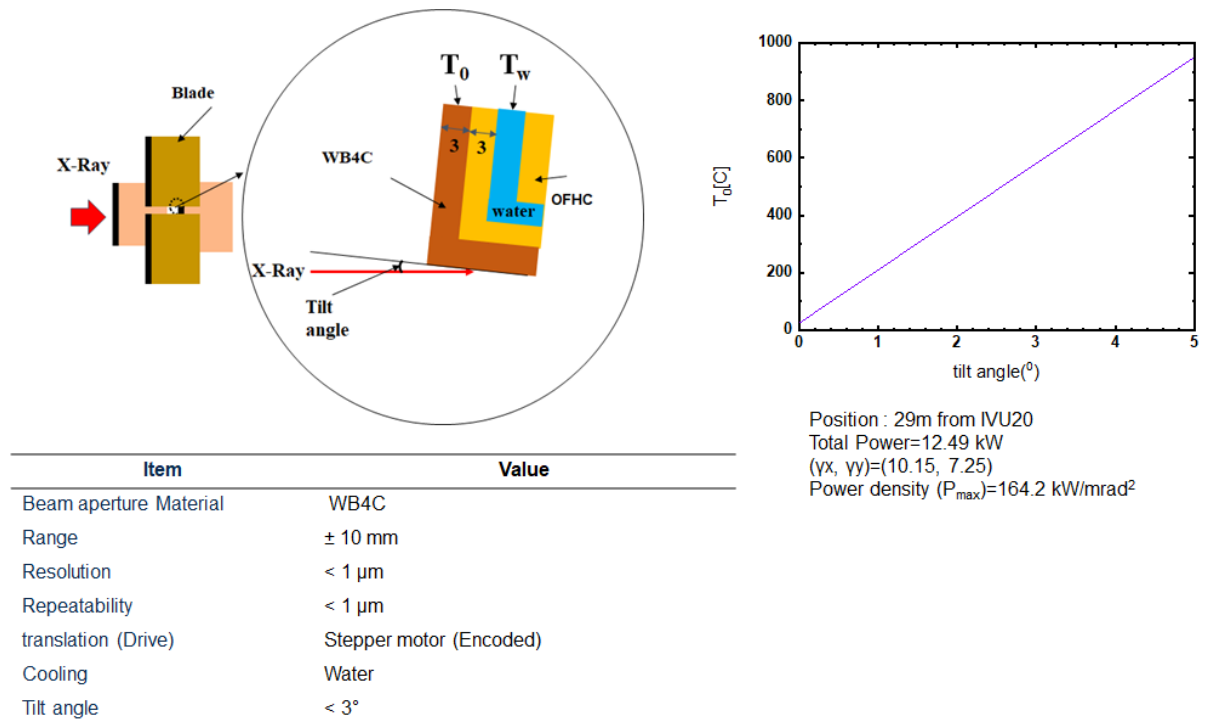
<Table 3.2.6.3> Main optics component list of COSAXS beamline

Distance [m]	Location	Component name	Description
0	Front-End	In-Vacuum Undulator	Period 20 mm, length of 3 m
22.5		Movable mask	
26.6	Optics hutch	Attenuator	White beam monitoring attenuator
27.5		Slit	Water cooled white beam slit
28		BPM	White beam positioning monitor with CVD
29		HHLM, M1	Plane, Two coated strips (Rh and Pt), horizontal reflection
30.5		HHLM, M2	Bendable, horizontal reflection
31.5		BPM	White beam positioning monitor with CVD
32.5		HDCM	Si (111) and Si (311). Side cooling with LN2, offset of 25 mm
33.5	Spool	CVD window	Separate vacuum (UHV and HV), thickness of 300 um
33.7		Slit	Beam defining slit (BDS), Tungsten carbide blades, 1 um precision, stepper motor
34.2		BPM	YAG crystal, retractable
35		CRL1 (Transfocator)	CRLs transfocator. Beam collimation or medium focus
40.5		BPM	YAG crystal, retractable
45		Slit	Tungsten carbide blades, 1 um precision, stepper motor
55		CRL2 (Transfocator)	CRLs transfocator. Beam collimation or medium focus
58		Slit	Tungsten carbide blades, 1 um precision, stepper motor
59		BPM	YAG crystal, retractable
62.8	Experimental hutch	Slit	Guard slits, Tungsten carbide blades, 1 um precision, stepper motor
63		Sample	Hexapod
71		Detector	Adjustable flight tube from 3 m to 8 m

○ Heat Load Considerations

The intense X-ray beam generated by the undulator in a fourth-generation storage ring imposes substantial thermal loads on upstream optical components. Effectively managing this heat load is essential for maintaining beam stability, preserving wavefront quality, and preventing damage or deformation of optical surfaces. To ensure reliable operation and high coherence performance, careful consideration must be given to material selection, cooling strategies, and optical configurations during the beamline design phase. In the following section, we detail the heat load management strategies implemented downstream of the front end, including the white beam slit, high heat load mirrors (HHLM), and the double crystal monochromator (DCM). To assess the thermal performance of the entire upstream optical system, detailed simulation studies will be presented at the end of this section.

The White Beam slit, located at 27.5 m, plays a crucial role in removing unwanted portions of the undulator beam and shaping the useful portion for incidence into the HHLM and DCM. It slits down the beam to approximately $0.75 \times 0.75 \text{ mm}^2$, which results in a beam size of $1 \times 1 \text{ mm}^2$ at the position of the DCM located at 32 meters from the source. By restricting the beam to its central cone, the slit reduces the total power transmitted to downstream optics, contributing to thermal load management. It results the power density of approximately 160 W/mm^2 on the DCM first crystal without HHLM. <Figure 3.2.6.13> illustrates the mechanical design of a typical slit assembly, including a simulation of blade surface temperature as a function of the tilt angle. The analysis indicates that the tilt angle should be limited to 3° or less to maintain the blade temperature within safe operating limits. The detailed specifications and thermal considerations of the White Beam slit are also summarized in <Figure 3.2.6.13>, supporting its suitability for high-power synchrotron beamlines.

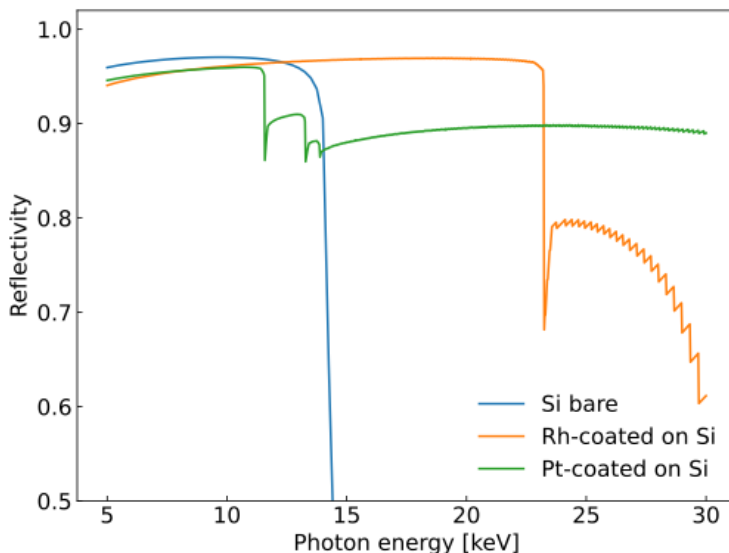


<Figure 3.2.6.13> The schematic structure of a typical slit and basic specifications.

A pair of High Heat Load Mirrors (HHLM) will be installed at 29 m and 30.5 m downstream of the source, reflecting the beam in the horizontal direction. The primary function of the HHLM is to suppress higher harmonic X-ray photon energies emitted from the IVU20 source via total reflection, thereby serving as a high harmonic rejection system while also absorbing a portion of the associated beam power. Each mirror will use a silicon substrate with dimensions of 600 mm in length, 50 mm in width, and 50 mm in thickness. Two reflective coatings, rhodium (Rh) and platinum (Pt), will be applied on the mirror surface in 5 mm wide, 600 mm long, and 100 nm thick stripes. At an incidence angle of 2.2 mrad, the Rh coated stripe provides a reflectivity of approximately 95 % up to 23 keV, while the Pt coated stripe ensures around 90 % reflectivity at higher photon energies when operated at an angle of 2.2 mrad (see <Figure 3.2.6.14>). For a beam size of 1 mm along the beam direction, the footprint on the mirror is estimated to be approximately 500 mm. Detailed information is summarized in <Table 3.2.6.4>.

To preserve the beam coherence, surface quality is critical. The surface roughness and overall figure error must be tightly controlled. In speckle based experiments, a slope error below approximately 1 μ rad is required to avoid contrast degradation. Therefore, a slope error well below 0.5 μ rad, including contributions from thermal distortion, is targeted. This imposes

a strict constraint on thermal management, and the surface temperature rise should be limited to less than 1 °C under full beam exposure. Thus, careful attention must be given to cooling strategies and mirror design to ensure thermomechanical stability during operation.



<Figure 3.2.6.14> The reflectivity as a function of photon energy for different coating materials. The incidence angle is 2.2 mrad for all cases and the coating thickness is 100 nm, calculated from Center for X-ray Optics database.

<Table 3.2.6.4> High heat load mirror target specifications

Parameter	HHLM1	HHLM2
Shape	Plane	Bendable
Source distance [m]	29	30.5
Incidence beam size [mm]	1 x 1	
Incident angle [mrad]	2.2 mrad	
Footprint [mm]	449 x 1	
Coating thickness [nm]	100 for Rh, 100 for Pt	
Substrate	Si	
Surface roughness	< 5 Å RMS	
Tangential slope error	<0.5 μrad RMS	
Sagittal slope error	<0.5 μrad RMS	

To improve both the wavevector resolution ($\Delta q/q$) and the longitudinal coherence length ($\lambda^2/\Delta\lambda$), energy monochromatization of the X-ray beam is essential in general synchrotron X-ray experiments. This is typically achieved using a Double Crystal Monochromator (DCM)

that employs Bragg diffraction in the hard X-ray regime. Since the energy resolution $\Delta E/E$ is governed by the Darwin width of the diffraction plane, two pairs of silicon single crystals, oriented along the (111) and (311) planes, will be installed in the DCM chamber to provide two different energy bandwidths of approximately 1.34×10^{-4} and 5×10^{-5} , respectively, at a photon energy of 10 keV. The translational degrees of freedom of the second crystal maintains a fixed exit beam height regardless of photon energy, unlike the channel-cut crystal type. The crystals will be mounted vertically, with the beam diffracted in the horizontal direction, known as the Horizontal DCM (HDCM). Previous studies have demonstrated that this configuration offers significant resistance to pitch vibrations and enables much more stable beam pointing at the sample (*Shi et al., 2017*), which is crucial in speckle based experiments such as XPCS that probe nano scale sample fluctuations. Although some intensity loss due to polarization may occur, the improvement in beam stability makes HDCM favorable. Detailed information on the DCM crystals is provided in <Table 3.2.6.5>.

<Table 3.2.6.5> HDCM specifications and criteria

	Crystal I	Crystal II
Crystal	Si (111)	Si (311)
$\Delta E/E$ @ E = 10 keV	$\sim 1.34 \times 10^{-4}$	$\sim 5 \times 10^{-5}$
Longitudinal coherence length ξ_l [nm] @ E = 10 keV	953	2,478
Photon energy range [keV]	8 to 30	
Operation	Fixed exit operation, closed loop (encoder) feedback	
Cooling	LN ₂ Side cooling	
First crystal size L_{1st} [mm]	50	
Second crystal size L_{2nd} [mm]	150	
Offset Z_0 [mm]	25	
Slope Error (incl. thermal distortions) [μ rad]	< 0.5	
Relative pitch vibration [μ rad]	< 0.1	

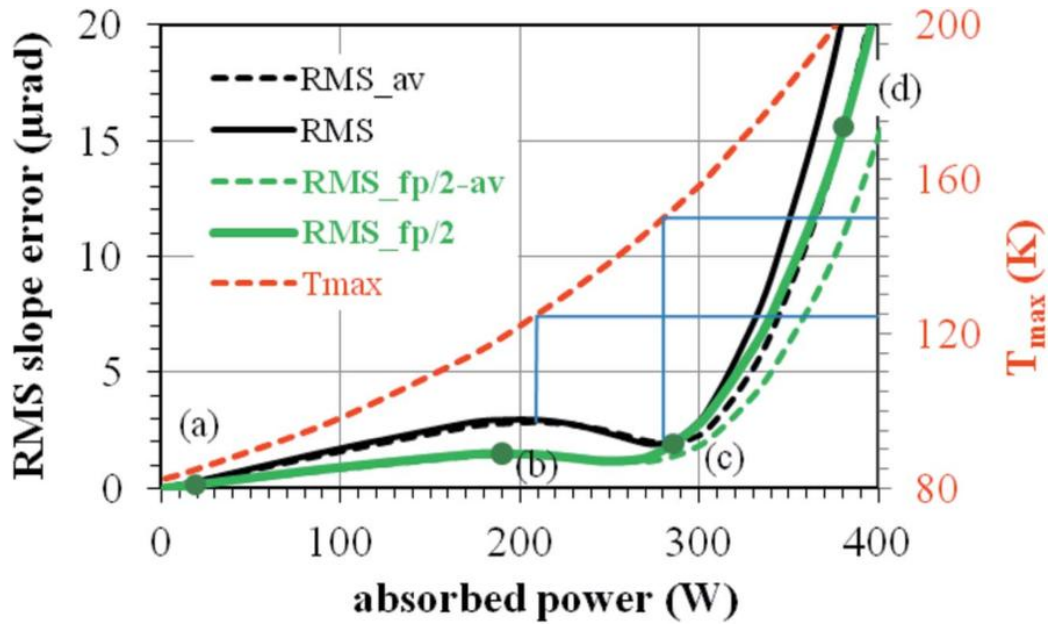
The residual heat after the HHLM will irradiate the first crystal of the DCM, and only a selective photon energy within the energy bandwidth ΔE will be diffracted to the second

crystal. Many previous studies, based on both theoretical calculations and practical measurements, have shown that the thermal load on the first crystal is the main concern when evaluating heat-induced distortions. At the COSAXS beamline, an advanced cooling method using liquid nitrogen side cooling will be applied to reduce thermal distortions in the DCM crystals. This design has already been demonstrated at three ESRF beamlines, including ID06, ID18, and ID26, under different experimental conditions (*Zhang et al., 2013*). In these studies, the absorbed power ranged from 19 W to 385.2 W, and the resulting RMS slope errors increased from 0.3 μrad to 22.03 μrad , as presented in <Table 3.2.6.6>.

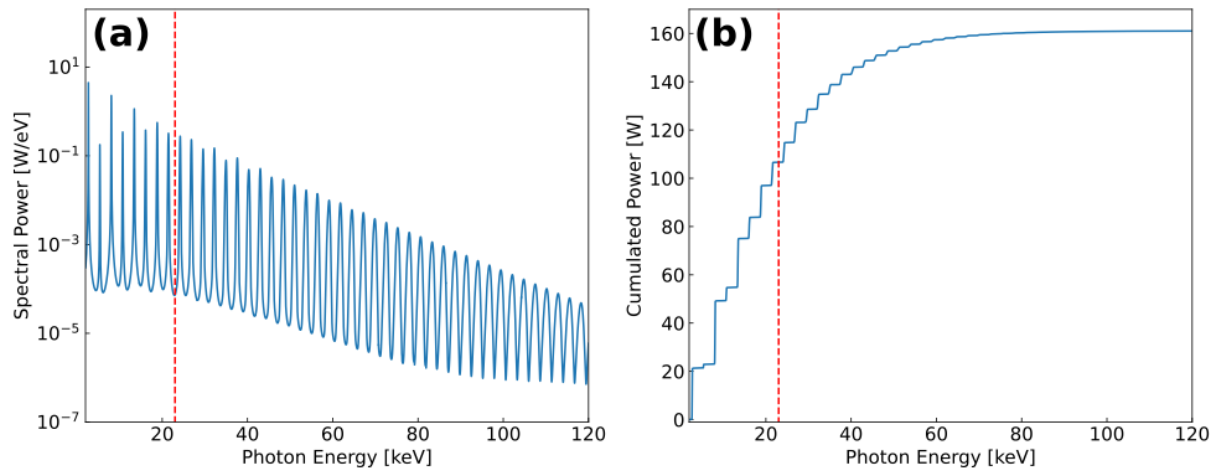
<Table 3.2.6.6> The heat load experiment conducted at ESRF (*Ref. Zhang et al., 2013*)

Electron beam current [mA]	Absorbed power [W]	T_{max} [K]	RMS slope error [μrad]
9.9	19.1	85	0.30
101	194.5	120.3	2.98
150	288.9	153.6	2.19
200	385.2	205.7	22.03

The IVU20 of the COSAXS beamline is expected to generate approximately 12.5 kW of total maximum power and a power density of 164.2 kW/mrad² under the full performance storage ring conditions of 4 GeV, 400 mA, and 1065 electron bunches. The WBS will trim the beam to produce a 1 x 1 mm² footprint on the first crystal of the DCM. Without the HHLMs, the power incident on the crystal is estimated to be around 160 W. When the mirrors are inserted into the beam path to suppress the high harmonic components from the undulator, approximately 50 W of power will be absorbed by the Rh-coated surfaces near 10 keV. As a result, about 110 W will reach the first crystal, corresponding to a power density of 42.64 W/mm² at a diffraction angle of 22.81 degrees. <Figure 3.2.6.15> presents the RMS thermal slope error measured at beamline ID06 of ESRF using side cooled silicon crystals. The slope error remains relatively stable up to an absorbed power of 300 W, after which it increases rapidly. For the COSAXS beamline, the expected slope error is around 1 μrad or even lower when the high heat load mirrors are used.



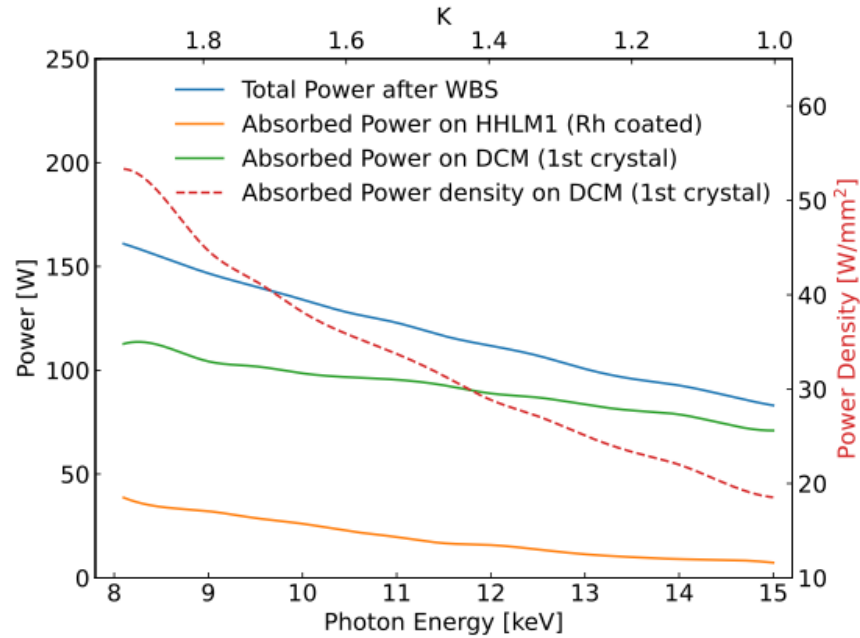
<Figure 3.2.6.15> RMS thermal slope error and the maximum temperature of the ID06 LN2-cooled silicon crystal as a function of absorbed power. (Zhang *et al.*, 2013)



<Figure 3.2.6.16> (a) Spectral power and (b) cumulated power as a function of photon energy, estimated by SRW within the OASYS framework. The vertical red dashed line indicates the cutoff energy of Rh-coated high heat load mirror.

<Figure 3.2.6.16> shows the estimated spectral power and corresponding cumulated power from IUV20, assuming the beam is slit down to $1 \times 1 \text{ mm}^2$ at DCM position (32 m) by WBS. The total cumulated power is about 160 W, and the HHLM with Rh coating will effectively

absorb the photon energy above 23 keV, substantially suppressing X-rays beyond the 9th harmonics. Approximately the cumulated power of 110 W is expected to be delivered to downstream optics, which is DCM first crystal.



<Figure 3.2.6.17> Heat load calculation on the HHLM and DCM as a function of photon energy and K.

To take into account more detailed beamline configurations such as mirror grazing angle, reflectivity, and the diffraction angle of the DCM crystal as a function of photon energy and K, XOPPY simulations within the OASYS framework have been performed, as shown in <Figure 3.2.6.17>. The blue solid line indicates the total power generated by the undulator, which decreases with increasing photon energy up to 15 keV. For the Rh coated mirrors, the first and second HHLMs absorb approximately 15% and 6% of the total power, respectively. The power density on the first DCM crystal (red dashed line), calculated based on the Bragg angle of the Si (111) plane and the beam footprint, exhibits a more rapid decline at higher photon energies due to the lower diffraction angles.

○ Beam focusing strategy

All focusing schemes of the optical elements were modeled using ray tracing, and the resulting beam sizes at the sample position were obtained. These simulated results showed excellent agreement with analytically derived beam sizes calculated using demagnification ratios $M = f_p/f_q$. For XPCS applications, both CRL1 and CRL2 transfocators are applied for beam collimation and focusing, respectively, as shown in <Figure 3.2.6.12>. The CRL combinations were identified that produces a focused FWHM beam size of approximately 13 μm horizontally and 4 μm vertically in the photon energy range between 8.5 and 12 keV (see <Table 3.2.6.7>). To ensure optimal focusing performance while preserving the wavefront quality of the coherent X-ray beam, the COSAXS beamline adopts compound refractive lenses (CRLs) fabricated from HPHT (High Pressure High Temperature) synthetic diamond crystal. Although diamond exhibits higher X-ray absorption than beryllium, it offers key advantages for use in high-coherence, high-flux environments. In particular, HPHT diamond provides excellent thermal conductivity, outstanding mechanical strength, and superior radiation hardness, making it highly suitable for optical elements exposed to intense synchrotron beams (Celestre et al., 2022). Furthermore, the use of advanced laser ablation techniques allows precise machining of diamond lenses, enabling the fabrication of CRLs with apertures exceeding 1 millimeter, which is critical for preserving beam throughput and wavefront quality in any scattering experiments.

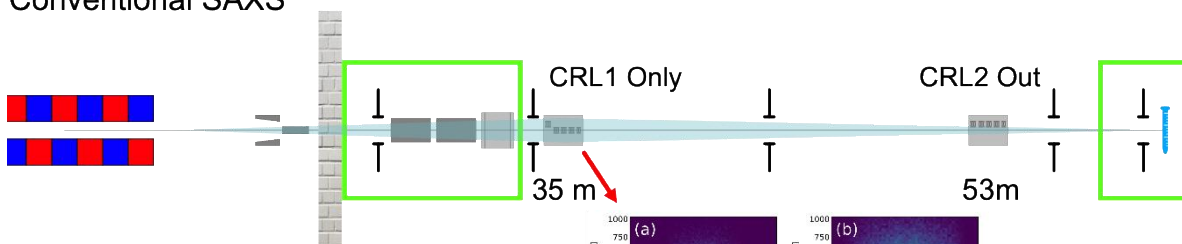
<Table 3.2.6.7> CRL configurations for XPCS measurements.

The minimum beam sizes at the sample position were evaluated for various photon energies using ray tracing simulations based on the OASYS framework.

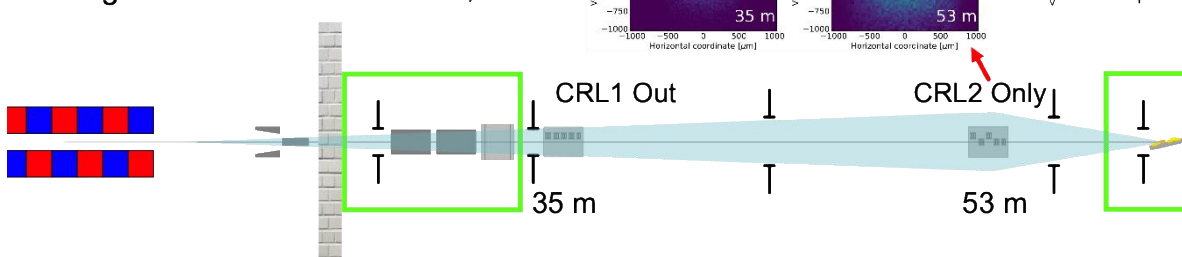
X-ray photon energy [keV]	CRL1		CRL2		Beam size in FWHM [μm]		Transmission (DCM and CRLs)	Photon flux [ph/s/0.1% bw]	Coherent Photon flux [ph/s/0.1% bw]
	Radius R [μm]	# of CRLs	Radius R [μm]	# of CRLs	Horizontal	Vertical			
8.5	725	1	805	4	12.97	4.230	0.228	3.67×10^{14}	6.74×10^{12}
9	650	1	723	4	12.71	4.052	0.253	3.79×10^{14}	6.56×10^{12}
10	520	1	588	4	12.75	3.967	0.304	3.95×10^{14}	6.21×10^{12}
12	350	1	412	4	12.86	3.743	0.38	3.44×10^{14}	4.55×10^{12}

Side view

Conventional SAXS



Grazing Incidence SAXS



<Figure 3.2.6.18> Focusing schemes for conventional transmission SAXS (upper) and grazing incidence SAXS (lower) experiments. In the conventional SAXS configuration, the beam size at the CRL1 translocator is approximately 700 μm in both the horizontal and vertical directions. For the GISAXS configuration, the beam size is around 1000 μm in both directions.

For SAXS experiments, either CRL1 or CRL2 will be used to focus the beam depending on the scattering geometry. For conventional transmission SAXS, where low beam divergence at the sample position is essential <Figure 3.2.6.10>, only CRL1, which is positioned upstream of CRL2, will be used to deliver a low divergence beam. In contrast, GISAXS requires optimized focusing at 53 meters from the source <Figure 3.2.6.11>, so the beam will bypass CRL1 and be focused only by CRL2. Recent advancements in large aperture diamond CRL fabrication allow both CRL1 and CRL2 to transmit input beams of approximately 700 μm and 1000 μm respectively, without significant intensity loss. The overall focusing schemes are illustrated in <Figure 3.2.6.18>, and the expected beam sizes along with corresponding CRL configurations are summarized in <Table 3.2.6.8>.

<Table 3.2.6.8> CRL configurations for Transmission and Grazing Incidence SAXS configuration. The minimum beam sizes at the sample position were evaluated for various photon energies using ray tracing simulations based on the OASYS framework.

X-ray photon energy [keV]		8.5	20	8.5	20
Scattering geometry		Transmission SAXS		Grazing Incidence SAXS	
CRL1	Radius R [μm]	946	455	-	-
	# of CRLs	3	8	-	-
CRL2	Radius R [μm]	-	-	588	430
	# of CRLs	-	-	4	14
Beam size in FWHM [μm]	Horizontal	35.9	33.90	8.21	8.22
	Vertical	11.31	9.215	2.62	2.28
Beam divergence in FWHM [μrad]	Horizontal	18.51	14.26	51.14	54.56
	Vertical	18.94	17.92	48	56.98
Transmission (DCM and CRLs)		0.351	0.407	0.13	0.254
Photon flux [ph/s/0.1%bw]		5.65×10^{14}	1.27×10^{14}	2.09×10^{14}	0.79×10^{14}

Note that the CRL configurations in <Table 3.2.6.7> and <Table 3.2.6.8> do not represent the final CRL configurations of COSAXS beamline. The beamline is currently being designed to support dynamic adjustment of beam sizes through flexible CRL transfocator settings. By applying the standard lens formula $f = \frac{R}{2N\delta}$, where f , R , N , δ are the focal length, radius of curvature, number of CRLs, and refractive index decrement of the element used, respectively, along with ray tracing simulations using the OASYS framework, the beamline can be configured to meet a wide range of experimental requirements with optimized focusing conditions. In addition, the use of one-dimensional CRLs is also being considered as an option to deliver a symmetric circular beam profile at the sample position when needed.

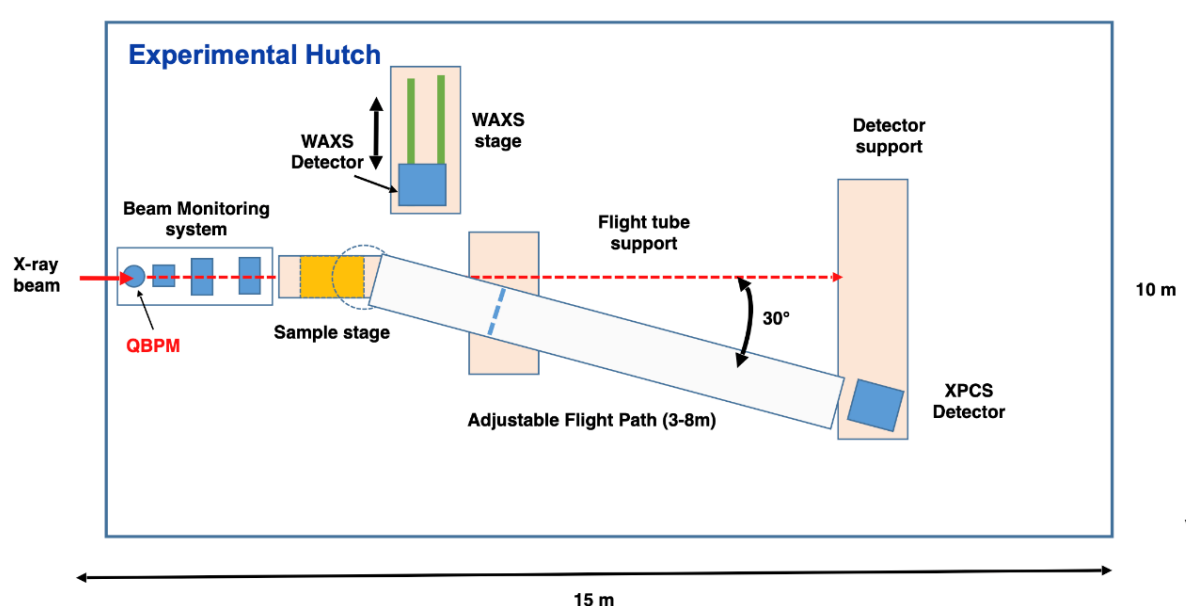
(7) Exp. system overview

This section provides an overview of the experimental systems to be implemented at the beamline in support of advanced scientific investigations. These systems are designed to fully

leverage the capabilities of the photon source and optics, while accommodating a broad range of X ray scattering experiments based on user requirements. The experimental station will feature state of the art instrumentation optimized for SAXS, XPCS, and related techniques. Key components include diverse sample environments with high adaptability and flexible detector configurations. The overall design emphasizes modularity, stability, and automation to ensure experimental reproducibility and user accessibility. The following sections describe each subsystem in detail, including sample stages, detector platforms, control systems, and auxiliary equipment, with a focus on their technical specifications, integration strategies, and expected performance.

○ Experimental hutch

The experimental hutch will accommodate various essential components, including precision sample stages, experimental chambers, area detectors, and auxiliary instrumentation such as beam position monitors and attenuators. Positioned 60 meters downstream from the X-ray source, the hutch itself measures 15 meters in length and 10 meters in width, providing ample space for flexible experimental setups. To enable long sample to detector distances up to a maximum of 8 meters, this beamline adopts a horizontal scattering geometry as the standard configuration, optimizing spatial resolution and angular coverage for both static and dynamic scattering experiments.



<Figure 3.2.6.18> Schematic of the experimental hutch of ID04.

○ **Beam positioning monitor and Ion chamber**

The beam positioning monitor will be installed upstream of the safety shutter and will track the beam position. A CVD thin crystal and an imaging camera, focused on the crystal surface at a 45-degree angle, will move vertically in and out of the beam path. With an objective lens magnification of $\times 10$ and a camera pixel size of $2\ \mu\text{m}$, the system will achieve a spatial resolution of $200\ \text{nm}$ and a field of view of $700 \times 400\ \mu\text{m}$. A feedback system will maintain beam alignment by adjusting the angle of the second mirror of HHLM. The beam positioning system, with a precision of a few hundred nanometers, ensures sufficient beam pointing stability at the sample position. Beam position feedback is enabled regardless of the safety shutter status.

An ionization chamber will be installed between the beam position monitor and the safety shutter to monitor the incident X-ray flux in real time. The chamber will operate with a gas mixture of argon and carbon dioxide (Ar/CO_2), which provides stable ionization characteristics and suitable absorption efficiency across the energy range of 7 to 30 keV. As X-rays pass through the chamber, they ionize the gas molecules. The resulting ion pairs are collected by electrodes under an applied bias voltage, supplied by a high-voltage power supply (HVPS), typically in the range of +100 V to +1000 V. The ionization current, usually in the picoampere to nanoampere range, is read out using a low-noise current amplifier or electrometer, which converts the current into a measurable signal for real-time monitoring. This setup enables continuous, non-invasive beam flux measurement, ensuring stable and normalized data collection for scattering experiments such as SAXS, WAXS, and XPCS.

○ **Attenuator and guard slits**

Solid-state attenuators are essential for reducing the intensity of the X-ray beam in order to protect beamline optics and samples from potential damage, and to prevent over exposure of the detector. The attenuator assembly is planned to be installed downstream of the safety shutter, where it can be reliably inserted or removed based on experimental requirements. The absorber materials currently under consideration include CVD diamond, silicon, and germanium single crystals. While metal foils such as aluminum, titanium, and copper are commonly used at synchrotron facilities, they must be carefully evaluated in this context, as they may disturb the X-ray wavefront and degrade beam coherence which is particularly important for coherent X-

ray scattering techniques.

Each material offers optimal attenuation over specific photon energy ranges:

- CVD diamond is effective for attenuating low-energy X-rays, particularly below 12 keV.
- Silicon crystals are suitable for medium-energy attenuation, typically between 10 and 20keV.
- Germanium crystals are appropriate for high-energy X-rays, particularly around 30 keV, and will be prepared in a range of thicknesses to offer flexible attenuation levels.

<Table 3.2.6.9> summarizes the calculated X-ray transmission values for these materials across relevant photon energies.

<Table 3.2.6.9> X-ray transmission values for different absorber materials and the photon energy

Thickness [um]	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV
CVD						
25	0.9	0.987	0.996	0.997	0.998	0.999
50	0.812	0.976	0.992	0.996	0.997	0.997
100	0.658	0.953	0.985	0.992	0.994	0.995
200	0.434	0.901	0.97	0.984	0.988	0.99
400	0.188	0.824	0.941	0.968	0.978	0.981
Si						
25	0.25	0.83	0.945	0.976	0.987	0.992
50	6.2E-02	0.688	0.891	0.953	0.975	0.985
100	3.88E-03	0.473	0.797	0.908	0.951	0.97
200	1.5E-05	0.224	0.636	0.824	0.904	0.941
400	2.26E-10	5.02E-02	0.405	0.68	0.808	0.886
Ge						
25	3.8E-02	0.618	0.288	0.566	0.73	0.83
50	1.46E-03	0.382	8.33E-02	0.32	0.543	0.694
100	2.15E-06	0.146	6.94E-03	0.102	0.295	0.482
200	4.65E-12	2.14E-02	4.82E-05	1.06E-02	8.7E-02	0.232
400	2.16E-23	4.58E-04	2.32E-09	1.12E-04	7.85E-03	5.4E-02

The guard slits will be installed immediately upstream of the sample position to remove beam tails and reduce parasitic scattering from upstream optics. The slit system will consist of four piezo-driven motorized stages equipped with titanium blades, enabling precise definition of the beam profile. This setup is particularly important for enhancing data quality in micro-SAXS measurements and improving speckle contrast in XPCS experiments. A flexible mounting structure will be implemented to allow the clean-up slits to be positioned as close as

possible to the sample, thereby maximizing beam definition at the interaction point and minimizing unwanted background.

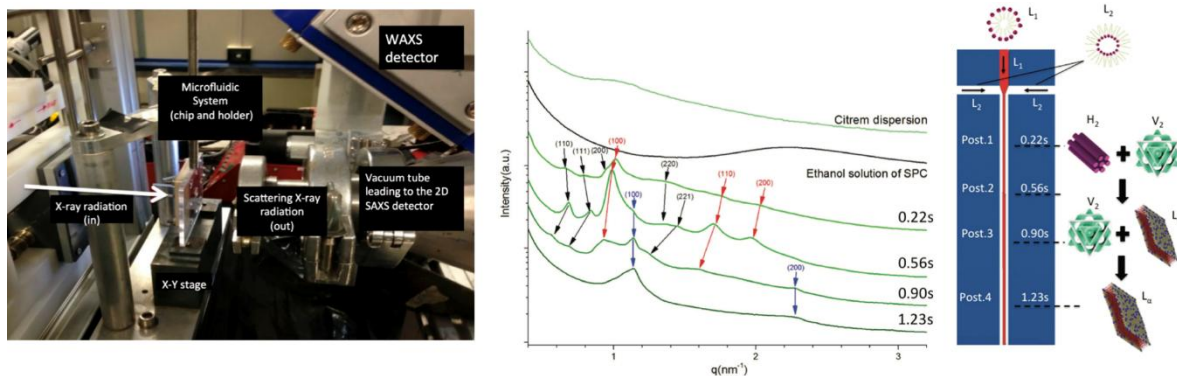
○ **Sample environments**

- Vacuum chamber

To facilitate windowless scattering experiments, a versatile vacuum chamber will be employed to significantly reduce photon loss caused by air gaps and window materials to facilitate windowless scattering experiments under photon-hungry conditions. The chamber will be equipped with two gate valves positioned upstream and downstream, effectively isolating it from the beamline and detector sections. In conjunction with an independent pumping system, this setup allows for rapid evacuation and venting of the chamber without affecting adjacent components, thereby minimizing sample loading and exchange times. Additionally, a copper sample holder integrated with a Peltier-based thermal control system will enable precise in-situ operando temperature-dependent measurements, offering stability and flexibility for a wide range of experimental conditions.

- Microfluidic system

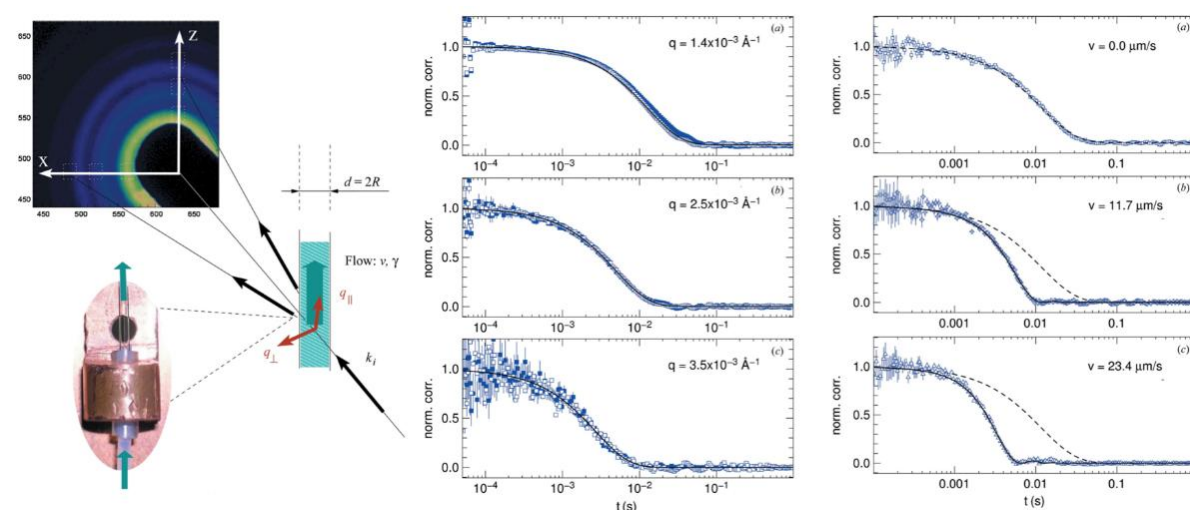
Microfluidics offers unique opportunities for the continuous synthesis of both hard and soft nanomaterials with controllable shapes and sizes, which are highly valuable in biomedical and pharmaceutical applications such as nanomaterial synthesis, drug delivery, vaccine development, and cell analysis. In addition to its high reproducibility and potential for integration with automated workflows, microfluidic platforms enable real-time chemical and biological analysis, rheological characterization, and structural screening. Key advantages include short measurement times, high precision in liquid handling, fine control over flow rates and timing, and minimal consumption of input materials <Figure 3.2.6.19>.



<Figure 3.2.6.19> Microfluidic system implemented at a synchrotron beamline. The X-ray scattering was obtained as a function of sample synthesis time. (Yaghmur & Hamad, 2022)

At this beamline, microfluidic chips will be mounted on the hexapod to facilitate structural investigations using both SAXS and WAXS techniques. The high-precision sample translation system allows for the capture of time-resolved structural evolution during synthesis processes. Furthermore, the fast repetition rate of the X-ray area detector enables the collection of speckle patterns, allowing for the analysis of dynamic behavior within the microfluidic flow. By accounting for the flow velocity shown in <Figure 3.2.6.20>, dynamic information can be extracted with high temporal resolution, providing insight into the kinetics of nanomaterial formation and transformations (Fluerasu et al., 2008).

- Sample scanner



<Figure 3.2.6.20> XPCS measurement at a microfluidic system. The flow effect on the dynamics was decoupled by the dedicated data analysis.

One of the primary challenges in XPCS measurements under high photon flux is the X-ray-induced heating effect, which can alter the intrinsic dynamics of the sample and compromise the measurement. To mitigate this issue, continuous sample translation methods are commonly employed to reduce the cumulative X-ray dose on any given region of the sample. However, the translation speed must be carefully optimized, as excessive movement can lead to forced decorrelation effects. These arise from reduced spatial overlap of the illuminated volume between successive frames, and are governed by both the beam size and the sample translation speed, given by (Lurio *et al.*, 2021).

$$g^{(2)}(q, \Delta t) = 1 + \beta \exp(-2\Gamma(q)\Delta t) \exp\left(-\frac{v^2 \Delta t^2}{a^2}\right), \quad (\text{Eq. 3.2.6.1})$$

where Γ , v , and a are the relaxation rate, translation speed and the beam size at the sample position respectively. Optimizing experimental conditions is essential in XPCS, requiring careful consideration of the expected sample relaxation time, X-ray dose effects, beam size, and sample translation speed. At this beamline, a high-speed sample scanning unit, which is consisting of horizontally and vertically coupled piezo-driven translation stages, will be mounted on top of the hexapod. This system offers a travel range of 100 mm, sufficient to scan standard glass or quartz capillaries. When operating at its maximum speed of 200 mm/s, the scanner can effectively mitigate dose accumulation and support the investigation of sample dynamics with characteristic times faster than 50 μ s, assuming a beam size of 10 μ m. This configuration ensures compatibility with a broad range of soft and hard matter systems, while preserving the integrity of dynamic measurements under high-flux conditions.

To enable flexible experimental configurations described above, a PI hexapod (model H-825) will be installed atop a Huber 2-circle goniometer, which also supports the positioning of the flight tube. The hexapod is capable of handling loads up to 30 kg and provides precise motion with translational travel ranges of approximately ± 27.5 mm (x-axis), ± 25 mm (y-axis), and ± 14 mm (z-axis), as well as rotational ranges of $\pm 11.5^\circ$ (x-axis), $\pm 10.5^\circ$ (y-axis), and $\pm 19^\circ$ (z-axis). The high degree of motion control provided by the hexapod enables precise alignment of a wide range of sample environments, including vacuum chambers, fast sample scanners, and contactless liquid sample environment. To further support full 3D scanning configurations, particularly those requiring incident angles that exceed the rotational capabilities of the hexapod, an additional rotation axis integrated into the Huber goniometer (aligned along the z-direction beneath the hexapod) will provide extended angular adjustment,

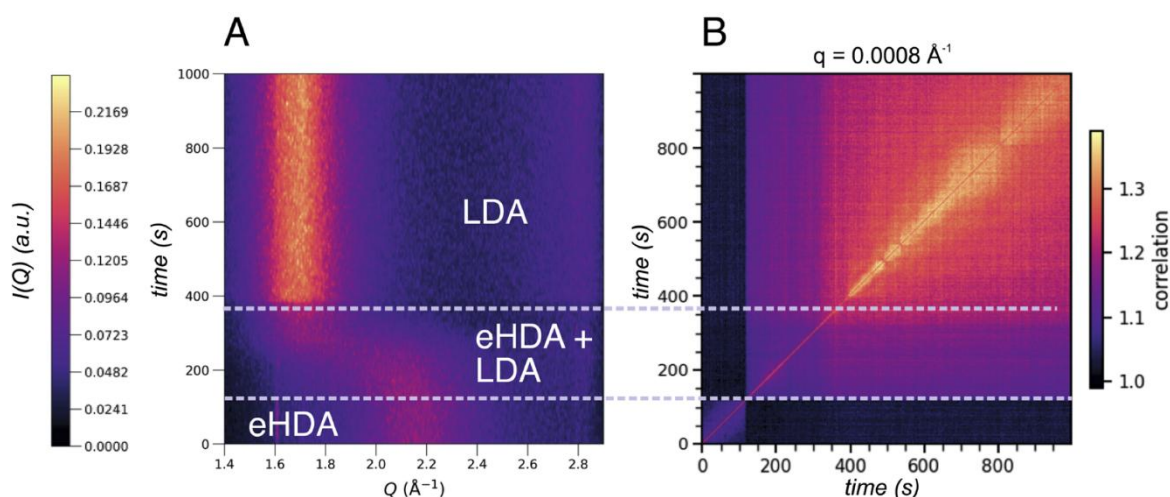
ensuring optimal sample positioning even under constrained conditions of the hexapod.

○ **Detector system**

- Flight tube

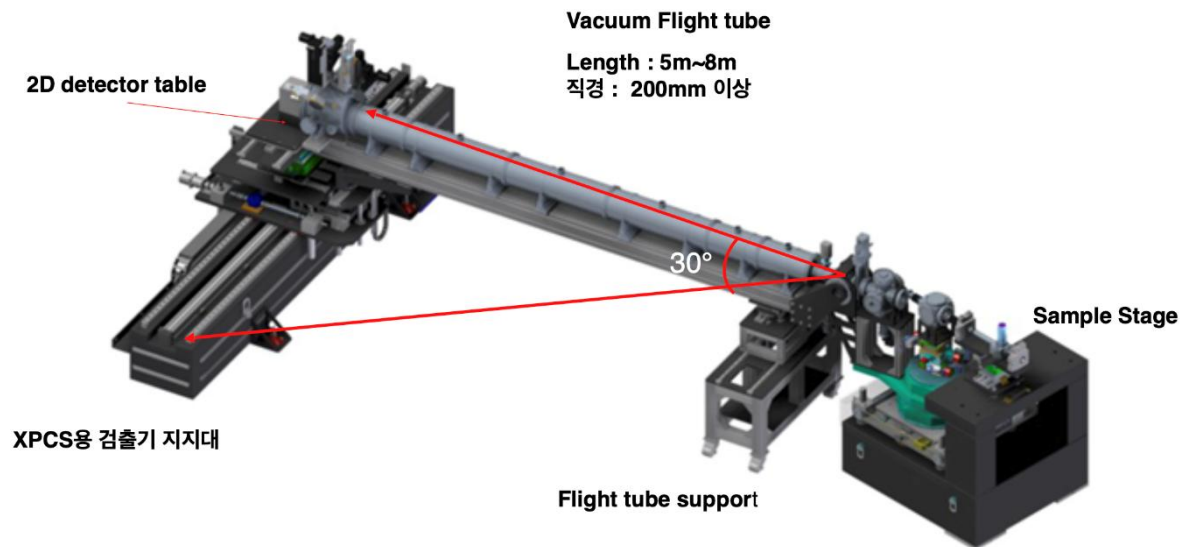
A vacuum flight tube will be installed between the sample interaction position and the detector to mitigate data contaminations from air scattering. The flight tube will consist of three modular sections, connected via O-rings to ensure vacuum integrity while allowing flexible assembly and maintenance. The system will maintain a vacuum level of low high vacuum (HV), and the total length will be continuously adjustable from 3 to 8 meters. This adjustability enables optimization of the accessible wave vector q range and enhancement of speckle contrast for XPCS and related measurements. For windowless experiments, the upstream of the flight tube will be directly connected to a gate valve after the sample chamber to maintain a continuous vacuum path to the detector system. The exit diameter of the tube will exceed 200 mm, providing sufficient clearance to fully accommodate large-area detectors such as the Eiger 4M ($155.1 \times 162.1 \text{ mm}^2$), ensuring full detector coverage and minimizing vignetting. For the standard air configuration, the entrance of the flight tube will be sealed with a flange equipped with a CVD window (6 mm in diameter, with optional water cooling) to maintain the vacuum inside the tube. When the window is positioned 10 cm downstream from the sample, the resulting acceptance scattering angle is 3.43° , corresponding to a projected coverage of 179 mm in one direction at the minimum detector position of 3 m.

Two support structures, which are one for the flight tube and another for the detector system, will be positioned 1.5 m and 8 m downstream of the sample position, respectively. Both structures will be mounted on linear translation stages, allowing motion in the horizontal direction. Additionally, a rotational stage beneath the base will enable the entire assembly to swing, facilitating automated adjustment of the scattering angle from 0° to 30° . The system is mechanically coupled to the 2-circle goniometer, ensuring that the center of rotation remains fixed at the sample position during angular adjustments.



<Figure 3.2.6.21> (a) X-ray scattering signals from low- and high-density amorphous ices at WAXS regime, and (b) the XPCS result at SAXS regime.

The maximum scattering angle of 30° corresponds to a wave vector q of $2.52 \text{ \AA}^{-1}$ at an incident energy of 9.613 keV which is a scientifically relevant range for probing the length scales characteristic of low- and high-density amorphous ice structures (*Ladd-Parada et al., 2022b*) <Figure 3.2.6.21>. In the standard experimental configuration (e.g., SAXS and μ SAXS), the area detectors will be positioned at 0° scattering angle. A beam stopper, aligned with the direct beam using precision manipulators, will protect the detector from beam damage. The stopper has a diameter of 4 mm, enabling access to low q values essential for μ SAXS measurements. A photodiode integrated at the center of the beam stopper will continuously monitor the direct beam intensity and is useful in beam alignment. The detectors for SAXS and XPCS will be mounted on a dedicated detector table equipped with three rotational axes (pitch, yaw, and roll) and three translational axes (x, y, and z). This full six-degree-of-freedom motion allows precise alignment of the detector plane, ensuring it remains perpendicular to the incident beam, particularly when the detector is positioned at an angle.



<Figure 3.2.6.22> The schematic of X-ray flight tube and detector stages.

- WAXS detector stage

Experiments requiring scattering angles greater than 30° will be conducted using an alternative configuration with a dedicated WAXS detector stage. In this setup, the minimum sample-to-detector distance is 0.25 m, allowing access to scattering angles from 0° to 31° , assuming the direct beam passes near the edge of the Eiger 4M detector. Additional linear translation of the detector in the high-angle direction further extends the accessible scattering range. Precise determination of the detector position and tilt angle will be carried out using reference samples, such as LaB_6 (lanthanum hexaboride) or CeO_2 (cerium dioxide), to ensure accurate angular calibration. To accommodate the WAXS detector at close proximity to the direct beam, the SAXS flight tube will be decoupled from the Huber goniometer and retracted. Nevertheless, simultaneous SAXS and WAXS measurements remain feasible at this beamline, offering comprehensive structural characterization across multiple length scales.

- Detector system

The ability to perform measurements with short exposure times, enabled by a photon flux approximately 100 times greater than that of 3rd generation synchrotron radiation facilities, allows not only the analysis of a larger number of samples within the same period but also the exploration of dynamic processes via time resolved X-ray scattering and XPCS. In particular,

for XPCS, the beamline will in principle provide speckle patterns of comparable intensity with 100 times shorter exposure, thereby enabling access to temporal resolutions down to the μs regime.

Achieving such temporal performance requires more than just high coherent flux. It is essential that these advancements are supported by the development of fast area detectors and matched with highly capable data acquisition systems. The temporal resolution of XPCS is fundamentally governed by both the available photon flux and the detector frame rate, but also critically depends on the speed and efficiency of the associated data acquisition and processing pipeline.

Ongoing developments in detector technology have led to several advanced X-ray detectors capable of operating at high frame rates with minimal dead time. <Table 3.2.6.10> summarizes state-of-the-art 2D area detectors that were surveyed in 2025 and may be considered for implementation at the COSAXS beamline. Among these, the EIGER detector provides a high dynamic range and a large sensitive area, making it well suited for routine X-ray scattering experiments that do not demand fast temporal resolution.

For XPCS applications requiring fast frame rates under low photon flux conditions, other detectors are more appropriate. The SPARTA detector, based on Adaptive Gain Integrating Pixel Detector (AGIPD) technology as used at the European XFEL (*Jo et al., 2025*), offers frame rates up to 6 MHz. However, its use in storage ring environments must be carefully evaluated due to the complexity of integrating pixel data structures and the relatively lower photon flux compared to XFEL sources (*Jo et al., 2021, 2023*).

The XSPA detector developed by Rigaku offers a practical compromise (*Mendez et al., 2023*), with frame rates of up to 970 kHz in burst mode. When operated in a 2 bit counting mode, capable of resolving photon counts from 0 to 3, this detector enables XPCS measurements with temporal resolutions ranging from 1.03 to 11.34 μs , well suited for studying dynamic processes in nanoparticle systems.

Furthermore, recent advances in event driven detector technologies based on Timepix4 chips have demonstrated extraordinary potential to push temporal resolution below the nanosecond scale. These detectors operate by recording individual photon events with precise time stamping, and their unique acquisition method leads to significantly reduced data volume compared to traditional frame based detectors. One such example, the TEMPUS detector, has

demonstrated a time resolution of approximately 200 picoseconds (*Correa et al., 2024*). However, it remains under active commissioning with ongoing improvements to data processing algorithms and operational stability.

As the Korea 4GSR project continues to evolve, the development and selection of suitable detector systems remains an open and critical topic, particularly for high speed XPCS applications. Final decisions will depend on the continued advancement of detector performance, data acquisition technologies, and the specific scientific requirements of the beamline.

<Table 3.2.6.10> The specification of variable 2D area X-ray detectors surveyed in 2025

	Pixel size [μm x μm]	Max. Frame rate	(Max.) Image depth /Dynamic range	Acquisition conditions	Type	Data format	Remarks
EIGER2X	75 x 75	0.5 kHz	32 bit	4 Mega pixels	Photon counting	HDF5/N eXus	Double gating with different energy thresholds
		2 kHz		1 Mega pixels			
Lambda	55 x 55	24 kHz	1 bit		Photon counting	HDF5/N eXus	
		4 kHz	6 bit				
		2 kHz	12 bit				
		1 kHz	24 bit				
SPARTA	200 x 200	6 MHz	1:10 ⁴ ph/pixel/frame @ 12.4 keV	Burst mode (352 frames)	Integrati ng pixel detector	HDF5	AGIPD based technique/ dynamic gain switching
		1 kHz		Normal operation			
Rigaku XSPA	76 x 76	50 kHz	2 bit	Normal operation	Photon counting	HDF5	
		8.5 kHz	16 bit	Normal operation			
		970 kHz	1, 2, and 3 bit	Burst mode (24, 11, and 7 frames)			
TEMPUS	55 x 55	40 kHz	8 or 16 bit	Normal operation	Photon counting	HDF5	Under developme nt
		Resolving 200 ps		Event driven			
CITIUS	72.6 x 72.6	17.4 kHz	1:1800 ph/pixel/frame @ 12 keV		Integrati ng pixel detector		High saturation count rate (600 Mcps/pixel)
Jungfrau	75 x 75	2.2 kHz	1:10000 ph/pixel/pul se @ 12 keV	Normal operation	Integrati ng pixel detector	HDF5	Dynamic gain switching
		150 kHz		Burst mode (16 frames)			

- Clean booth

To ensure stable and controlled measurement conditions, such as maintaining consistent temperature and humidity levels, and minimizing external disturbances including dust and airborne particles, a clean booth surrounding the sample stage is under consideration. This enclosure will help reduce environmental noise, which is particularly important for sensitive measurements such as XPCS, SAXS, and time-resolved experiments where stability is critical. The clean booth will have dimensions of $2\text{ m} \times 1\text{ m} \times 2\text{ m}$ ($L \times W \times H$) and will be designed to be retractable, allowing for convenient access to the sample stage and experimental components during setup or maintenance. The structure will be compatible with other beamline equipment, ensuring that it does not interfere with sample exchange, alignment, or detector movements. Depending on experimental needs, the booth may also be equipped with HEPA filtration and active temperature or humidity regulation to meet cleanroom-like conditions around the sample environment.

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3.2.7 ID23 RealTime XAFS Beamline

A. Introduction

X-ray Absorption Spectroscopy (XAS) is a powerful tool for probing the electronic and local structures of specific elements in a material. The absorption threshold corresponds to the energy required to excite core electrons from the K-, L-, and M- shells (principal quantum numbers $n = 1, 2$, and 3). When the incident energy exceeds this threshold, the absorption coefficient increases sharply, showing a feature known as the absorption edge.

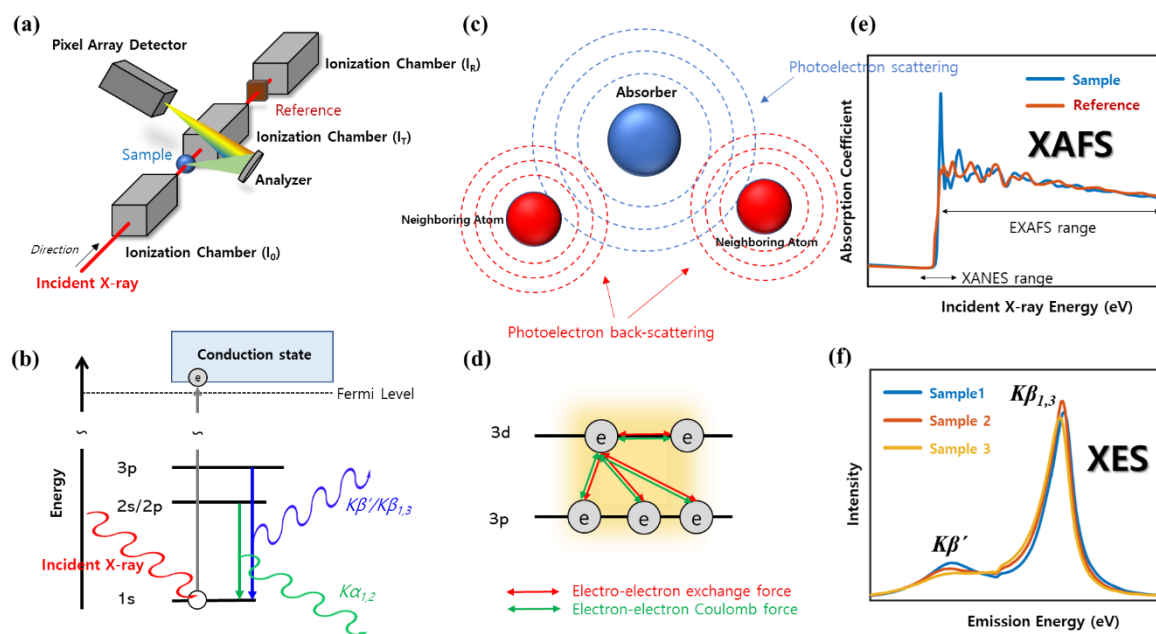
The X-ray Absorption Near Edge Structure (XANES) region spans -20 to 150 eV above the absorption edge and is primarily dominated by transitions of core electrons to quasi-bound states. This region is highly sensitive to the local electrical and structural properties around the absorbing atoms. In contrast, the Extended X-ray Absorption Fine Structure (EXAFS) region, extending from the upper end of XANES to approximately $1,000$ eV, is influenced by photoelectron scattering and backscattering. EXAFS provides detailed insight into local structural properties, including distances, coordination numbers, and structural disorder between absorber and neighboring atoms. The XAFS (X-ray Absorption Fine Structure) spectrum consists of the XANES and EXAFS regions. Typically, XAFS measurements utilize a synchrotron-based X-ray source, ionization chambers, fluorescence detectors, and a double crystal monochromator (DCM). The step-scan is commonly employed, where the DCM incrementally adjusts the incident angle to satisfy Bragg's law.

Recently, the on-the-fly scan method has been developed to reduce measurement time by allowing motors to move continuously from the start to the end point without stopping. While the traditional step-scan requires 10 to 20 minutes per scan, the on-the-fly scan can complete an XAFS measurement in 3 minutes. Additionally, the adoption of the Quick DCM, featuring enhanced DCM motor speed, enables measurement times to reach the sub-microsecond range. This method is known as Quick XAS.

Each scanning method—step-scan, on-the-fly scan, and Quick XAS—has unique advantages. As the scanning time decreases, the signal-to-noise ratio significantly improves, leading to higher spectrum quality. Whereas, fast scanning is particularly advantageous in specific applications, such as measurements on biological tissues, where minimizing radiation damage is critical. Moreover, these methods facilitate the study of transient states and kinetic

processes, including redox reactions in battery materials, catalytic processes, and phase transitions in metastable materials. The Real-time XAFS (RXAFS) beamline is the only facility dedicated to XAFS among the first-phase beamlines of Korea-4GSR. It is designed to support step-scan, on-the-fly scan, and Quick XAFS, utilizing the bright undulator source of Korea-4GSR. The RXAFS beamline delivers highly focused and intense X-ray beams across a broad energy range of 4 to 40 keV, enabling XAFS measurements for elements with atomic numbers greater than 21.

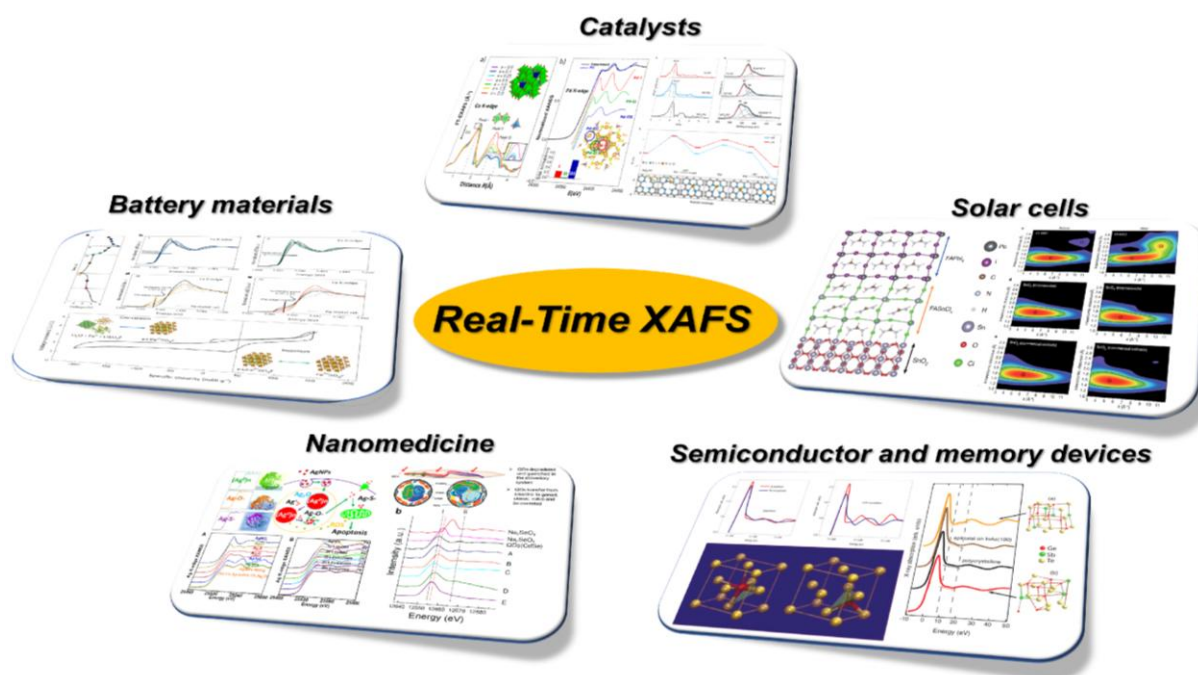
In addition to these beam properties, the RXAFS beamline offers X-ray Emission Spectroscopy (XES), which detects fluorescence emitted during core-to-core or core-to-valence transition. The XES spectrum provides critical insights into oxidation states, spin states, and ligand environments, making it a valuable complement to XAFS. With the ability to measure XAFS and XES simultaneously, the RXAFS beamline enables comprehensive analysis of material properties.



<Figure 3.2.7.5> (a) Schematic diagram of simultaneous XAFS and XES measurements. A monochromatic beam excites the electrons in atoms, and both transmitted and emitted signals are collected. (b) Schematic of atomic energy levels showing excitation and emission process. (c) Principle of XAFS: A photoelectron excited by the incident X-ray is backscattered by neighboring atoms. This interference modulates the absorption coefficient, allowing the analysis of local environment. (d) Principle of XES: Electronic interactions, such as exchange and Coulomb forces surrounding electrons, cause shifts in fluorescence energy (e) Example of XAFS spectra showing both XANES and EXAFS regions for sample and reference (f) Example of XES spectra showing the variation in emission features for different samples.

B. Scientific Objective

XAFS analysis provides element-specific insights into the local properties between absorber and neighboring atoms, making it an invaluable tool for studying material properties across diverse research fields, such as catalysis, semiconductors, solar cells, nanomedicine, and battery technologies <Figure 3.2.7.2>.



<Figure 3.2.7.2> Expected scientific applications of RXAFS beamline.

The RXAFS beamline is specifically designed to support XAFS as a core technique, with its development closely aligned with the scientific objectives established by the Korea Synchrotron Radiation User Association (KOSUA). This alignment ensures the beamline meets the rigorous demands of cutting-edge research. The RXAFS beamline design goals are listed in <Table 3.2.7.1>.

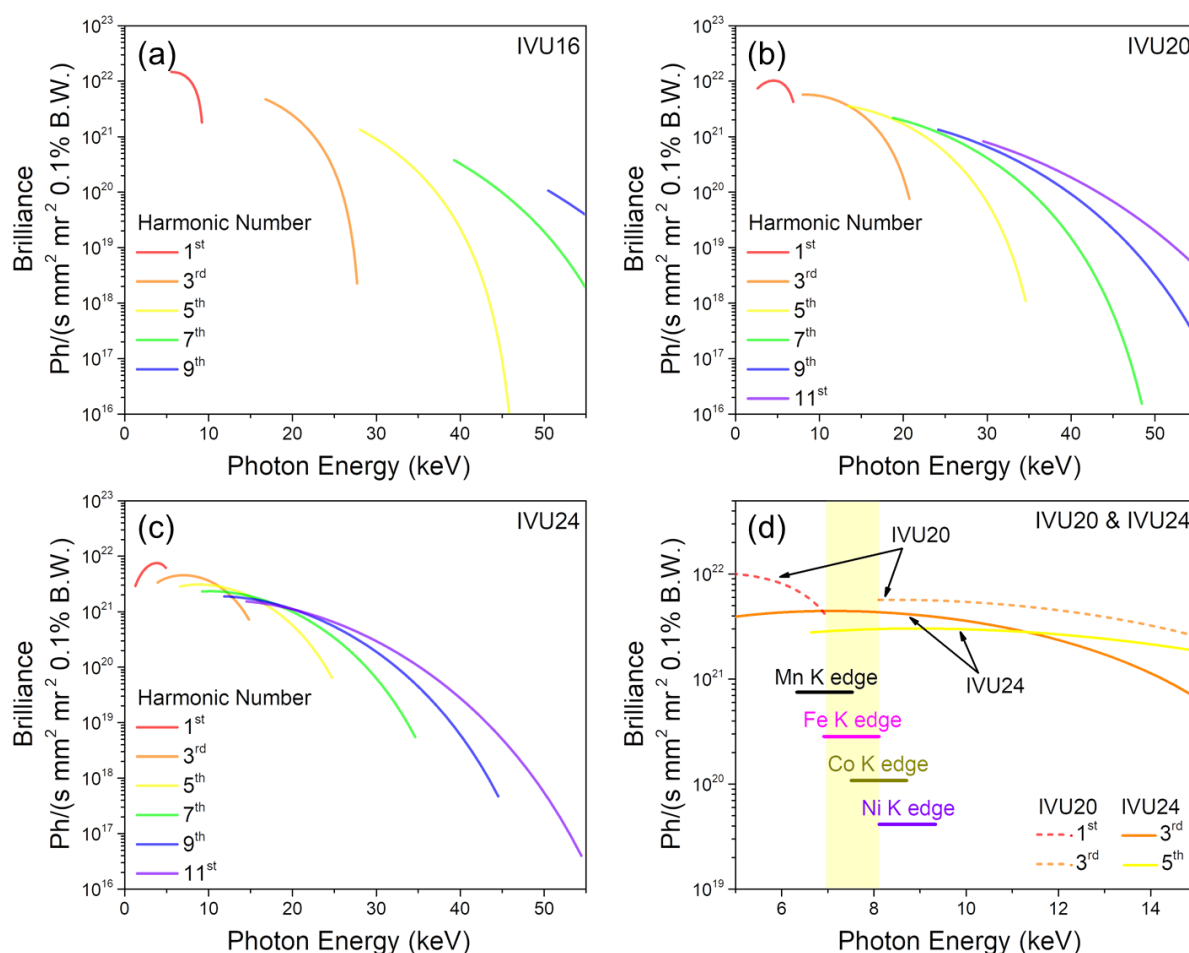
<Table 3.2.7.1> Beamline design goals

Light Source	In-vacuum Undulator (IVU24, 3m)	
Energy Range	4 to 40 keV	
Measurement time for one EXAFS data	Quick XAFS	~ 50 ms
	Normal XAFS	~ 3 min (on-the-fly scan) ~ 20 min (step-scan)
Energy resolution ($\Delta E/E$)	~ 1.4×10^{-4} Si(111) / ~ 3×10^{-5} Si(311)	
Beam size at sample position (@ 10 keV)	18 (H) $\times$ 8 (V) μm^2 (focused beam, @ 75 m) 1020 (H) $\times$ 810 (V) μm^2 (unfocused beam, @ 60 m)	
Beam flux at sample position (ph/s)	Tuned Undulator	~ $9 \times 1,013$ (@ 5 keV) ~ $4 \times 1,012$ (@ 40 keV)
	Tapered Undulator	~ $2 \times 1,012$ (@ 7 keV) ~ $3 \times 1,011$ (@ 25 keV)
Main equipment	- High Heat Load Mirror (HHLM) - Continuous-scan Double Crystal Monochromator (C-DCM) - 60 Hz Quick Double Crystal Monochromator (Quick DCM) - Energy Dispersive Fluorescence Detector - Fast-response Gas Ionization Chambers - 2D Position Sensitive Detector (2D PSD)	
Experimental equipment	- High-throughput sample holder & Sample auto-changing system - von Hamos spectrometer	
	In situ experiments	- Electrochemistry & Battery cell - Cryogenic cooling cell (> -196 °C) - Heating cell (< 1,200 °C) - High-temperature cell for thermocatalysis (heating & gas environment) - Mass analyzer

C. Beamline Insertion Device

An intense X-ray beam is crucial for the RXAFS beamline to enhance the signal-to-noise ratio, enabling shorter measurement times for both XAFS and XES spectra. Additionally, as listed in <Table 3.2.7.1>, the capability to cover a continuous energy range from 4 to 40 keV is essential for XAFS measurements.

To achieve these requirements, we evaluated three types of in-vacuum undulators (IVUs): IVU16, IVU20, and IVU24 with magnetic period lengths of 16 mm, 20 mm, and 24 mm, respectively, and a total length of 3 m. The optimal undulator was selected based on the brilliance simulations for undulator gap settings ranging from 5 mm to 16 mm, as shown in <Figure 3.2.7.3>.



<Figure 3.2.7.3> The brilliance of harmonics for (a) IVU16, (b) IVU20, and (c) IVU24 as a function of photon energy. (d) comparison of energy continuity between IVU20 and IVU24 near 7 to 8 keV.

The IVU16 exhibits energy discontinuities between harmonic X-ray beams, and the IVU20 has a gap in coverage near 7 to 8 keV. In contrast, the IVU24 provides seamless energy coverage, spanning the entire range without discontinuities. For this reason, the RXAFS beamline chooses IVU24 as its source <Table 3.2.7.2>.

<Table 3.2.7.2> IVU24 undulator parameters

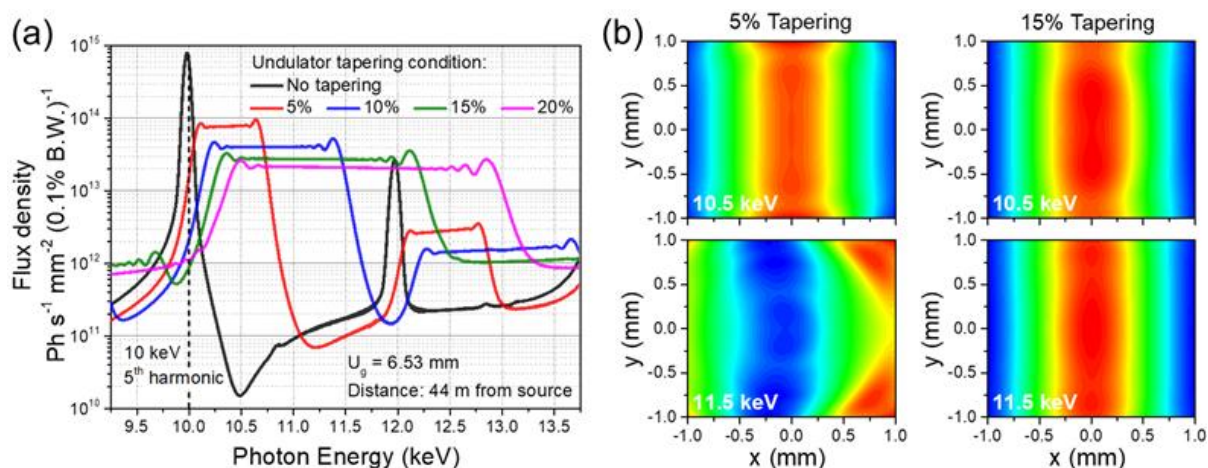
Undulator	Period (mm)	Length (m)	U _g (mm)	K _{max}	Power (kW)	Power density (kW mrad ⁻²)	Max. power after FE (kW)
IVU24	24	3	5 to 16	2.747	17.9	165	0.87 Through 2(h)×2(v) mm ² FE mask

The photon energy bandwidth of IVU24 is approximately 1% of the photon energy. For certain XAFS measurements that encompass both the XANES and EXAFS spectra, a broader bandwidth of 1.5 keV is necessary. This can be achieved through two approaches: Tuned Undulator mode and Tapered Undulator mode.

In Tuned Undulator mode, the undulator gap is adjusted in synchronization with the DCM's set energy. This mode is suitable for both the step-scan and the on-the-fly scan. However, in Quick XAFS, synchronizing the undulator motor speed with the DCM's energy setting is challenging.

The Tapered Undulator mode, by contrast, fixes the undulator gap while introducing a magnetic field gradient along the electron beam trajectory. Although this approach reduces monochromatic X-ray beam flux compared to the Tuned Undulator mode, it provides a broader energy bandwidth, enabling Quick XAFS measurement without undulator gap adjustment.

<Figure 3.2.7.4 (a)> illustrates the flux and photon energy bandwidth of the beam passing through the white beam slit of the RXAFS beamline with a 2 mm (h) x 2 mm (v) opening, under varying taper ratios. It is noteworthy that the taper ratio allows for easy control of the bandwidth. Interestingly, the taper ratio also affects the beam shape. As shown in Figure 4b, with a taper ratio of 5% with a 6.53 mm initial gap, the beam shape distorts as photon energy increases. With a taper ratio of 15%, however, the beam shape change becomes negligible. The simulation results suggest that sufficiently large range of the taper ratio control is necessary to maintain the beam shape across the bandwidth.



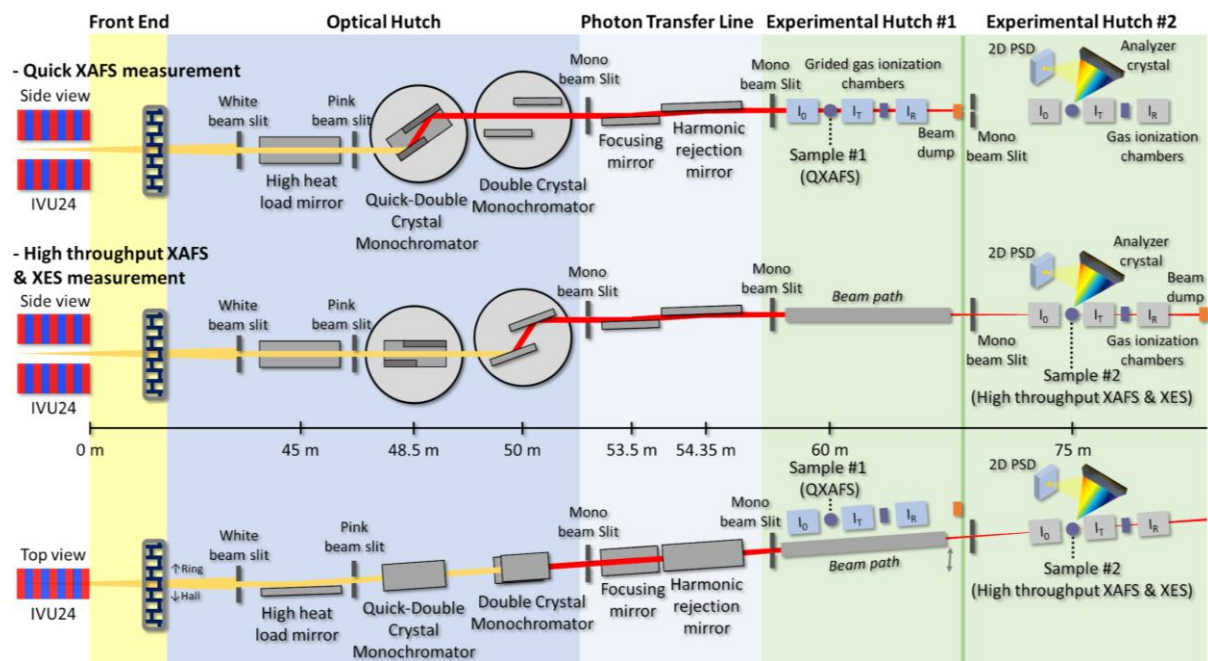
<Figure 3.2.7.4> The effect of taper ratio control on photon beam flux and beam shape. (a) Flux and photon energy bandwidth at an initial gap of 6.53 mm under different taper ratios. (b) Beam shape variation with increasing photon energy at different taper ratios.

D. Beamline Front End

The RXAFS beamline adopts the standard Front End (FE) design used for IVU beamlines at Korea-4GSR (ref). The FE can handle the 17.9 kW power output of the IVU24. The exit mask features a windowless aperture with a 2 mm (h) x 2 mm (v) opening.

E. Beamline Layout

The beamline layout of RXAFS is illustrated in <Figure 3.2.7.5>. Following the FE section, the Optical Hutch (OH), Photon Transfer Line (PTL), and two tandem Experimental Hutches (EH) are positioned consecutively.



<Figure 3.2.7.5> Schematic illustration for RXAFS beamline layout.

<Table 3.2.7.3> lists the main components of the RXAFS beamline and their distances from the source.

<Table 3.2.7.3> Main components

Component	Distance from source	Specification	Usage
PBPM-3	41 m	Pick-up type	Diagnosing white beam position
Movable Mask	42 m	Water Cooled	Aligning the white beam
Attenuator	43.7 m	Water Cooled, CVD Diamond, B ₄ C, Si	Removing low-energy X-ray beam
White Beam Slit	44 m	Water Cooled, Max. opening size: 1.2(h)×1.2(v) mm ²	1) Removing the heat load by the white beam 2) Preventing the accidents due to malfunction of the movable mask 3) Diagnosing beam position through electron current readout function
HHLM (High Heat Load Mirror)	45 m	In-Ga eutectic cooled 1× sagittal cylinder mirror (Rh 5 nm/Pt 50 nm)	1) Removing of heat load by high-energy X-ray beams 2) Collimating the X-ray beams
Pink Beam Slit	47 m	Water Cooled	1) Aligning the pink beam 2) Removing the scattered beams 3) Diagnosing beam position through electron current readout function
Pink Beam Screen	47.4 m	Water Cooled, YAG+CCD	1) Aligning the HHLM 2) Diagnosing pink beam shape
Quick DCM	48.5 m	Si(111)&(311) LN2 Cooled	1) Monochromatization of the X-ray beam 2) Fast energy scanning speed of 10 to 50 Hz
DCM	50 m	Si(111)&(311) LN2 Cooled	Monochromatization of the X-ray beam
Pink Beam Stop	50.8 m	Water Cooled, YAG+CCD	1) Blocking the pink beam 2) Aligning the DCM
Mono Beam Slit	52.4 m	4 way-slit	1) Aligning the mono beam 2) Removing the scattered beams
Diamond screen monitor	52.6 m	CVD diamond. Thickness: 50 μm	1) Aligning the mono beam 2) DCM 2 nd crystal feedback
HFM (Horizontal Focusing mirror)	53.5 m	2×sagittal cylinder mirror (Si, Rh 5 nm/Pt 50 nm)	1) Focusing the beam in the horizontal direction 2) Removing high-harmonic X-ray beams

HRM (Harmonic Rejection Mirror)	54.35 m	Flat mirror 3×Strip (Si, Rh 5 nm/Pt 50 nm, Pt 50 nm)	1) Focusing the beam in the vertical direction 2) Removing high-harmonic X-ray beams 3) Parallelizing the beam path
Mono Beam Slit	55.5 m	4 way-slit	1) Aligning the mono beam 2) Removing the scattered beams
Mono Beam Screen	55.8 m	YAG+CCD	1) Blocking the mono beam 2) Diagnosing mono beam shape 3) Aligning the DCM
Diamond screen monitor	58 m	CVD diamond Thickness: 50 μ m	1) Diagnosing mono beam position 2) HRM feedback (long-term)
Hutch Shutter	58.6 m		Blocking the mono beam
Hutch Slit	59.2 m	4 way-slit	Defining the mono beam
Sample Position #1 (Quick XAFS)	60 m	Gridded Gas Ionization Chamber, PIPS, In Situ Cell	Quick XAFS experiment stage
Mono Beam Screen	66 m	YAG+CCD	1) Blocking the mono beam 2) Diagnosing mono beam shape
Hutch Slit	72 m	4 way-slit	Defining the mono beam
Nanobeam position monitor	74.5 m	Kapton, Thickness: 75 μ m Positional resolution: < 100 nm	Diagnosing mono beam shape and position
Sample Position #2 (XAFS+XES)	75 m	Gas Ionization Chamber Analyzer Crystals (JJ-X ray), Energy Dispersive Fluorescence Detector, 2D PSD	XES & High-throughput XAFS experiment stage

F. Optics Review

The detailed specifications for the optics are listed in <Table 3.2.7.4>.

<Table 3.2.7.4> Optics specifications

	HHLM	QDCM	DCM	HFM	HRM
Distance from source (m)	45	48.5	50	53.5	54.35
Incident Angle	2 mrad	4.5 to 30° (Si 111) 5.0 to 15° (Si 311)	4.5 to 30° (Si 111) 5.0 to 15° (Si 311)	2 to 3 mrad	2 to 3 mrad
Shape	Sagittal cylinder	Flat	Flat	Cylindrical	Flat
Tangential Radius (km)	7 to 40 km (bender)	-	-	∞	12 to 25 km (bender)
Sagittal Radius (mm)	180	-	-	61.4 (2 mrad): [Rh 5 nm/Pt 50 nm] 92.0 (3 mrad): [Si]	∞
Surface Normal direction	Horizontal	Vertical			
Substrate	Si	Si(111) / Si(311)	Si(111) / Si(311)	Si	Si
Coating Materials (Thickness, nm)	[Rh 5 nm /Pt 50 nm]	-	-	[Si] [Rh 5 nm /Pt 50 nm]	[Si] [Rh 5 nm /Pt 50 nm], [Pt 50 nm]
Beam size (H×V) @ 10 keV ($\mu\text{m} \times \mu\text{m}$)	1,200×1,160	1,290×1,190	1,330×1,190	1,410×1,170	1,360×1,120
Footprint (L × H) (mm×mm)	600×1.2	18×1.2	18×1.2	600×1.2	600×1.2
Substrate size	800×50×55	55×40×50	60×25×50	600×60×50	800×50×50

(L×W×H) (mm×mm×mm)		(1 st crystal)	(1 st crystal)		
Focus distance (m)	∞	-	-	21.5 m	∞
Roughness, σ (r.m.s.)	< 0.3 nm	< 1 μm	< 1 μm	< 0.3 nm	< 0.3 nm
Slope error (Tangential / sagittal) (μrad, r.m.s.)	<1.5/<5.0	<1	<1	<1.5/<5.0	<0.25/<1.0
Max total heat load (W)	16.3	56.1	52.8	-	-
Max surface heat load (W mm⁻²)	0.0326 (@4 keV)	28.1 (@4 keV)	26.4 (@4 keV)	-	-

(1) Optical Simulation

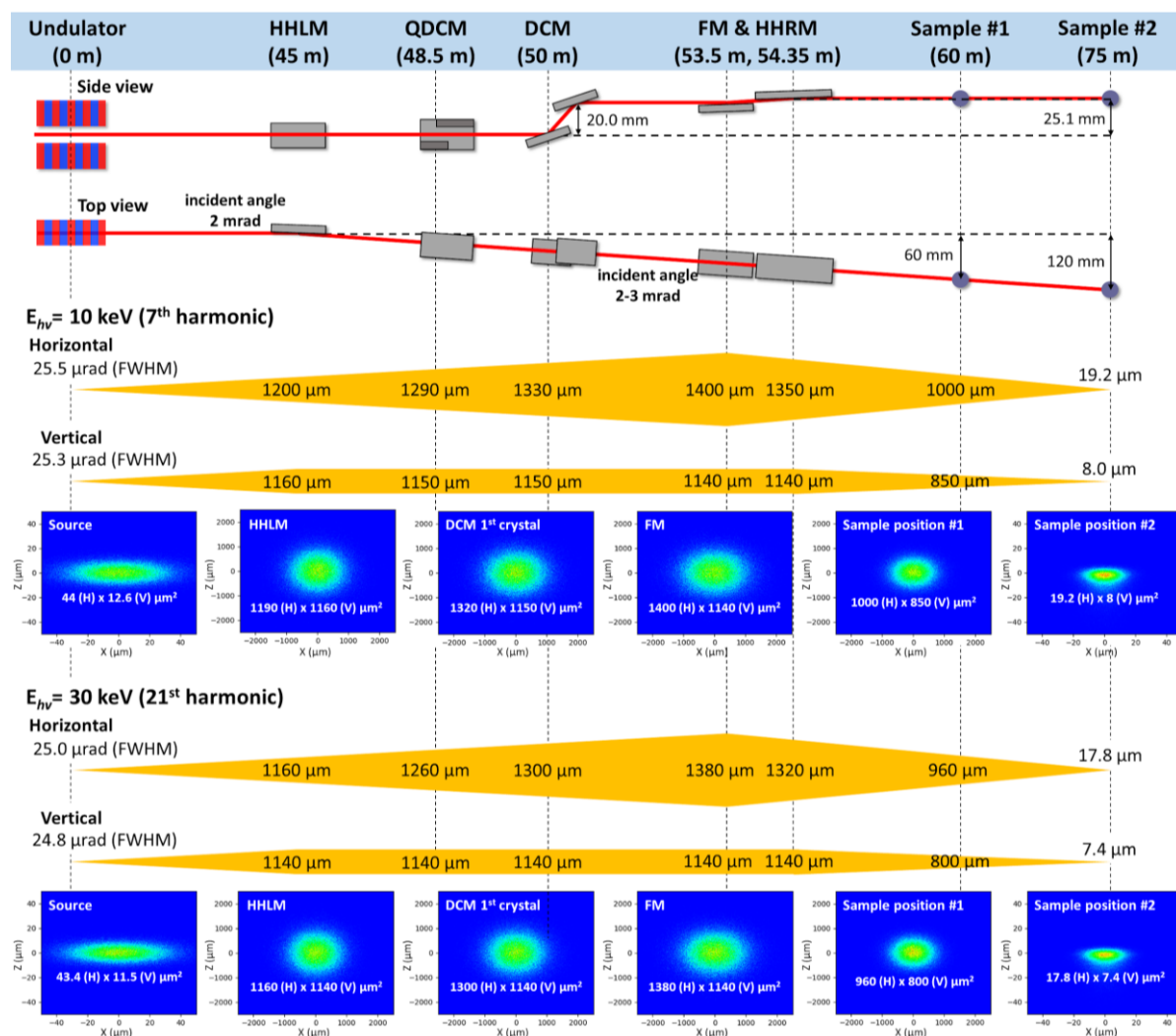
A ray-tracing simulation was conducted to predict the photon beam characteristics, including the photon beam's size and flux at various optics positions, including sample positions #1 and #2. The SHADOW OUI in the OASYS software was utilized for this simulation (source: <https://www.aps.anl.gov/Science/Scientific-Software/OASYS>).

<Figure 3.2.7.6> displays the ray-tracing results for photon energies of 10 and 30 keV, corresponding to the 7th and 21st harmonics, respectively. The expected photon beam size at the source is approximately 44 μm (horizontal) x 12 μm (vertical). The HFM, located at a distance of 53.5 m from the source, will focus the photon beam horizontally toward sample position #2 with a 2.5:1 focusing ratio. The HRM will also focus the beam vertically using the bender. Consequently, the expected photon beam size at sample position #2 will be around 20 μm (horizontal) x 8 μm (vertical).

For sample position #1, designated for the Quick XAFS experiment, a defocused beam will be used. This approach minimizes changes in vertical photon beam position caused by Bragg angle scanning of the Quick DCM by positioning sample position #1 as close to the Quick DCM as possible. The expected beam size at sample position #1, across the entire photon

energy range provided by this beamline, will be approximately 1,000 μm (horizontal) x 800 μm (vertical).

The results in <Table 3.2.7.7> show the ray-tracing data, including the source size, flux, and beam size at the sample positions. The predicted photon flux at the sample position can reach as high as 10^{12} to 10^{13} photons per second across the entire photon energy range of this beamline. These results are based on a tuned undulator with a constant magnetic gap along its length. However, for tapered undulator cases, the flux at the sample position will decrease by about 10^1 or 10^2 orders of magnitude, depending on the degree of tapering. Under typical Quick XAFS measurement conditions, the undulator gap will be tapered by 10% to broaden the photon beam's bandwidth for measuring the XAFS region. In such a case, the flux is expected to decrease by about 10^1 of magnitude.



<Figure 3.2.7.6> Ray-tracing results.

<Table 3.2.7.7> Summary of ray-tracing results

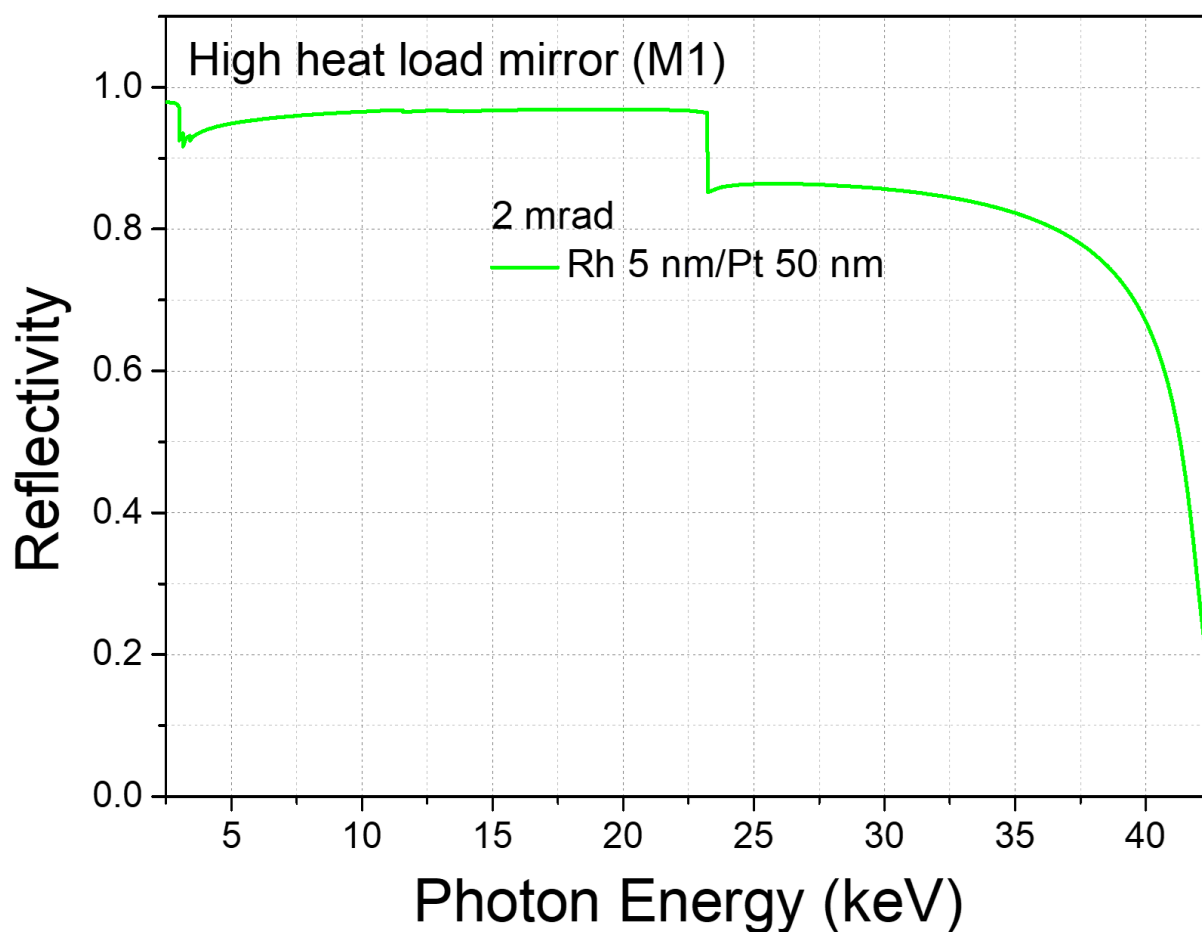
Energy (harmonic)	K	Source size, (H×V, FWHM)	Source flux (ph/s/0.1% B.W.)	Beam size at sample #1 (@60 m) (H×V, FWHM)	Beam size at sample #2 (@75 m) (H×V, FWHM)	Flux at sample (ph/s)
5 keV (3 rd)	2.366	44×14 μm^2	1.7×10^{15}	930×790 μm^2	19.4×8.8 μm^2	9.0×10^{13}
10 keV (7 th)	2.620	44×13 μm^2	9.8×10^{14}	1,000×850 μm^2	19.2×7.4 μm^2	6.8×10^{13}
20 keV (15 th)	2.738	43×12 μm^2	4.1×10^{14}	1,000×830 μm^2	17.8×7.2 μm^2	2.9×10^{13}
30 keV (21 st)	2.620	42×11 μm^2	1.7×10^{14}	960×800 μm^2	17.8×7.4 μm^2	9.7×10^{12}
40 keV (29 th)	2.680	44×11 μm^2	7.9×10^{13}	980×810 μm^2	17.8×7.2 μm^2	3.9×10^{12}

(2) High Heat Load Mirror (HHML or M1)

The High Heat Load Mirror (HHLM), located 45 m from the source, will serve the following purposes:

- Beam collimation
- High heat load management

The HHLM is the first optical component of the RXAFS beamline. To deliver photon beams with an energy range of 4 to 40 keV, Rh 5 nm/Pt 50 nm bilayer will be used as a coating material for the mirror surface. The incident angle of the beam will be set at 2 mrad and fixed during operation to satisfy the ease of the beam alignment process. <Figure 3.2.7.7> shows the reflectivity curve of the HHLM corresponding to photon energy, with no noticeable reflectivity decrease across the entire energy range of 4 to 40 keV. The HHLM reflects the beam horizontally and is cylindrical in the sagittal direction of the mirror crystal. Accordingly, it can collimate a beam vertically, thereby enhancing the energy resolution of a monochromatic beam and reducing flux loss due to the limited Darwin width of the Si crystal in the monochromator.



<Figure 3.2.7.7> Reflectivity curve of the HHLM.

(3) Quick Double Crystal Monochromator (Quick DCM)

The Quick Double Crystal Monochromator (Quick DCM), located 48.5 m from the source, will serve the following purposes:

- **Quick-monochromatization**

The crystal stage of the Quick DCM consists of two liquid nitrogen-cooled channel-cut crystals (Si(111) and Si(311)) placed next to each other, and the crystals can be switched depending on the photon energy to be used. The Quick DCM will have a maximum scanning speed of 60 Hz, enabling XAFS measurements every ten milliseconds when XAFS data are obtained in both forward and reverse scanning directions. The step-scan and on-the-fly scan time for traditional XAFS using standard DCM is a few seconds to a few minutes. It is important to note that Quick DCM is essential equipment for the RXAFS beamline because the main goal of the beamline is to provide real-time measurement methods during various in

situ/operando experiments.

The Quick DCM will be operated under various Bragg rotation speeds using two types of motors: a Goniometer-based step motor and a torque motor on the goniometer. <Table 3.2.7.5> provides a summary of each motor's specifications. The selection of motor type depends on the chemical reaction rate of the system. The photon energy from the source can be adjusted by tuning the magnetic gap of the undulator. However, changing the photon energy of a beam from the undulator at a speed required by Quick DCM is challenging. Therefore, it is important to perform undulator tapering, which effectively broadens the energy bandwidth of the photon beam, when using Quick DCM.

<Table 3.2.7.5> DCM motor specifications

Scan mode	Movement	Range	Motor Speed (frequency)
Bragg angle Step mode (θ_s)	Goniometer-based step motor	4° to 25°	1° s ⁻¹ (~ 0.2 keV s ⁻¹ @ 5 keV) (~ 1 keV s ⁻¹ @ 10 keV)
Bragg angle Fast scan mode (θ_f)	Torque motor on the goniometer	± 2.1°	0.1 to 60 Hz

(4) Standard Double Crystal Monochromator (DCM)

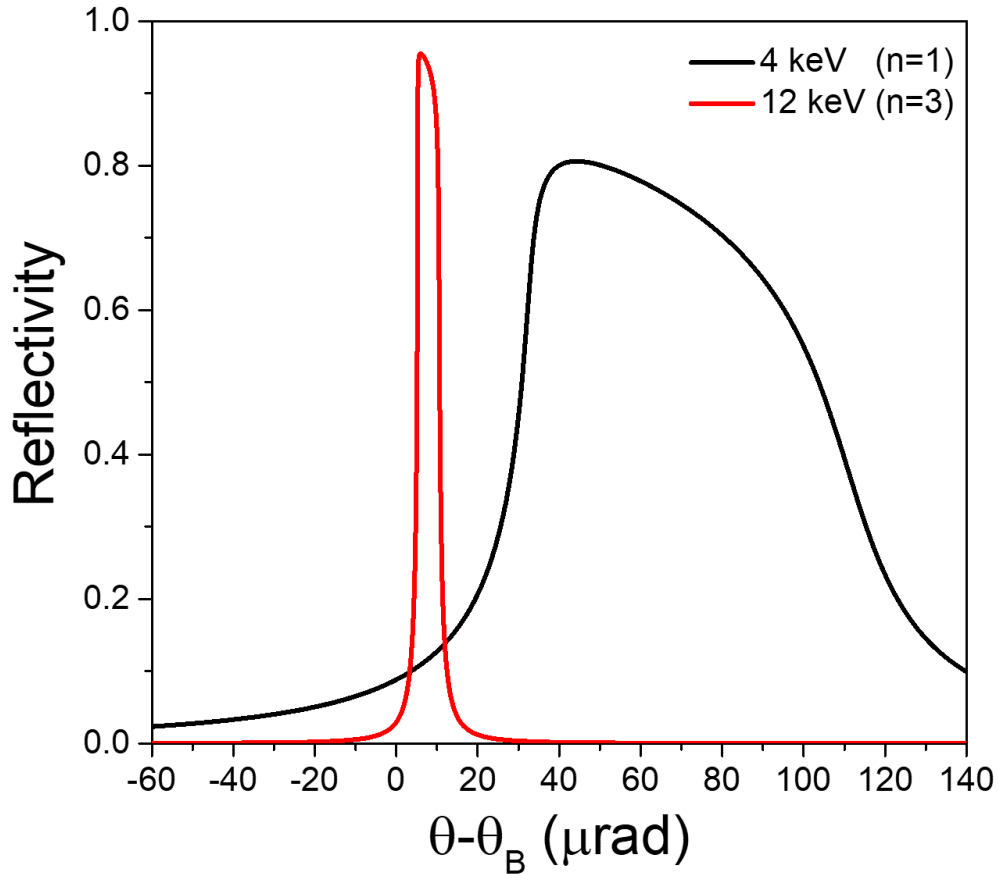
The Standard Double Crystal Monochromator (DCM), located 50 m from the source, will serve the following purposes:

- **Monochromatization**

The crystal stage of DCM consists of two liquid nitrogen-cooled Si crystals, Si(111) and Si(311), which can be interchanged depending on the required photon energy. The DCM will be used for the step-scan and on-the-fly scan, with a measurement time ranging from a few seconds to several minutes. Additionally, XES measurements requiring a stable beam during the procedure will be performed using this equipment. The angular stability over an extended period ranging from hours to days should be maintained within a variation of approximately 20 to 50 nrad to ensure beam stability.

Even after passing through the DCM, the monochromatic beam may still contain high-order harmonics that share the same diffraction condition as the desired beam energy. This issue can

be overcome by slightly detuning the 2nd crystal of the DCM, thereby rejecting the high-order harmonics. <Figure 3.2.7.9> illustrates the Darwin width curves of the Si(111) crystal for two different harmonics. By detuning the second crystal by approximately 70 μrad relative to the Bragg axis, it is possible to effectively suppress the high-order harmonic due to differences in the reflectivity of each harmonic energy.



<Figure 3.2.7.9> Darwin width curve of Si(111).

The energy resolution of the monochromatic beam passed through the DCM can be determined using the following equation:

$$\Delta E/E = \cot\theta_B[\omega_D^2 + \varphi^2]^{1/2} \quad (\text{Eq. 3.2.7.1})$$

In (Equation 3.2.7.1), θ_B , ω_D , and φ represent the Bragg angle, the Darwin width of the Si crystals, and the photon beam divergence, respectively. <Table 3.2.7.6> provides an overview of the calculated energy resolution of the RXAFS beamline, taking into account the beam collimation effect. For Si(111), the energy resolution with a collimated beam is smaller than the natural bandwidth for a specific element, indicating that it is possible to obtain XAFS

data without any distortion caused by photon beam divergence. On the other hand, if the beam is not collimated, the energy resolution may exceed the natural bandwidth, potentially leading to distortion of the XAFS data.

For a monochromatic beam obtained from a Si(311) crystal, the energy resolution is smaller than the natural bandwidth for a specific element. However, it is important to note that the Darwin width of the Si(311) crystal, within the energy range of 15 keV to 40 keV, is ranging from 7.9 to 2.8 μ rad (FWHM). In the same energy range, the vertical divergence of the photon beam is approximately 26 μ rad (FWHM). A significant flux loss may occur in these cases due to the small Darwin width of the Si(311) crystal compared with the photon beam divergence. Therefore, a collimated beam is necessary to reduce photon beam divergence effectively and mitigate flux losses for this case.

<Table 3.2.7.6>The calculated energy resolution of a monochromatic beam

Si(111)			Edge Energy (keV)	$\Delta E/E$ (w.o. collimation)	$\Delta E/E$ (with collimation)	Natural Bandwidth (FWHM, eV)
Energy (keV)	$\Delta E/E$ (10^{-4}) (w.o. collimation)	$\Delta E/E$ (10^{-4}) (with collimation)				
5	1.56	1.4	Ti K (4.966)	0.77	0.70	0.94
10	1.94		Zn K (9.659)	1.87	1.35	1.67
15	2.46		Rb K (15.200)	3.74	2.13	2.99
20	3.04		Mo K (20.000)	6.08	2.80	4.52
25	3.50		Pd K (24.350)	8.52	3.41	6.24

Si(311)			Edge energy (keV)	$\Delta E/E$ (w.o. collimation)	$\Delta E/E$ (with collimation)	Natural Band Width (FWHM, eV)
Energy (keV)	$\Delta E/E$ (10^{-4}) (w.o. collimation)	$\Delta E/E$ (10^{-4}) (with collimation)				
15	1.06	0.3	Rb K (15.200)	1.61	0.46	2.99
20	1.41		Mo K (20.000)	2.82	0.60	4.52
25	1.68		Pd K (24.350)	4.09	0.73	6.24
30	2.04		Sb K (30.491)	6.22	0.91	9.16
35	2.40		Cs K (35.985)	8.64	1.08	12.3
40	2.76		Ce K (40.443)	11.2	1.21	15.1

The scanning speed of the Bragg angle for this DCM should be adjustable from 0.001°/sec

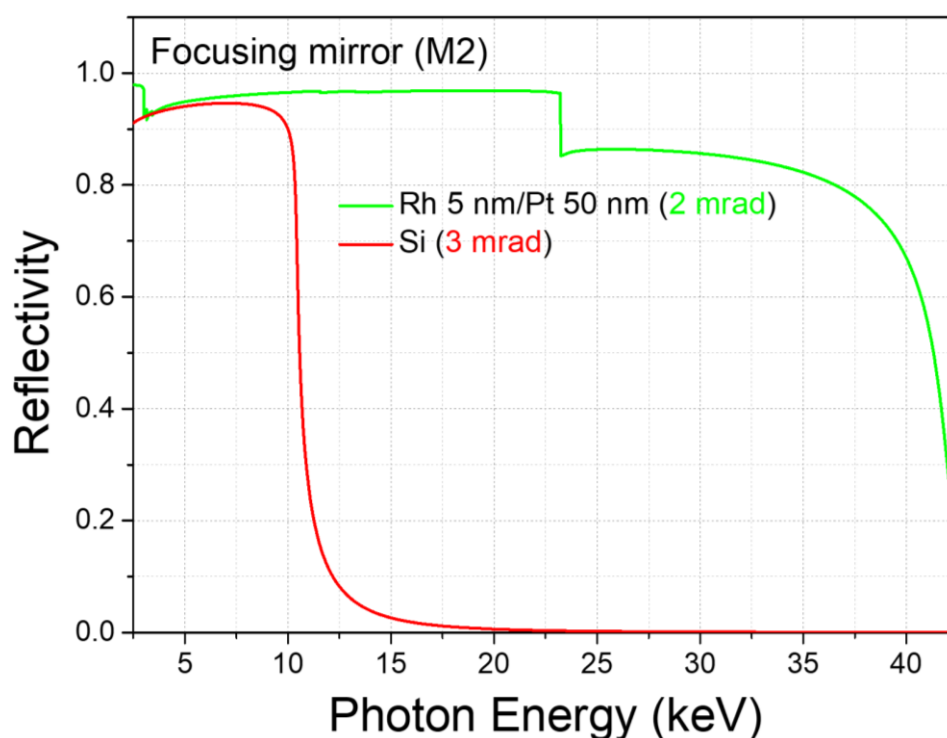
to 4°/sec without any hardware or software modifications. This flexibility enables us to swiftly switch between measurement modes. Additionally, the beam offset should align with that of the Quick DCM, ensuring easy optical alignment when switching between the two monochromators. Several manufacturers offer products that meet these specified criteria.

(5) Horizontal Focusing Mirror (HFM or M2)

The Horizontal Focusing Mirror (HFM), located 53.5 m from the source, will serve the following purposes:

- Beam focusing in a horizontal direction
- High harmonic rejection

The HFM is designed to reflect the beam vertically (up-bounce) and feature a sagittal cylindrical shape, allowing it to focus the beam horizontally. It consists of two mirror surfaces with different coatings and sagittal radii, enabling it to focus the beam and reject high harmonics by changing the incident angle. <Figure 3.2.7.10> illustrates the reflectivity curve of the HFM with two mirror surfaces: a Rh 5 nm/Pt 50 nm bilayer and Si, for incident angles of 2 mrad and 3 mrad, respectively.



<Figure 3.2.7.10> Reflectivity curve of the HFM.

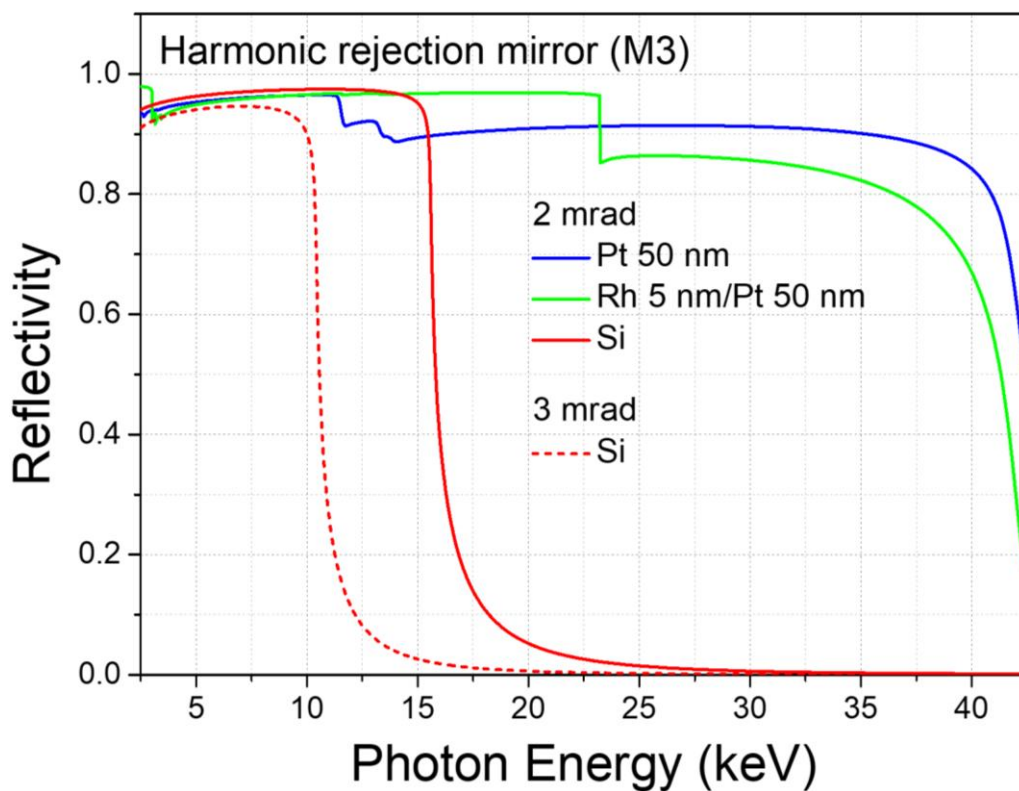
The RXAFS beamline will deliver photon beams with energies starting from 4 keV.

Therefore, it is essential to remove high harmonics when using the beam around this energy. When users need to adjust the photon energy across a wide range of 4 to 40 keV in a single beamtime, they will use a mirror with a Rh 5 nm/Pt 50 nm coating in a fixed mode. Harmonic rejection will then be achieved by detuning the 2nd crystal of the DCM for effective beamline management. By allowing users to easily switch between different photon energies, the HFM provides a flexible and efficient solution for a wide range of experimental requirements.

(6) Harmonic Rejection Mirror (HRM or M3)

The Harmonic Rejection Mirror (HRM), located at 54.35 m from the source, will serve the following purposes:

- Beam focusing in a vertical direction
- High harmonic rejection



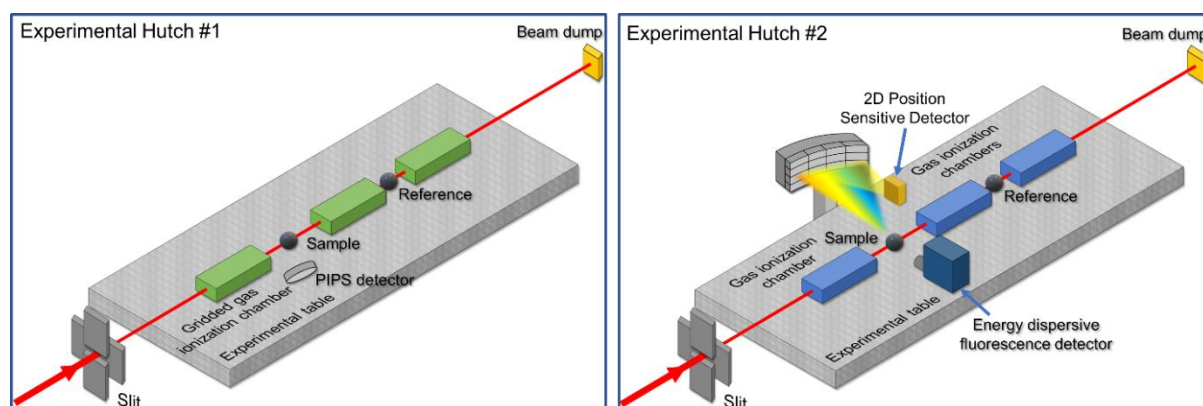
<Figure 3.2.7.11> Reflectivity curve of HRM.

The HRM will be designed to reflect the beam vertically (down-bounce) and has an originally flat shape, allowing it to focus the beam vertically using a bender. It consists of three

mirror surfaces: Si, Rh 5 nm/Pt 50 nm, and Pt 50 nm. The mirror surface can be interchangeable depending on the required photon beam energy. When the beam energy is below 15 keV, the Si surface will be used to remove the high harmonics effectively. Adjusting the incident angle from 2 mrad to 3 mrad is an additional option to remove the high harmonics when using the beam with energy around 4 to 5 keV. Since it is difficult to remove the high harmonics by detuning the crystal in the Quick DCM, which is equipped with the channel-cut Si, the effective rejection of high harmonics through this HRM becomes important during the Quick XAFS measurement. For traditional XAFS, the Rh 5 nm/Pt 50 nm coating will be used, and the high harmonics can also be removed by detuning the 2nd crystal of DCM.

(7) Experimental System Overview

The end-stations of the RXAFS beamline will be used for conducting XAFS, Quick XAFS, and XES experiments aimed at investigating the electronic, chemical, and structural properties of novel materials, including nanomaterials, catalysts, batteries, and nanomedicine, during specific chemical reactions. Therefore, the beamline has broad applications across various scientific fields, each requiring distinct sample environments. To accommodate this diversity, the RXAFS beamline will operate two separate end-stations, designated as Experimental Hutch #1 (EH #1) and Experimental Hutch #2 (EH #2), located 60 m and 75 m from the source, respectively. <Figure 3.2.7.11> provides a schematic illustration of the experimental setups for each hutch, featuring gas ionization chambers, X-ray fluorescence detectors, a 2-dimensional position-sensitive detector, and analyzer crystals.



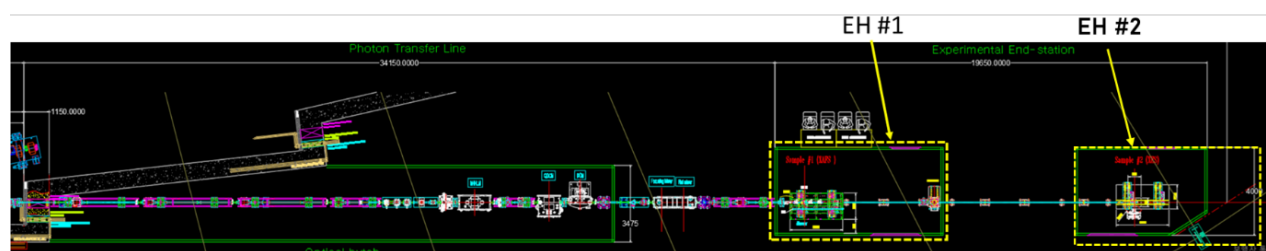
<Figure 3.2.7.11> Schematic overview of end-stations.

○ Experimental Hutch I

EH #1 will include gridded gas ionization chambers as the main equipment to capture the XAFS spectrum within a few milliseconds, which is essential for Quick XAFS measurements. Passivated Implanted Planar Silicon (PIPS) detectors will be used to detect the X-ray fluorescence signal from the sample within a similar time frame. A range of in-situ cells, including electrochemical cells, a Linkam heating stage with controllable interior gas composition, and capillary cells, will be available for users interested in conducting in-situ/operando XAFS measurements. The equipment would be installed on an optical table to facilitate easy setup and removal.

Many in-situ/operando Quick XAFS measurements require a specific gas environment. A gas supplier with several channels for different gases, including hydrogen, oxygen, nitrogen, and carbon dioxide, will be installed inside the hutch. The specific gases to be supplied would be reassessed in future meetings with users to meet their demands.

<Figure 3.2.7.12> shows the location of EH #1, where the equipment for Quick XAFS mentioned above will be installed.



<Figure 3.2.7.12> Location of EH #1 and EH #2.

○ Experimental System II

In the second hutch (EH #02) as shown in the <Figure 3.2.7.12>, equipment for X-ray Emission Spectroscopy (XES) experiments will primarily be installed. XES has emerged as a necessary tool in synchrotron science due to its unparalleled capability to probe the electronic structure, chemical environment, and spin states of a wide variety of materials. Unlike conventional X-ray absorption techniques, XES offers element-specific and site-selective information into occupied electronic states, enabling the study of both ground and excited states with high sensitivity. The application of XES is particularly crucial for investigating systems containing transition metals and rare-earth elements, where subtle changes in the local electronic configuration can influence physical and chemical properties.

The XES equipment, equipped with a von Hamos spectrometer, is designed with a diverse set of scientific experiments in mind, each addressing fundamental questions in materials science and chemistry. Primary application is the study of catalytic mechanisms in transition metal complexes and heterogeneous catalysts, where XES can reveal oxidation states, ligand fields, and spin states at active sites under working conditions. Another area is battery and fuel cell research: XES enables the tracking of redox processes and degradation pathways in electrodes and electrolytes during operation, offering insights essential for the design of next-generation energy storage materials. These experiments demonstrate the potential of XES in addressing key challenges in the fields of energy, environment, and technology.

The spectrometer will be capable of accommodating up to 16(4x4) segmented cylindrically bent analyzer crystals, each mounted on an independent crystal holder equipped with stages that allow for both linear and tilt adjustments. Candidate analyzer crystals include Si(100), Si(111), Si(220), Si(311), and Si(331), enabling detection of fluorescence signals in the 5–20 keV energy range. This range covers the K emission lines of transition metal elements. The spectrometer will be coupled with a two-dimensional position-sensitive detector (2D-PSD).

To maximize the versatility of the XES beamline, the von Hamos spectrometer will support several principal experimental configurations. The first is the conventional XES measurement, optimized for high-resolution detection of $K\beta$ and $K\alpha$ emission lines from transition metal samples. This setup employs cylindrically bent analyzer crystals and a position-sensitive detector, achieving energy resolutions on the order of 0.3 to 0.5 eV, suitable for discerning subtle valence and spin state variations. The second configuration is an in situ/operational XES for changes in electronic structure during chemical synthesis or transformation. The third setup is resonant XES (RXES), in which the incident X-ray energy is tuned across absorption edges while monitoring emission, providing two-dimensional maps of electronic excitations including HERFD-XAS. Each of these setups can be further adapted for in situ or operando measurements, supporting a broad spectrum of cutting-edge research programs.

The contents of this chapter may be modified depending on the direction of beamline construction and are not in a final state.

3.2.8 ID22 BioNX Beamline

A. Introduction

The Bio Nanocrystallography (BioNX) beamline is the first designated MX beamline for the Korea-4GSR during its initial phase. This beamline will conduct Macromolecular crystallography (MX) technique to determine atomic resolution crystal structures of biological macromolecules such as protein, DNA, RNA, and their complexes. To date, approximately 200,000 atomic-resolution structures of biomacromolecules have been determined, with 85% of these structures resolved using macromolecular crystallography performed in synchrotron(1). Due to these high-resolution three-dimensional structures, modern biology can understand how biomolecules interact each other, their roles in biological processes, and their contributions to health and disease. This knowledge has significantly advanced the fields of biology and pharmacology, and more recently, it has been actively utilized in drug discovery research.

Recent developments in MX technique focus on extending its applicability to challenging crystals. Membrane proteins, for instance, are notoriously difficult to crystallize and often too delicate to endure conventional handling methods due to their fragility on physical contact and radiation damage (2). Although cryo-cooling of crystals effectively slows down radiation damage, it is hard to get the diffractive crystals and high resolution data with the conventional rotational crystallography. To overcome these challenges, two innovative approaches, serial synchrotron crystallography (SSX) and in situ crystallography (ISX), have emerged (described in B. Scientific objective) (3,4). In contrast to conventional rotational crystallography, serial synchrotron crystallography and in situ crystallography determine crystal structures by collecting snapshots or wedge data from microcrystals. After collecting as many snapshots or wedge datasets as possible from numerous crystals, the individual snapshots and datasets are integrated and merged to produce one complete structural dataset (5). This method offers the advantages of eliminating the optimization step to generate large membrane protein crystals and allows experiments to be conducted at both room temperature and cryogenic temperature since radiation damage to a single crystal can be reduced below the Garman limit (6–8). Due to highly coherent and low divergence beam of the 4th generation storage ring, BioNX beamline facilitates these technique for facing challenging problems in structural biology.

Furthermore, the high beam flux and ultra-fast detector enhance imaging speed, allowing a

larger number of samples to be processed each day and thereby increasing the capacity for high-throughput screening (HTS). This improvement has accelerated the drug design process to generate a final lead compound, reducing both the cost and time required for drug development (9). Therefore, leveraging the advantages of Korea-4GSR, the BioNX beamline aims to incorporate cutting-edge scientific technologies to design a world-class advanced beamline.

The design of the BioNX beamline was referred by the FMX beamline at NSLS-II (10). Design goal of BioNX beamline is summarized in <Table 3.2.8.1>. Key features include a target beam size at the sample position ranging from 1 x 1 to 13 x 13 μm^2 , photon energies between 8 and 25 keV, and a photon flux of 10^{13} to 10^{14} ph/s. To enable rapid changes in beam size, a CRL (Compound Refractive Lens) defocusing method has been adopted. Additionally, a horizontally bounced Double Crystal and Multilayer Monochromator (hDCMM) will be employed to stably deliver the micron size beam and provide a high flux. These specifications are comparable to those of recently upgraded international MX beamlines <Table 3.2.8.2>. It is anticipated that this will elevate the standard of MX in Korea to a world-class level.

<Table 3.2.8.1> Design goal of BioNX beamline

Content	Details
Light source	In-vacuum undulator 20 (3 m)
Photon energy (keV)	8 to 25
Wavelength (Å)	0.5 to 1.55
Energy resolution ($\Delta E/E$)	$<2 \times 10^{-4}$
Beam size (μm^2)	1 x 1 to 13 x 13 in FWHM
Photon flux (ph/s)	10^{13} to 10^{14}
Techniques	SSX, ISX, HTS
Measurement speed	> 100 Hz

<Table 3.2.8.2> Comparison of MX Beamline Specifications at international Synchrotrons

	4GSR BioNX	ANSTO MX3	Diamond VMXm	ESRF ID29	MAX-IV microMAX	NSLS-II FMX
Beam size (μm^2, VxH) (minimum)	1x1	2x2	0.3x0.5	0.5x0.5	1x1.5	1x1.5
Beam size (μm^2, VxH) (maximum)	13x13	8x2	10x13	6x5	5x5	10x10
Photon flux @sample (ph/s)	10^{13} to 10^{14}	6×10^{13}	$> 10^{13}$	$> 5 \times 10^{15}$ @10keV	10^{13} (DCM) 10^{14} to 10^{15} (DMM)	3.5×10^{12}
Energy range (keV)	8 to 25	10 to 15	7 to 28	10 to 25 and 35	5 to 25 (DCM) 10 to 13 (DMM)	5 to 30
Undulator	IVU20 (3m)	IVU17.2 (3m)	IVU21	IVU21	IVU18 (3 m)	IVU21 (1.5 m)
Monochromator (Energy resolution)	hDCMM	hDMM (0.9%, 0.5%, 0.3%)	hDCM	-	hDCM (2×10^{-4}) DMM (0.4%, 1%)	hDCM (3×10^{-4})
CRL defocus	O	O	x	-	O	O
Diffractometer	MD3-UP	MD3-UP	-	MD3-UP SSX	MD3-UP	Nelson Air SP150
Detector	EIGER2 XE 16M	Eiger2 XE 16M	EIGER2 X CdTe 9M (high energy) Pilatus3 6M (medium X-ray energy)	Jungfrau 4M	EIGER2 X CdTe 9M	EIGER X 16M
Operation status	Under designing	Commissioning	Commissioning	Operation	Commissioning	Operation

B. Scientific objective

(1) Serial synchrotron crystallography (SSX)

The primary technique of the BioNX beamline is serial synchrotron crystallography (SSX). The demand for analyzing the crystal structures of challenging proteins has recently increased

(11). Challenge proteins are difficult to crystallize, and optimizing them to large sizes is time and resource consuming work. Therefore, technology capable of obtaining diffraction patterns from microcrystals has become essential, leading to the development of SSX. The principle of SSX is to obtain diffraction patterns from microcrystals while minimizing radiation damage. This is achieved by a small beam with high flux, for which a snapshot from a single crystal can be obtained before it is destroyed with a short exposure time (12). At the same time, methods for delivering microcrystals have been developed as the liquid jet and fixed target. In the liquid jet method, protein crystals are mixed with a viscous solution and slowly flowed so that the crystals are delivered into the path of the X-ray beam. The fixed target method involves spreading microcrystals onto a chip with small wells, and diffraction patterns are obtained by raster scanning the X-ray beam over the chip. Using these methods, the goal is to collect as many snapshots as possible to reconstitute one complete dataset (<Figure 3.2.8.1>, left panel) (5). Essential components for this approach include a beamline design that provides high flux and a small beam size, fast detector and data acquisition (DAQ) infrastructure for rapid data collection, and software for data processing (13).

To meet this demand, BioNX beamline is planned to be designed to utilize a 1-micron beam and a photon flux 10^{13} to 10^{14} photons per second. In addition, not only a diffractometer with a sphere of confusion value below 200 nm for precise sample alignment but also an ultra-fast detector, capable of capturing images at up to 560 Hz in full frame mode are required. This composition is expected to construct a high-performance SSX system, enhancing the efficiency and accuracy of the data collection. The sample delivery system would primarily provide fixed-target method. Compared to the serial femtosecond crystallography (SFX) beamlines at XFEL, where beamtime is limited, BioNX beamline will improve accessibility to serial crystallography experiments, allowing users to more easily perform this technique.

(2) In-situ crystallography (ISX)

In-situ crystallography (ISX) is a technique used to study the structural properties of crystals directly in their native environment, without the need for crystal extraction or transfer. This method minimizes potential damage and artifacts that can arise during handling and exposure to non-native conditions. By maintaining the crystals in their natural state, ISX can provide more accurate and high quality data on the molecular structure of the protein crystal. This

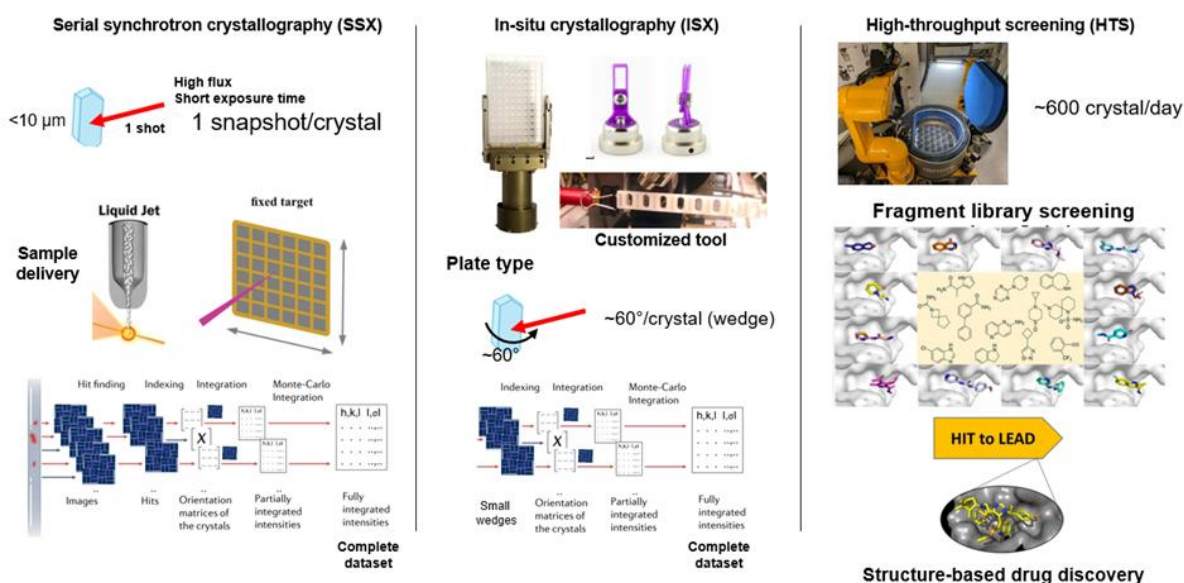
approach is particularly useful for studying fragile and difficult-to-crystallize proteins and other macromolecules (4).

To implement this technique, a 96-well plate or a customized tool produced by a 3D printer can be used (<Figure 3.2.8.1>, middle panel). When employing plate-type data collection, around 60 degrees of data can be collected per sample, referred to as a "wedge." By collecting multiple wedges and subsequently integrating and merging them, a complete dataset can be generated. This approach is known as small-wedge synchrotron crystallography (SWSX) (7,14,15). The technique requires a specialized goniometer head capable of mounting the plate, a beam size of approximately 10 μm or less, and a photon flux ranging from 10^{11} to 10^{12} photons per second. The BioNX beamline is designed to meet these requirements and aims to establish a user-friendly environment.

(3) Automated high-throughput screening (HTS)

Automated high-throughput screening using MX beamlines at synchrotrons has significantly accelerated the identification of potential drug candidates by rapidly analyzing numerous protein-ligand complexes. This is achieved by automating sample handling and data collection, which facilitates the efficient screening of large compound libraries (<Figure 3.2.8.1>, right panel) (16).

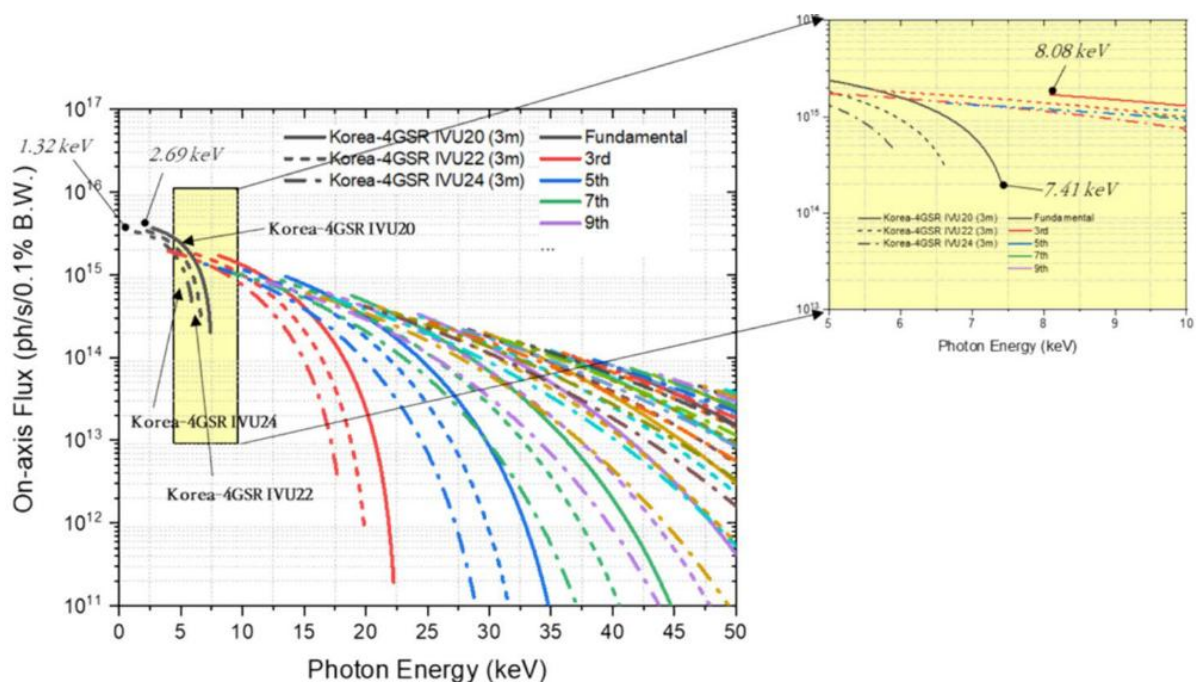
The BioNX beamline will support remote sample delivery and experimentation, enabling the screening of around 600 samples per day. Additionally, a dedicated high-throughput fragment screening laboratory will be established, allowing users to conduct experiments directly at the accelerator facility (described in section “H. (1) Sample preparation laboratory”). This approach not only accelerates the speed and precision of drug discovery but also provides detailed insights into the interaction between target proteins and chemical compounds at atomic resolution. It enables a deeper understanding of the mechanism of action of potential therapeutic agents, thereby enhancing the overall drug development system.



<Figure 3.2.8.1> Beamline sciences of the BioNX beamline.

C. Beamline Requirements for the Insertion Device

The primary objective of the BioNX beamline is to maximize data acquisition from challenging small crystals with high flux beam and short exposure times. To achieve this, it is necessary to adopt an in-vacuum undulator capable of generating high flux. Among the three undulators planned for the Korea-4GSR (IVU20, IVU22, and IVU24), the IVU20 offers the highest flux (see <Figure 3.2.8.2>, <Table 3.2.8.3>). Additionally, it has the advantage of having the lowest heat load at 12 kW. However, the IVU20 exhibits a spectral discontinuity between 6.8 keV and 8.08 keV, which limits experiments within this energy range (17). For instance, element scans of cobalt (Co) might be restricted. Nevertheless, since these elements are present in biological samples at trace levels of less than 1% (18), it is anticipated that few users will require this capability. The BioNX beamline will cover an energy range of 8-25 keV with primary operations planned at 12.4 keV and 20 keV. At this energy range, the photon flux at the sample position is expected to be approximately 10^{13} to 10^{14} ph/s. The IVU20 undulator to be used in the BioNX beamline has a length of 3 m, a period of 20 mm, and a gap size adjustable between 5 and 18 mm. The source parameters of BioNX are summarized in <Table 3.2.8.4>.



<Figure 3.2.8.2> Predicted photon flux and spectral discontinuity of the IVU20 (17).

<Table 3.2.8.3> Comparison of the three undulator of Korea-4GSR (17)

IVU Type	IVU20	IVU22	IVU24
On-Axis Flux	Best	90% of IVU20's between 10 to 30 keV	80% of IVU20's between 10 to 25 keV
Coherent Flux	Best	80% of IVU20's between 10 to 30 keV	60% of IVU20's between 10 to 30 keV
Spectral Continuity	Missing/compromised between 7.41 keV and 8.08 keV	Perfect at gap size <5.58 mm	Perfect at gap size <6.46 mm
Heat Load on Beamline by Off-Axis Radiation	Best: 12 kW at the minimum gap size	15 kW at the minimum gap size	17 kW at the minimum gap size

<Table 3.2.8.4> Source Parameter for BioNX beamline

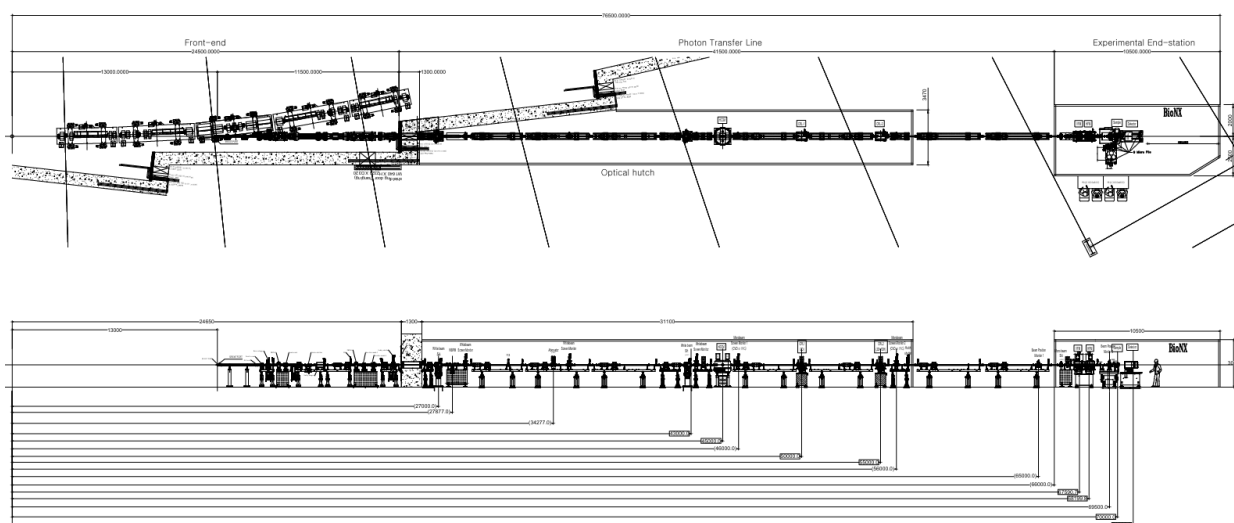
Undulator	Period (mm)	Length (m)	Gap size (mm)	$K_{\max}$	Max total power (kW)	Power density (kW/mrad ²)
IVU20	20	3.0	5 to 18	1.91	12.5	165

D. Beamline Requirements for Front End

The Front End of the BioNX beamline will incorporate the latest High Heat-Load Front End, capable of handling up to 12 kW of power and specifically designed to support the X-ray beam from the IVU20. More detailed information can be found in the 'Front End' section of this report.

E. Beamline Layouts

The layout of the BioNX beamline consists of a front-end, an optical hutch, and an experimental hutch. Two separate enclosed hutches, the optical hutch and the experimental hutch, will be operated and located at sector ID22. In the optical hutch, a Double Crystal and Multilayer Monochromator (DCMM) and various diagnostic devices will be installed to monochromatize the white beam before transmitting it to the experimental hutch. The experimental hutch will enclose Compound Refractive Lenses (CRLs) and focusing mirrors, which focus the monochromatized beam from the optical hutch down to a minimum of 1 micron. By placing the mirror devices within the same hutch as the sample, the influence of temperature fluctuations on the beam would be minimized. Additionally, beam conditioning devices will be installed as well. The distance from the undulator to the sample is 70 m (<Figure 3.2.8.3>). <Table 3.2.8.5> presents all major components and their respective locations along the beamline.



<Figure 3.2.8.3> Beamline layout of BioNX.

(1) Beamline Component Table

<Table 3.2.8.5> Component list of BioNX beamline

Hutch distance (m)	Distance (m)	Component	Specification	Description
Optical Hutch 26 to 57 m	43	White beam slit	4-way slit, UHV	Beam conditioning
	43.5	White beam screen monitor	Retractable; CCTV Diamond BPM	White beam monitor
	45	horizontal DCMM	Si(111) crystal and Mo/B4C multilayer	Monochromator Monobeam
	46	Monobeam screen monitor	CCTV; cooled	Monobeam profiling
	48	Heat load chopper	Water cooled	Reducing thermal load and generate pulsed beam
	50	CRL1	2D, diamond lens	Beam focusing
	55	CRL2	2D and 1D, diamond lens	Beam size expansion
	56	Monobeam screen monitor	CCTV; cooled	Monobeam profiling
Spool 57 to 66 m	65	Beam position monitor	Diamond, Ultra high vacuum, feedback	Beam position & profile defining
End-station 66 to 77 m	67.2	Monobeam Slits	4-way slit, UHV	Beam conditioning
	67.7	VFM	Si/ Rh (50) /Pt (50)	Focusing vertical beam
	68.4	HFM	Si /Rh (50) /Pt (50)	Focusing horizontal beam
	69	Fast chopper	Water cooled	Generation of the pulsed beam
	69.8	Beam position monitor	< 100 nm resolution, feedback	Beam position & profile defining
	70	Sample stage	MD3-UP SOC: <200 nm	Beam diffractometer
	Up to 71	Detector	EIGER 2 XE 16M	Detection of diffraction pattern

F. Optics Overview

(1) Beam Delivery Specifications

The beam delivery system of the BioNX beamline has two distinct features. First, due to the small ratio of source-beam size, 4:1 (horizontal FWHM: 42 μm , vertical FWHM: 11 μm), and a beam divergence close to 1:1 (horizontal FWHM: 22.8 μrad , vertical FWHM: 21.6 μrad), a one-stage direct focusing using Vertical Focusing Mirror (VFM) and Horizontal Focusing Mirror (HFM) without employing a secondary source will be applied. This approach reduces the optical complexity and minimizes the decrease in beam flux that would result from using a secondary source. The stability of the micro-sized beam is ensured by adopting a horizontal bounced monochromator. This beam delivery system simplifies the optics and enhances manageability, which would provide the advantage of delivering a stable beam. Second, the beam size can be adjusted by expanding the beam using CRLs. By adding a CRL to the beam path, the focal point of the beam moves to upstream, which leads to increase the beam size at the sample position.

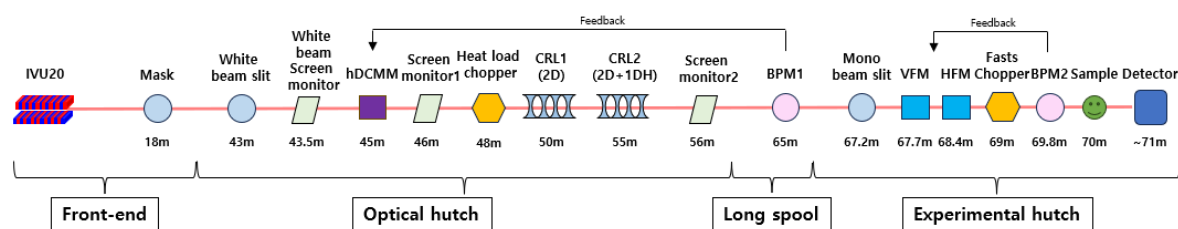
This defocused beam enables rapid changes in beam size without the need to fine-tune the focusing mirror requiring precise and delicate adjustments (10). For example, when focusing only with the focusing mirror without a CRL, the beam size is approximately $0.9 \times 0.3 \mu\text{m}^2$. To increase the beam size, CRLs can be added, allowing for beam sizes ranging from approximately $1 \times 1 \mu\text{m}^2$ to $13 \times 13 \mu\text{m}^2$ (as shown in <Table 3.2.8.6>). The variation in beam size due to focal point shifts with energy changes will be managed by limiting the number of CRLs and controlling the available beam sizes. The anticipated beam size and flux, calculated using OASYS, are summarized in <Table 3.2.8.6>.

<Table 3.2.8.6> Expected flux and beam sizes of the BioNX beamline

Energy (keV)	Optics	Beam size (FWHM, μm , HxV)	Flux (ph/s)
12.4	KB only	0.93x0.38	6.67×10^{13}
12.4	1 CRL-2D	1.83x2.72	4.87×10^{13}
12.4	2 CRL-2D and 1 CRL-1DH	7x5.34	4.68×10^{13}
12.4	4 CRL-2D and 1 CRL-1DH	9.74x10.47	4.5×10^{13}
20	KB only	0.98x0.37	2.11×10^{13}
20	1 CRL-2D	1.14x1.11	1.37×10^{13}
20	5 CRL-2D and 3 CRL-1DH	5.39x5.15	1.33×10^{13}

(2) Detailed Optical Layout

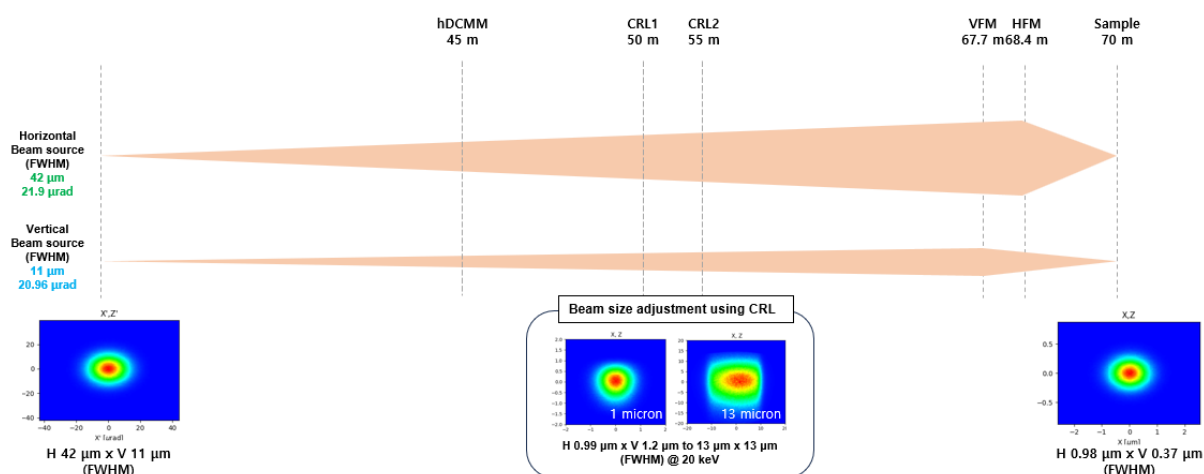
The optical layout scheme of the BioNX beamline is shown in <Figure 3.2.8.4>. The beamline is divided into three sections as the Front End, the optical hutch, and the experimental hutch. In the optical hutch, the white beam will be monochromatized. The experimental hutch will contain the beam focusing system and experimental equipment to obtain diffraction pattern from the sample. The distance from the light source to the sample position is 70 m. A 2D detector for collecting the result will be installed within 71 m.



<Figure 3.2.8.4> The optical layout of the BioNX beamline.

(3) Ray-tracing results

Optical simulations were carried out using the OASYS software. The source size and focal spot size of the BioNX beamline were simulated as well as with the distribution of the beam intensity <Figure 3.2.8.5>.



<Figure 3.2.8.5> Raytracing and simulation of beam size and intensity.

(4) Optics Specifications

<Table 3.2.8.7> Specification of the mirrors

Mirror system type	VFM	HFM
Mirror size	50 x 600 x 50 mm	50 x 600 x 50 mm
Optical footprint	1.62 x 450 mm (3 sigma)	0.9 x 400 mm (3 sigma)
Coating strip number	3 ea	3 ea
Coating strip size	10 x 580 mm	10 x 580 mm
Beam size	1.48 mm x 1.42 mm (FWHM)	1.5 mm x 1.44 mm (FWHM)
Coating material	Si, Rh (50), Pt (50)	Si, Rh (50), Pt (50)
Substrate material	Silicon	Silicon
Mirror surface shape	Elliptical	Elliptical
Reflection direction	Up	Hall
Cooling method	Not	Not
Mirror bender	Not	Not
Tangential radius	Ra=35 km, Rb=37.4 km	Ra=35 km, Rb=31.4 km
Sagittal radius	inf	inf
Tangential slope error	0.2	0.2
Sagittal slope error	0.2	0.2
Incident angle	3.0 mrad	3.0 mrad
Shot beam stability	0.1 um / 30 min	0.1 um / 30 min
Mirror surface height	1400	1400
Motor axis	Pitch, yaw, roll, x, y, z	Pitch, yaw, roll, x, y, z
Manual axis	Pitch, yaw, roll, x, y, z	Pitch, yaw, roll, x, y, z
Installation location (m)	67.7	68.4

○ Double crystal and multilayer monochromator (DCMM)

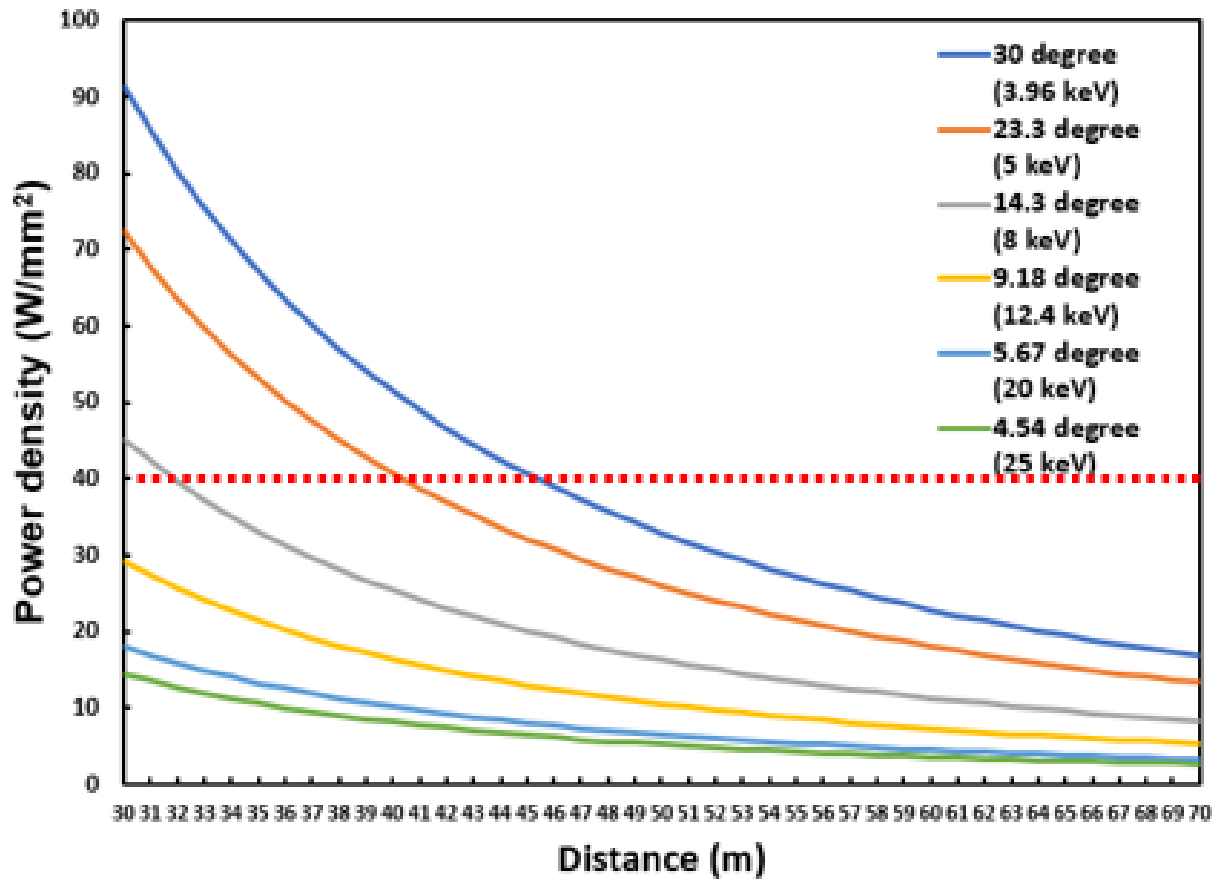
The monochromator employed will be a double crystal and multilayer monochromator (DCMM) with Si (111) and Mo/B4C multilayer <Table 3.2.8.8>. To minimize the high heat load from the 4GSR light source on the monochromator and determine its optimal position, the power density was calculated at various distances using Spectra.<Figure 3.2.8.6> shows how the power density received by the first crystal of the monochromator changes with distance

from the light source. As the Bragg angle and corresponding energy of the first crystal increases as 4.54° (25 keV), 5.67° (20 keV), 9.18° (12.4 keV), 14.3° (8 keV), 23.3° (5 keV) and 30° (3.96 keV), the power density increases simultaneously. Conversely, increasing the distance from the light source leads to decrease the power density. As the 30° is the maximum motion range of the crystal, the power density at a 30° angle was considered as the maximum condition. The first crystal of the monochromator can withstand a heat load limit of 40 W/mm². At a 30° angle, the power density drops below this threshold after approximately 45 m. As a result, the position of the monochromator has been set at 45 m to ensure that the heat load it receives remains at a safe level.

Maintaining beam stability is crucial for the BioNX beamline, particularly when focusing to a minimum size of 1 micron. One of the main factors impacting beam stability is the vibrations caused by the optics configuration. These vibrations are mainly induced from the first and second crystals of the monochromator and it is caused by the cooling system. The primary sources of these vibrations include liquid-nitrogen pulsation, two-phase flow of the gas and liquid, and pump vibrations(19,20). A horizontal bounce monochromator is the most effective solution to mitigate these effects, providing greater stability against vibrations in the vertical beam direction. This design is also compact and resists ground vibrations, making it more suitable for maintaining micron beam sizes compared to vertical configurations (10). It aligns with the polarization direction of the X-ray beam, resulting in considerable absorption within the 5 keV to 6 keV energy range. Consequently, the operational photon energy range for this beamline is confined to 6.5 keV to 20 keV. As mentioned in “Section C. Beamline Requirements for the Insertion Device”, the IVU20 of the Korea-4GSR is incapable of generating X-rays in the 6.8 to 8.1 keV energy range (17). After further optimization, the beamline will accommodate an expanded energy range of 8 to 25 keV, with a primary focus on energies around 12.4 keV and 20 keV. An ultra-high vacuum DBPM will be installed at 65 m to provide feedback for beam position adjustments and to define the beam profile <Table 3.2.8.5>.

<Table 3.2.8.8> Specification of the DCMM

Content	Specification
Photon energy	8 to 25 keV
Energy resolution	$\Delta E/E < 2 \times 10^{-4}$
Crystal and multilayer	Si (111) and Mo/B4C
Cooling	liquid-nitrogen (LN2)
Operation	fixed exit operation, closed loop (encoder) feedback
Sensors and interferometers	the crystal gap and stage vibrations
1stCrystal	50 mm
2ndCrystal	150 to 300 mm



<Figure 3.2.8.6> Power density prediction of the BioNX beamline based on distance from the light source. The red dotted line shows the heat load limitation of the monochromator.

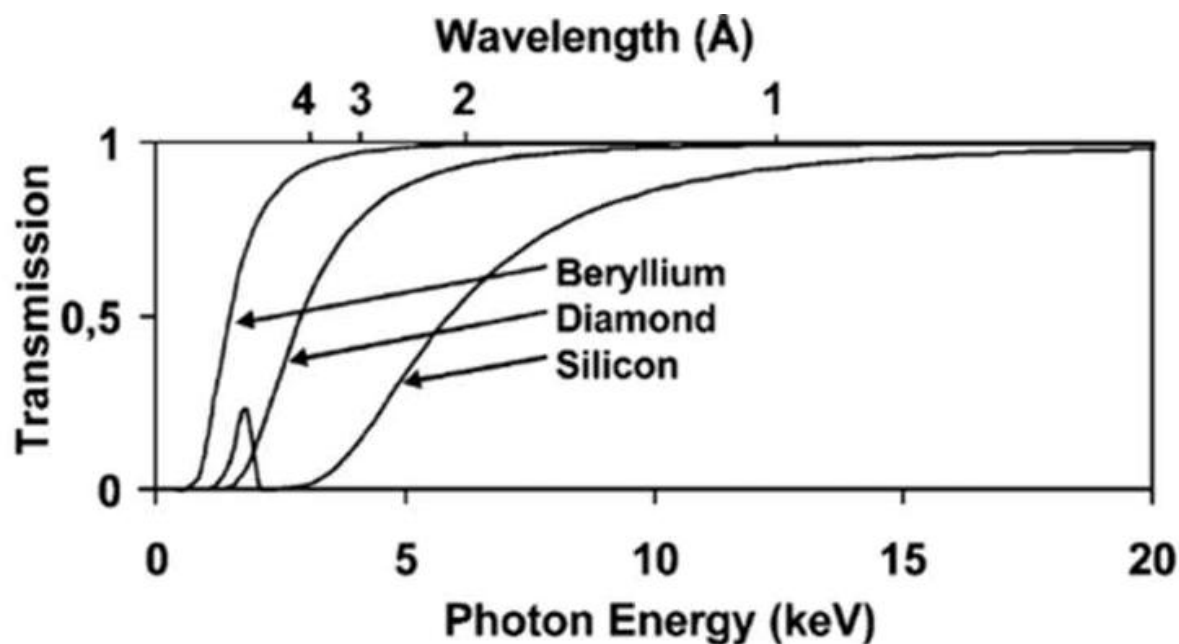
○ Compound refractive lens (CRL)

The CRL (Compound Refractive Lens) is composed of an array of individual lenses, each functioning as a biconcave lens. This arrangement allows for the adjustment of the focal length by modifying the beam's refractive index. As the number of CRLs increases, the focal length shortens, resulting in an increased beam size at a fixed sample position. This phenomenon, known as defocusing, enables the rapid adjustment of the beam size at the sample location (10).

Recent trends in upgraded MX beamlines show a growing adoption of CRL for beam size adjustment (e.g., ANSTO MX3, MAX-IV microMAX, NSLS-II FMX, as shown in <Table 3.2.8.2>). This is because adjusting the beam size by adding CRLs to the beam path is significantly faster than adjusting the beam size by bending a focusing mirror. Additionally, these beamlines often achieve a minimum beam size close to 1 micron, making stability during beam size adjustments critically important. CRLs offer better stability compared to focusing mirrors, particularly in terms of resistance to temperature changes and vibrations (9,21). For these reasons, many international beamlines appear to have opted for CRL defocusing methods to adjust beam size.

Following these advantages, the BioNX beamline will also adopt a CRL defocusing design to ensure stability and quick beam size adjustments with small beams. The beam size adjustments at 12.4 keV and 20 keV are expected to follow the specifications summarized in <Table 3.2.8.6>. The CRL system will use 1D and 2D CRLs for focusing in the horizontal and both direction, with multiple CRLs controlling via a transfocator. A CRL with a radius of curvature around 1 to 6 mm would be required for this setup. However, it has recently been reported that Beryllium, a material widely used for CRLs, has faced production issues, leading to discontinuation. Alternative materials such as diamond, silicon, and aluminum lenses are available, with diamond lenses offering the closest transmission properties to Beryllium (as shown in <Figure 3.2.8.7>).

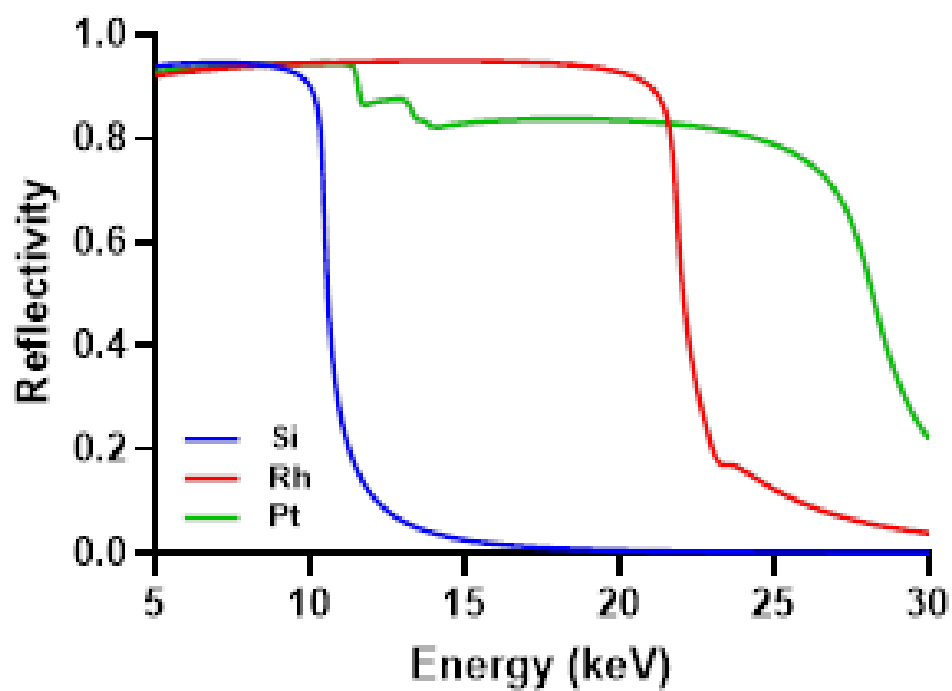
However, since diamond lenses are still under development, it remains to be seen if they can meet the required specifications, and adjustments may need to be made depending on future developments.



<Figure 3.2.8.7> Transmission comparison with three lens materials depending on photon energy (JJ X-ray provided).

○ Focusing Mirrors

Two mirrors, HFM (Horizontal Focusing Mirror) and VFM (Vertical Focusing Mirror), are employed to focus the beam in the horizontal and vertical directions and located at 68.4 m and 67.7 m, respectively. These mirrors will be elliptical with a fixed focal length, as specified in <Table 3.2.8.7>. To provide a stable micron-sized beam at the sample position, the mirrors will be placed close to the sample position and enclosed within an experimental hutch to minimize the vibration and temperature fluctuation affecting beam stability. For high-harmonic rejection, the incidence angle is set to 3 mrad, and the mirror surfaces will be coated in three strips with silicon, rhodium, and platinum. The reflectivity of each surface is shown in <Figure 3.2.8.8>. The mirror surface will be changed according to the monochromatic photon energy.



<Figure 3.2.8.8> Reflectivity based on coating material (Silicon, Rhodium, Platinum) of focusing mirror at 3 mrad of incidence angle.

G. Instrument Overview

(1) Scientific Scope

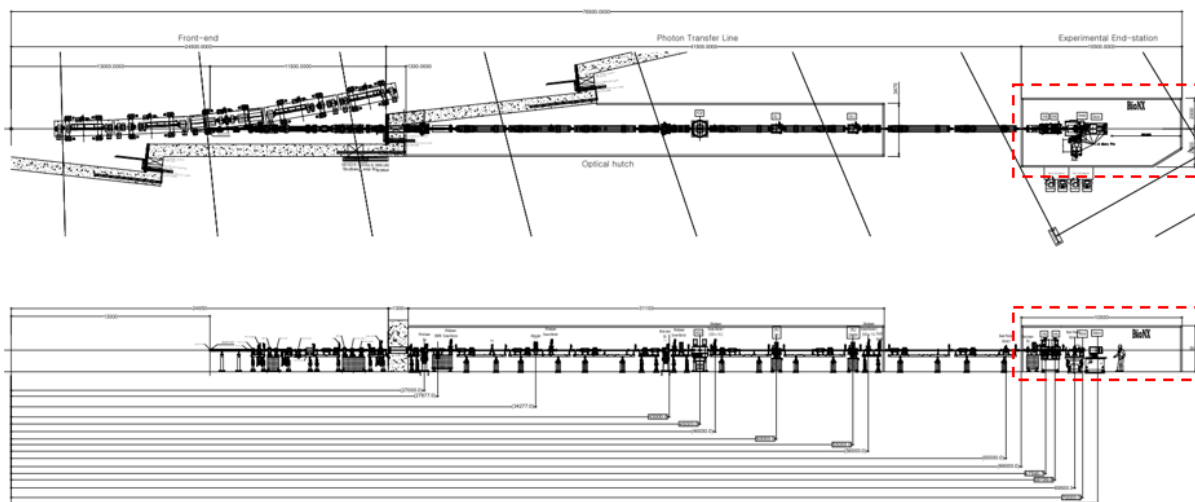
The design objective of the BioNX beamline is to construct a facility that enables both serial crystallography and high-throughput experiments to support drug development. To achieve this purpose, the beamline will be equipped to provide high flux and small beam sizes suitable for obtaining high-quality data from nano- or micro-sized protein crystals, which are commonly used in serial crystallography. Additionally, the beamline features a high-precision diffractometer and an ultra-fast 2D detector for precise alignment of the protein crystal on the micron beam and collects the diffraction data from the high hertz (>100 Hz) experiment. For high-throughput experiments, the end-station will be equipped with a 6-axis robot arm and a sample storage chamber capable of storing approximately 600 samples. The detailed specifications of each piece of equipment are described below.

(2) Instrument Definition

The instrument of the BioNX beamline includes an optical table with beam conditioning diagnostics, a sample diffractometer, a 2D detector, a 6-axis sample exchange robot arm, sample storage liquid nitrogen chamber as well as a silicon drift detector.

(3) Instrument Location

The instrument will be located in the experimental hutch of the ID22 section as indicated in <Figure 3.2.8.9>.



<Figure 3.2.8.9> ID22 section layout of the BioNX beamline. The experimental hutch is marked by the red dotted box.

(4) Instrument Operating Modes

The sample diffractometer will be designed to support easily interchangeable goniometer heads, including a fixed-target SSX-specific goniometer head and a plate-specific goniometer head. This allows for rapid switching between three types of experiments: rotational crystallography, fixed-target serial crystallography, and in-situ crystallography. Consequently, the following four operating modes will be supported:

1. Rotational crystallography mode
2. Fixed-target serial crystallography mode
3. In-situ crystallography mode
4. Automated high-throughput screening with rotational crystallography mode

Each mode can accommodate both cryogenic and room temperature experiments upon user's request.

(5) Instrument Specifications

○ High-precision diffractometer

To handle nano- or micro-sized protein crystal samples, a high-precision diffractometer with a sphere of confusion (SOC) value below 200 nm is required to position samples accurately on

a micron-sized beam. A high-resolution microscope must be able to observe the crystal samples along the same axis as the beam to precisely align micron-sized samples within the beam. All devices for sample alignment and movement must operate with precision of several hundred nanometers and must exhibit repeatability and high reproducibility. The diffractometer should operate in conjunction with a sample exchange robot and be capable of sending hardware trigger signals to the detector based on rotation angles and positions.

Additionally, to set the appropriate rotation axis for crystals with large unit cells, a multi-axis goniometer (κ/ϕ) is necessary to minimize the overlap of diffraction spots. Furthermore, helical scan and raster scan capabilities should be supported to reduce radiation damage and perform serial crystallography. <Table 3.2.8.9> shows the required specifications of the BioNX beamline. These features fulfill the requirements for the beamline's science, enabling delicate adjustments and various scan modes, which are essential for handling microcrystals.

<Table 3.2.8.9> Required specifications of the sample diffractometer

Sample alignment	
Design resolution	5 nm
Range	Y axis : 110 mm/ Z axis : 6 mm / X axis : 6 mm
Static accuracy	$\pm$ 100 nm
Scan axis (Omega)	
Sphere of confusion (SOC)	< 100 nm
Rotation speed	> 100 deg/s
Design angular resolution	< 0.1 mdeg
Static accuracy	< $\pm$ 1 mdeg
Kappa range	0° to 90°
Kappa angular resolution	< 0.1 mdeg
Phi angular resolution	< 0.1 mdeg

○ 2D detector

X-ray diffraction will be measured using a photon-counting detector that offers high sensitivity and supports high-speed imaging at rates exceeding 30 Hz. To measure diffraction

from crystals with large unit cells such as membrane proteins and large protein complexes, the detector should have an active area of at least 300 mm. This prevents overlapping of diffraction spots even the detector is positioned farther back to resolve individual spots, while it allows high-resolution data collection. <Table 3.2.8.10> presents the required specifications of the detector. These specifications are sufficient to perform serial crystallography and to collect the large amounts of data produced in a short time. It would be also possible to enable the separation of individual spots in densely packed diffraction patterns from large unit cells larger than 1,000 Å (22).

<Table 3.2.8.10> Required specifications of the detector

Content	Specification
Type	2D photon-counting detector
Active area (W x H) (mm ²)	> 300 x 300
Pixel array (W x H) (pixels)	4,148 x 4,362
Pixel size (W x H) (μm ²)	75 x 75
Count rate (photons/s/mm ²)	Up to 10 ⁷
Frame rate	700 Hz (8 bit) / 560 Hz (16 bit)

○ Sample exchange robot with sample storage chamber

A sample exchange robot is essential for high-throughput screening experiments. It automatically replaces the pins holding mounted crystals on the sample diffractometer, drastically reducing the time researchers spend opening and closing the experimental hutch to manually exchange the samples. This automation also minimizes human errors that can occur when placing protein crystals in the cryogenic stream, enabling consistent collection of high-quality diffraction data without ice rings. For rapid sample exchange, a 6-axis robot arm equipped with a double sample gripper is required. Additionally, an LN₂ sample storage chamber capable of holding a large number of samples should be employed for high-throughput experiments. The current goal of the BioNX beamline is to process 600 samples per day. Therefore, a dewar capable of storing approximately 600 samples simultaneously is needed. This setup will enable rapid screening of the compound libraries with target proteins, thereby accelerating drug development projects.

H. Beamline support facility

(1) Sample preparation laboratory

To support drug discovery research, a sample preparation laboratory will be provided alongside the BioNX beamline. Aiming to collect data from 600 crystal samples daily for high-throughput experiments, it is recommended that users avoid transporting a large number of delicate protein crystals, as they are highly sensitive to temperature, humidity, and physical shock unless they are frozen. Instead, an on-site biological sample preparation laboratory will be provided within the Korea-4GSR accelerator, allowing users to prepare large quantities of samples on-site.

This facility should be equipped with a crystallization robot to assist in the high-volume production of crystals, as well as an automated imaging device for screening crystallization conditions. The sample preparation lab should be outfitted with essential equipment for crystallization experiments, including microscopes, incubators, and lab tables.

Additionally, the sample preparation lab will support fragment library screening, which is an efficient way in drug discovery. After the high-throughput production of protein crystals, fragment compound solution can be dispensed onto these crystals for soaking method, allowing on-site screening of protein-compound binding. To support this, a device using ultrasound technology to dispense small amounts of compounds is required. Moreover, a motorized device with X, Y, and Z axis movement is required to facilitate repetitive tasks by mounting numerous crystals onto sample pins. It enable the collection of up to 100 crystals per hour. This setup will enhance the efficiency of the fragment library screening in terms of analyzing the prepared sample immediately with the high-throughput screening system in the beamline. This facility makes it an excellent resource for drug development research.

I. Computing infrastructure

To support the massive data collection and processing demands of the BioNX beamline, a robust computing infrastructure is essential. The system must handle the large volumes of data generated by the 2D photon-counting detectors operating at high frame rates, especially during serial crystallography experiments. Real-time data processing capabilities are required to provide immediate feedback to users, enabling on-the-fly adjustments during experiments. The

computing infrastructure should include high-performance data storage solutions with sufficient capacity and fast data acquisition speeds. Parallel processing capabilities, utilizing multi-core CPUs and GPUs, are necessary to accelerate data analysis workflows, including image processing, integration, and merging of diffraction data.

Additionally, user-friendly software interfaces should be developed to facilitate data management, visualization, and analysis. Secure remote access options can further enhance user accessibility, allowing users to monitor experiments and analyze data from off-site locations. Implementing a scalable and flexible computing system will ensure that the BioNX beamline can meet current and future computational demands, supporting advanced research in structural biology and accelerating scientific discoveries.

(1) Data acquisition

Due to the nature of MX beamlines, data acquisition software requires a user-friendly GUI and a system that enables easy remote access. Traditionally, the software has been installed on the local computer at the beamline, requiring users to install additional remote access programs to connect directly to the local computer for data acquisition. This setup has several disadvantages: it requires the installation of a separate remote access program, and direct connection to the local computer generates a high volume of data transfer sending the full graphical interface, causing delays in beamline control that vary depending on the user's local network conditions (23). Additionally, using remote access programs for this type of connection is vulnerable to security issues, making it unsuitable for the BioNX beamline, which requires rapid and massive data collection.

A recent trend in MX beamline data acquisition software is the development of web-based GUIs, which allow users to access the system without installing additional programs and with any types of web browser. This approach also reduces data transfer significantly compared to connecting to a local computer, providing a seamless experimental environment that is less affected by network conditions. Moreover, partially limiting user accessibility to the software can strengthen the overall security of the beamline system, while introducing advanced security such as a two-factor authentication system further enhances the security level for user access (24,25).

Examples of such web-based user interfaces (WUI) include WIFIP (FIP2 beamline at ESRF),

YAIBEX (ANSTO), MXCuBE3 (ESRF), Daiquiri (ID21 beamline at ESRF), and Finback (SSRF). In line with this trend, the BioNX beamline plans to either develop its own software or adopt existing software that meets its requirements, depending on future staffing availability.

(2) Data management

A user-friendly system for sample shipping, experiment history tracking, and collected data management is essential for users to conduct remote experiments. Currently, the 5C beamline at Pohang Accelerator Laboratory uses web-based software, MXLive, which allows users to monitor sample status, download collected data, and review past experiment records after completion (26). This type of data management system has been well-received by users for its convenience, as the web-based platform enables easy access anytime.

Similarly, the BioNX beamline requires a data management system at this level, which must also be compatible with the data acquisition system. Additionally, it should support setting an experimental strategy that allows for automated high-throughput experiments. This setup would enable users to efficiently plan and execute experiments by transferring these strategies to the data acquisition software.

Apart from MXLive, ISPyB is another web-based software commonly used for data management across European accelerators, including ESRF, Soleil, DLS, MAX IV, HZB, EMBL, DESY, and ALBA (27). With development efforts supported through collaboration among these institutions, ISPyB is known for its high system stability. The BioNX beamline plans to either develop an in-house data management system or adopt an existing software solution that meets these requirements, with potential adjustments depending on future staffing levels, same as the plan for the data acquisition system.

(3) Computing power

To achieve the targeted beamline science objectives of SSX, ISX, and HTS on the BioNX beamline, the desired frame rate is at least 30 Hz. Based on the detector specifications outlined in section 3.2.8 “(5) Instrument Specifications - 2D detector”, an uncompressed data file would be approximately 72 MB. This may result in an estimated data rate of 2.16 GB/s, and collecting data with a full 360° rotation at 0.1° oscillation yields about 259.2 GB. For high-throughput

experiments with 600 crystal samples per day, approximately 155.5 TB of storage capacity would be required.

To meet the minimum design goals of the BioNX beamline, computing infrastructure must support the specifications summarized in <Table 3.2.8.11>.

<Table 3.2.8.11> Estimation of the data size of single crystal data collection

Data acquired rate	30 Hz
1 File size (uncompressed)	72 MB
Data rate	2.16 GB/s
Data size of 1 set (360°, 0.1° oscillation)	259.2 GB
Data size for 600 crystals	155.5 TB

The data center planned in Korea-4GSR project will provide online HPC for data storage and analysis, with further details available in the data center section. To ensure stable data storage and analysis, a local HPC server is also necessary, with specifications outlined in <Table 3.2.8.12> as minimum requirements. These may be subject to change with future upgrades to the computer system.

<Table 3.2.8.12> Minimum requirements of local HPC server

Master server-Dell PowerEdge R760 Server	
CPU	2*Intel Xeon Gold 6426Y 2.5G, 16C/32T, 16GT/s, 38M (185W)
RAM	256GB(4*64GB) 4800MT/s DDR5 Dual Rank RDIMM
SSD	2*480GB SSD SATA Read Intensive 6Gbps 512 2.5"
HDD	2*12TB 7.2K RPM SATA 6Gbps 512e 3.5in Hot-plug HDD
CPU node server-Dell PowerEdge R960	
CPU	4*Intel Xeon Gold 6418H 2.1G, 24C/48T, 16GT/s, 60M cache, Turbo, HT (185W) DDR5-4800
RAM	512GB(16*32GB) 4800MT/s DDR5 Dual Rank RDIMM
SSD	2*960GB SSD SATA Read Intensive 6Gbps 2.5" Hot-plug
Storage-Dell PowerVault ME5084 Storage Array	
HDD	528 TB (24 x 22 TB SAS 12Gbps)

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3.2.9 BM10 High Energy Microscopy Beamline

A. Introduction

The BM10 High-Energy Microscopy (HEM) beamline is designed to provide full-field X-ray imaging in the high-energy range of 20 to 150 keV, with a particular emphasis on non-destructive, three-dimensional (3D) microtomography (μ CT) and dynamic (4D) imaging. The beamline utilizes the highly collimated and intense synchrotron radiation emitted from a bending magnet source and delivers a large beam up to 200 mm $\times$ 30 mm at the sample position located 100 meters downstream, enabling wide field-of-view imaging for large and complex samples.

The HEM beamline focuses on high-speed, high-resolution X-ray imaging using indirect detection microscope. This approach is well-suited for the study of internal microstructures such as porosity, grain morphology, defects, and interfaces, in a wide range of materials including metals, composites, biomaterials, geological samples, and industrial parts [1-4]. Sub-micron resolution is achieved through scintillator-based indirect optics, and the imaging system supports multi-scale measurements by allowing flexible magnification and detector configurations.

The broad energy ranges up to 150 keV offers deep penetration power, enabling imaging of dense or large samples and compatibility with in-situ/operando environments. This makes the beamline ideal for dynamic studies of structural evolution under conditions such as thermal loading, mechanical stress, fluid flow, and phase transitions [5-7]. Additionally, the high-energy white beam allows for faster acquisition and reduced motion artifacts, critical for time-resolved experiments.

The beamline adopts a simple and robust optical layout with minimal optical components to preserve beam coherence and maintain long-term stability. This design enables stable imaging over long propagation distances and supports phase-contrast imaging techniques to enhance contrast in low-absorption materials.

Scientific objectives of the HEM beamline include:

- Non-destructive 3D/4D imaging of industrial and functional materials
- In-situ analysis of internal structural changes during processing or operation

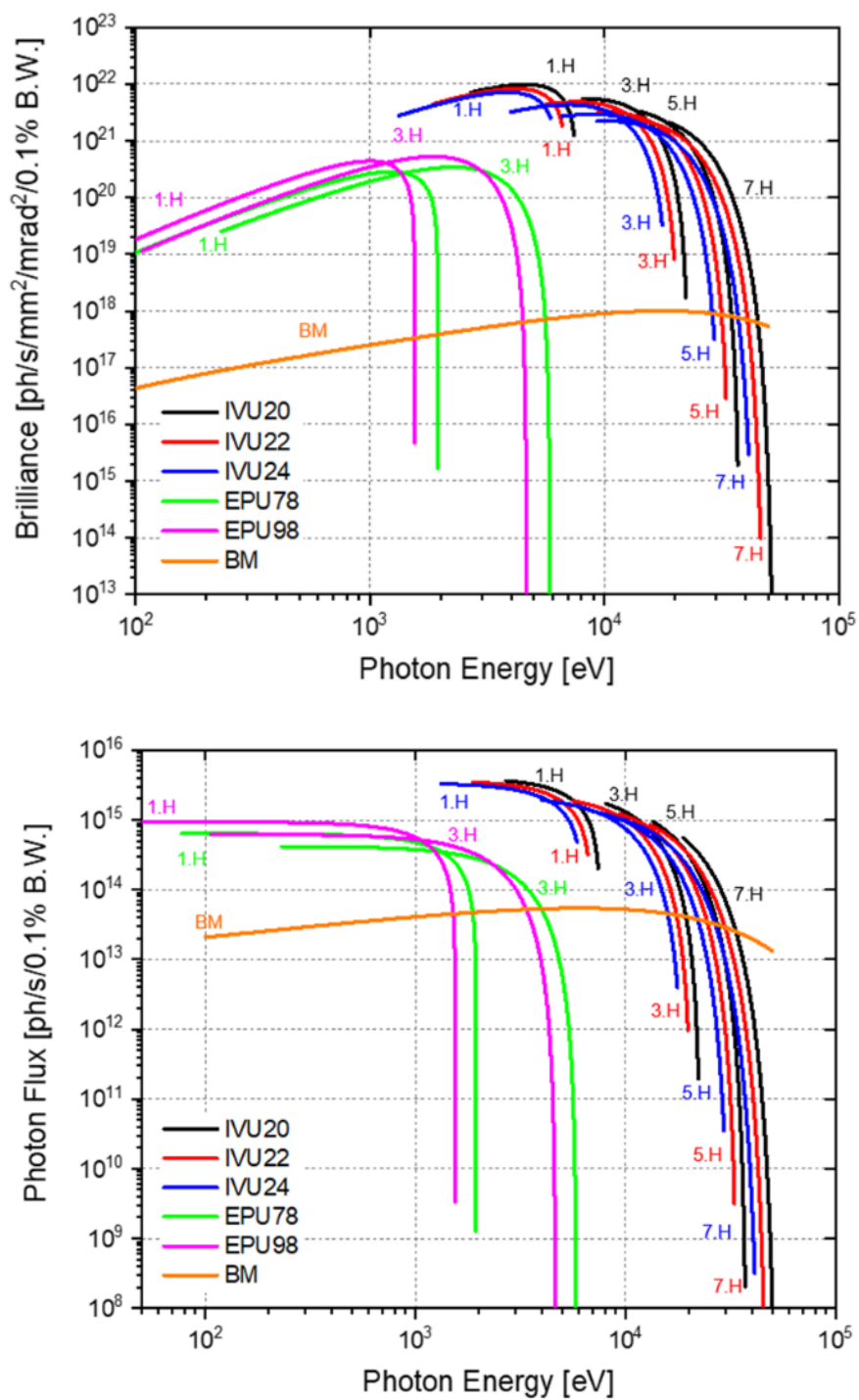
- High-resolution imaging of biological and biomedical specimens
- Development of new imaging techniques for multi-scale and phase-sensitive studies

To support these goals, the beamline incorporates high-heat-load optical components, motorized white beam slits, precision sample stages, and large-area detectors with high-speed data acquisition. The beamline infrastructure is also designed for future expansion, including advanced detectors, automated sample handling systems, and integration with image reconstruction tools.

B. Beamline Requirements for the Insertion Device (Bending magnet)

HEM beamlines require high-brightness sources that can cover the X-ray energy spectrum above 150 keV and small source sizes to maximize phase contrast effects. To meet these requirements, bending magnets or super-bend magnets are needed that can provide high fields at short device periods.

Bending magnets are essential components of synchrotron facilities used to steer electron beams along circular paths, and the performance of the magnets is critical to the overall functioning of the beamline in terms of brilliance and flux. <Figures 3.2.9.1> and <Table 3.2.9.1> illustrate the brilliance and flux curves for bending magnets, showing their capabilities at various photon energies.



<Figure 3.2.9.1> Predicted brilliance and flux of the Insertion Devices.

<Table 3.2.9.1> Source Parameters for High-Energy Microscopy beamline

Source Type	Magnetic Field	Magnetic Radius	Total Power	Critical Energy
Bending magnet	2T	6.67 m	1.36 kW	21 keV

Bending magnets have magnetic fields as high as 2 Tesla, with a critical energy of 21 keV and a usable energy range of up to 150 keV. The extended energy range covering up to 150 keV supports a wide array of experimental techniques and applications, including studies of dense materials and high-energy processes. High flux and brightness enable more detailed, higher resolution imaging and analysis, which are essential for advancements in materials science, biology, and chemistry.

Bending magnets can be upgraded to super-bend magnets in the future to provide an immediate improvement in beamline performance while preserving the existing beamline design. Super-bend magnets are specialized magnets designed to enhance the performance of synchrotron beamlines by generating higher flux and brilliance, particularly at higher photon energies. High photon energy allows for more accurate and detailed investigations in various scientific domains such as imaging, X-ray absorption fine structure (XAFS), and scattering. We anticipate meeting future scientific requirements by keeping open the option to upgrade our imaging beamline.

C. Beamline Requirements for the Front End

The layout of the beamline is split into two parts separated by a ratchet-shaped storage ring tunnel wall, and the inside of the ring tunnel wall is the Front-End (FE). The FE is designed to protect both personnel and equipment on the beamline, as well as the machinery in the event of a vacuum failure on the beamline.

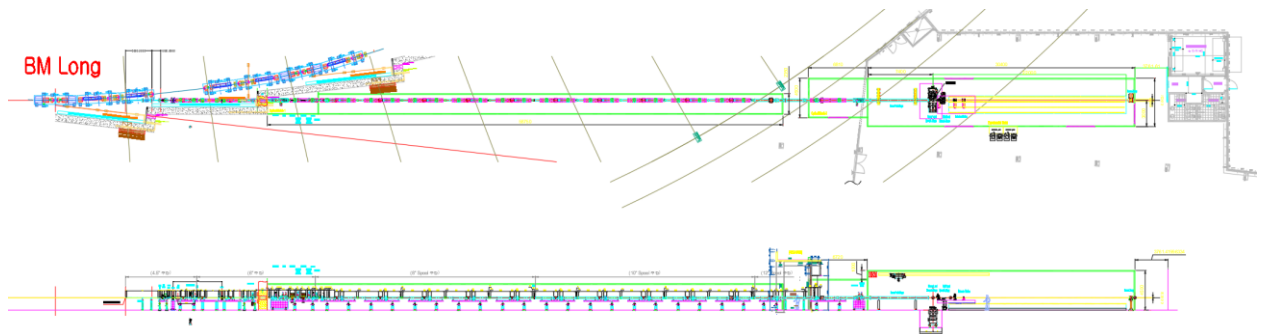
The HEM beamline requires a new high heat load Front End capable of handling a total power of 1.36 kW with a beam divergence of 2.2 mrad horizontally and 0.6 mrad vertically. The Front-End of the HEM beamline is designed to respond to beamline issues while minimizing entry and exit. <Table 3.2.9.2> shows an overview of the components and functions of the HEM beamline Front-End.

<Table 3.2.9.2> Component list of the Front-End in the High-Energy Microscopy beamline

Distance from source (m)	Component	Description/Comments
0	Bending Magnet	Source (2 T)
12	Parasitic Mask	(H) 2.2 mrad x (V) 0.6 mrad
12.5	Beam Stopper	Absorb of high-energy Bremsstrahlung radiation
13	Diamond Window	Vacuum separate
13.5	PBPM1	Diamond-blade
14	Safety Magnet	Electron Stop
15.3	Photon Shutter 1	Main beam blocking
19.5	PBPM2	diamond-blade
21	Safety Shutter 1	beam diagnostics & Shockwave Blocking

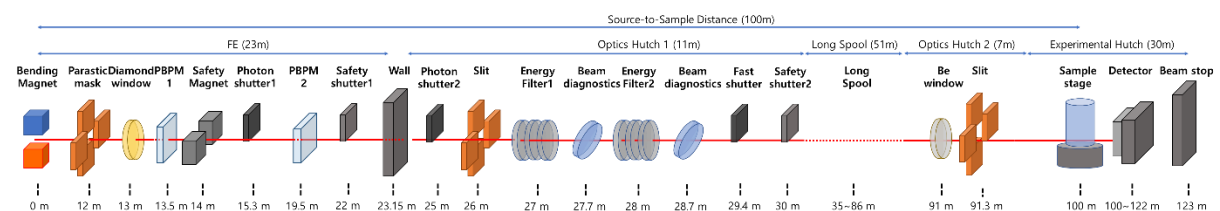
D. Beamline Layout

HEM beamline will be one of two long beamlines built at the Korea-4GSR. Located at BM-10, HEM beamline extends beyond the exterior wall of the storage ring building, allowing for a sample position that is located at 100 meters from source.



<Figure 3.2.9.2> Layout for High-Energy Microscopy beamline.

The conceptual layout of beamline shown in <Figure 3.2.9.3> displays X-ray optics, sample environments, and detector.



<Figure 3.2.9.3> Conceptual layout of the High-Energy Microscopy beamline indicating diagnostics, x-ray optics, sample location, and detector.

(1) Beamline Component Table

<Table 3.2.9.3> shows all major beamline components and lists them in order of distance from the source.

<Table 3.2.9.3> High-Energy Microscopy beamline component table

Location	Distance from source (m)	Component	Description/Comments
Front End (0 to 23 m)	0	Source	Bending magnet (2T)
	12	Parasitic Mask	(H) 2.2 mrad x (V) 0.6 mrad
	12.5	Beam Stopper	Absorb of high-energy Bremsstrahlung radiation
	13	Diamond Window	Vacuum separate
	13.5	PBPM1	Diamond-blade
	14	Safety Magnet	Electron Stop
	15.3	Photon Shutter 1	Main beam blocking
	19.5	PBPM2	diamond-blade
	21	Safety Shutter 1	Bremsstrahlung Blocking
Wall (23.15 to 24.95 m)	23.15	Wall	Front End Radiation blocking (1.8m)
Optical Hutch 1 (24.95 to 35 m)	25	Photon Shutter 2	Main beam blocking
	26	Slit	Beam size defining and heat absorption (H) 2.0 mrad x (V) 0.3 mrad
	27	Energy Filter	Polychromatic Beam Filtering
	27.7	On-line Diagnostics	beam diagnostics
	28	Energy Filter	Polychromatic Beam Filtering
	28.7	On-line Diagnostics	beam diagnostics
	29.4	Fast shutter	Reduction of radiation damage
	30	Safety Shutter 2	Bremsstrahlung Blocking
Long spool (35 to 86 m)	35	Long spool	Beam transfer (UHV)
Optical Hutch 2 (86 to 93 m)	91	Exit Window	Be window (UHV, > 200 mm, water cooled)
	91.3	Exit Slit	Final Beam size defining
Exp. Hutch (93 to 123 m)	100	Sample Stage 1	Heavy Load Air-Bearing Stage
	101.2	Sample Stage 2	Light Load Air-Bearing Stage
	100 to 122	Detector Station	Phase contrast effect
	100 to 122	Detectors	X-ray microscope
	123	Beam Stop	White Beam Stop, Fixed, Cooled

E. Optics Overview

(1) Beam Delivery Specifications

The HEM beamline operates in the energy range of 20 keV to 150 keV. The X-ray beam generated from the bending magnet has an opening angle of approximately 2 mrad in the horizontal direction and 0.3 mrad in the vertical direction. As a result, at the sample position located 100 meters downstream from the source, a large beam footprint of approximately 200 mm $\times$ 30 mm is achieved.

The optical layout of the HEM beamline is deliberately kept simple and robust. Projection images are obtained from samples positioned 100 meters from the source without the use of complex optical components such as focusing mirrors or monochromators. This minimalist approach enhances beam path stability and simplifies alignment and maintenance over long distances.

The energy filters are employed to optimize the bandwidth of the polychromatic (white) beam. To preserve the coherence properties of the source, all filter surfaces must be precisely polished to minimize wave-front distortion.

The Energy filters are placed near the light source to allow for the controlled injection of a low-divergence beam. Since the attenuator and filters are constantly exposed to the full white beam, active cooling is essential to ensure thermal stability and prevent material degradation.

Overall, beam performance is governed by the combination of white beam slits, energy filters, and attenuators, which together define the beam size, energy spectrum, and intensity. The expected beam parameters under different configurations are summarized in <Table 3.2.9.4>.

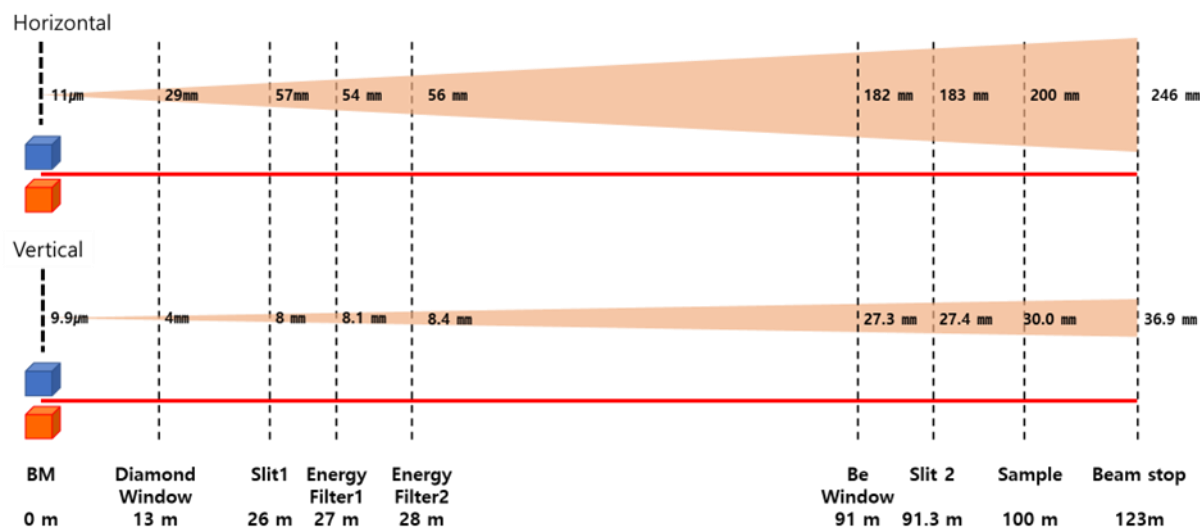
<Table 3.2.9.4> Performance parameters of filtered polychromatic beam in the High-Energy Microscopy beamline

Distance from source (m)	Component	Beam size FWHM (H x V, mm)	Incident beam power (W)	Absorption beam power (W)
0	Source	0.011 x 0.0099	448.0	0
13	Diamond window	28.6 x 3.9	468.0	103.2
26	4-Slit	57.2 x 7.8	364.8	47.1
27	Energy filter (Al ₂ O ₃ 0.5mm)	54 x 8.1	317.7	180.0
28	Energy filter (Mo 1mm)	56 x 8.4	137.7	127.2
91	Be window	182.0 x 27.3	10.5	0.1
91.3	4-Slit	182.6 x 27.4	10.4	0
100	Sample	200.0 x 30.0	10.4	0
123	Beam stop	246.0 x 36.9	10.4	10.4

(2) Detailed Optical Layout

○ Ray-tracing (Horizontal, Vertical)

Optics configuration for projection imaging is shown in <Figure 3.2.9.4>.



<Figure 3.2.9.4> Optics configuration (horizontal/upper, vertical/lower) for projection imaging.

(3) Optics Specifications

○ Windows

The window located at the Front End of the beamline plays a critical role in thermal management and in maintaining optimal beamline vacuum conditions. It protects sensitive downstream components by reducing the thermal load before the beam reaches the white beam slits, energy filter, and end station.

Chemical Vapor Deposition (CVD) diamond is selected as the window material due to its high thermal conductivity and low X-ray absorption, allowing it to effectively manage high thermal loads while minimizing beam attenuation. Compared to beryllium, CVD diamond can be polished to a mirror-like finish, which helps preserve the wave-front quality of the X-ray beam emitted from the source.

These CVD diamond windows are specifically designed to withstand high heat load conditions while maintaining beamline performance. In addition to thermal management, the windows serve a crucial safety function by separating the ultra-high vacuum (UHV) environment of the storage ring from the beamline. In the event of a vacuum failure downstream, the window prevents UHV degradation and protects the accelerator system.

The Front-End diamond window has a maximum aperture of 38×9 mm, which is sufficient to fully transmit the beam and has been demonstrated to reduce the heat load by approximately 103 W under normal operating conditions.

A second window is installed at the downstream end of Optical Hutch 2, which is the final vacuum interface point before the beam enters the experimental hutch. This window separates the UHV section from the downstream ambient pressure environment, where detectors and sample stages are located.

Since the HEM beamline is designed to provide a beam width of up to 200 mm at the sample position, this window must accommodate a large aperture. Therefore, it is engineered to meet both structural stability and thermal resistance requirements under wide-beam and high-heat-load conditions.

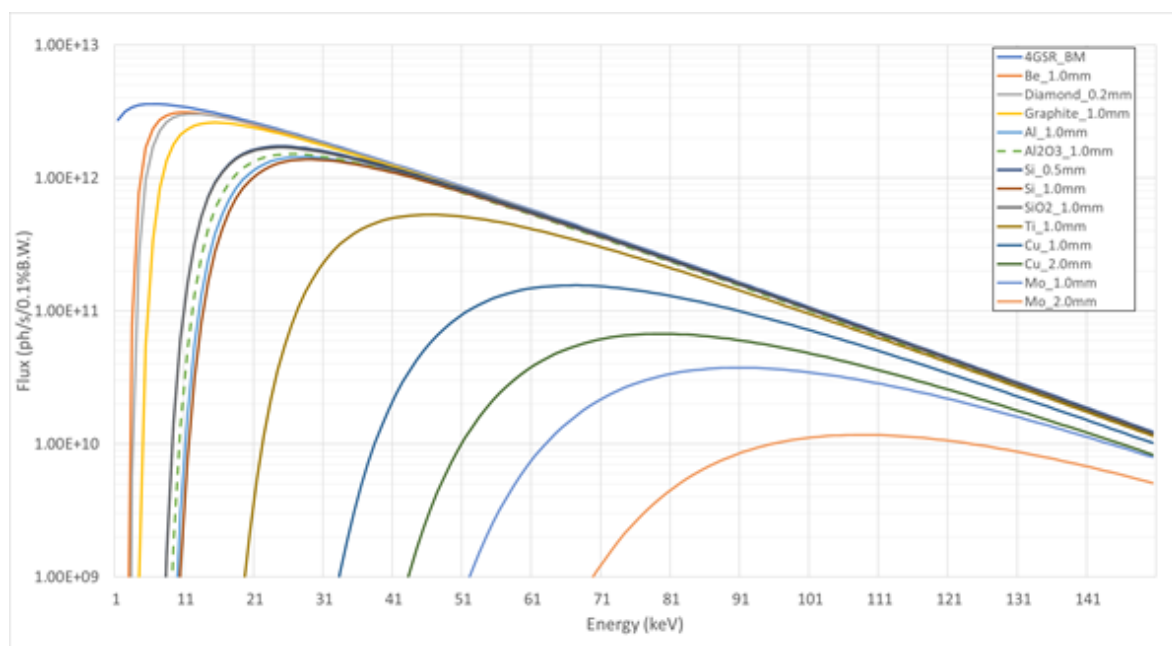
○ Energy Filters

In high-energy imaging beamlines, an energy filter is a critical component used to remove unwanted low-energy photons and to define the energy bandwidth of the X-ray beam. This process optimizes the beam quality, ensuring that only the desired high-energy photons are used for imaging.

The low-energy cut-off filter operates by selectively absorbing or reflecting photons below a specific energy threshold, allowing only higher-energy photons to pass through. By eliminating these low-energy components, the filter reduces background noise and significantly improves the signal-to-noise ratio (SNR) of the imaging system. This leads to sharper and more accurate images, which are essential in high-resolution tomography.

In addition to improving image quality, low-energy photons are a major contributor to the thermal load on downstream optical elements and detectors. Filtering out these photons not only protects temperature-sensitive components but also enhances their performance stability and operational lifespan.

At the HEM beamline, beam quality and performance are finely tuned using a set of energy filters. The expected performance characteristics resulting from different filter configurations are shown in <Figure 3.2.9.5>.



<Figure 3.2.9.5> Performance of beam by filter material in the High-Energy Microscopy beamline.

Materials with high atomic numbers (Z) such as aluminum (Al), copper (Cu), or molybdenum (Mo) are commonly used for low energy cut-off filters due to their high absorption efficiency for low-energy photons. The low energy cut-off filter is placed early in the beamline, before other optical elements and the sample, to maximize its protective and quality-enhancing effects.

○ Slits

The white beam slits are critical components of the HEM beamline, serving essential functions in thermal management, beam conditioning, and white beam experiments. These slits are equipped with motorized actuators that allow precise control of the beam aperture, adjusting the X-ray white beam size with high accuracy.

Due to the high power density of the synchrotron white beam, especially under worst-case conditions such as operator inattention or during beam diagnostics each slit must be capable of intercepting the full beam and must be designed with adequate cooling systems to withstand significant thermal loads.

The HEM beamline requires two sets of high-heat-load slits:

- The first set of slits is located upstream of the energy filter. These slits adjust the beam size incident on the energy filter and simultaneously serve to reduce the thermal load delivered to the second slit system downstream.
- The second set of slits functions as the final beam-defining aperture for the experiments. It precisely shapes the beam before it reaches the sample, ensuring optimal illumination conditions.

As an imaging beamline, HEM must deliver a beam with adjustable dimensions that match the field of view and resolution requirements of various samples. Therefore, the slits must provide high stability, reproducibility, and thermal robustness to maintain beam quality across a wide range of experimental conditions.

○ **Beam Shutter and stops**

Effective management of x-ray beams, both white and monochromatic, requires a series of shutters and stops strategically placed along the beamline. These components ensure that the beam can be safely blocked or directed as needed, protecting equipment and allowing for safe operation and maintenance.

The photon shutter in the Front-End is capable of blocking the beam from entering the beamline, including the optical hutch. Located at the very start of the beamline, it controls the initial entry of the X-ray beam. The photon shutter operates frequently on the imaging beamline, so we configure them in pairs to prepare for accidents.

The beam stop is located at the downstream end of the experimental hutch. The final component will be a cooled, fixed stop for both white and monochromatic beams.

○ **Beam transports and Vacuum**

The HEM beamline consists of three sections:

- Optical Hutch 1 extends from the safety wall to the Energy filers. It determines the performance of the white beam.
- Long Spool facilitates transport between Optical Hutch 1 and Optical Hutch 2. It uses appropriate vacuum tube hardware because the beam size expands during delivery.
- Optical Hutch 2 includes a slit for defining the beam size, and a window for vacuum separation.

The photon transfer line (PTL) is maintained at ultra-high vacuum (UHV) from the front to the exit window. This UHV environment ensures the integrity of the X-rays in the end station.

F. Instrument Overview

The HEM end-station instruments at Korea-4GSR are designed to provide world-class high-energy X-ray imaging capabilities. Covering a broad energy range, accommodating large beam sizes, and supporting multiple imaging modalities, these instruments are equipped to address

diverse scientific challenges from detailed microstructural analysis to large-scale studies of materials under extreme conditions. The strategic layout and configuration of the end stations ensure maximum flexibility and operational efficiency, enabling a wide range of advanced research applications.

(1) Scientific Scope

○ Full-Field Imaging

Full-field imaging captures the entire field of view in a single exposure, rather than scanning the sample point by point. This approach is widely used in scientific and industrial applications, including microscopy, medical diagnostics, and materials analysis.

The bending magnets of the HEM beamline provide strong magnetic fields up to 2 Tesla enabling high-energy X-ray beams reaching up to 150 keV. Beam sizes range from tens of microns to 200 mm, offering high flexibility for different experimental requirements.

Direct-beam full-field imaging (radiography/tomography) allows for the widest field of view, making it ideal for non-destructive 3D imaging and structural analysis. This modality is particularly well-suited for examining internal structures across a range of sample sizes and compositions.

○ Multiscale Imaging

Modern materials often exhibit hierarchical structures spanning nanometers to millimeters. Understanding such systems requires imaging techniques that are adaptable across scales, both in spatial resolution and field-of-view.

The HEM beamline supports multi-scale full-field imaging through:

- Variable magnification setups using different scintillator–lens combinations
- Detectors with small pixel sizes for sub-micron resolution, and large sensor areas for wide coverage
- Long propagation distances that preserve coherence and enable phase-contrast enhancement at multiple scales

This flexibility allows researchers to investigate both fine internal features (e.g., microcracks, fiber networks) and broader phenomena (e.g., component deformation or flow paths) within a single experiment. Such integrated capability enables a more complete understanding of material behavior and supports imaging-driven design and validation.

○ Propagation-based phase contrast imaging (PBI)

Propagation-based phase contrast imaging (PBI) is a powerful full-field X-ray imaging technique that utilizes the phase shift of X-rays as they propagate through a sample. [8-9] This method is particularly effective for visualizing low-density materials, biological tissues, polymer composites, and internal interfaces that are difficult to detect using traditional absorption-based contrast.

When X-rays travel through matter, they undergo changes not only in amplitude (due to absorption) but also in phase, as a result of variations in the material's refractive index. The complex refractive index is expressed as $n=1-\delta+i\beta$, where δ is the real part that governs phase shifts, and β is the imaginary part responsible for absorption.

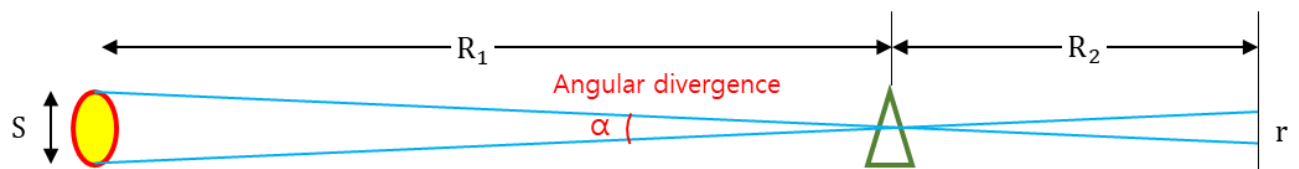
As shown in comparative data across materials and energy levels, β (absorption) decreases rapidly at high energies, leading to poor image contrast in absorption-based imaging. In contrast, δ (phase) remains significant—even at high X-ray energies—and is often more than three orders of magnitude greater than β . This makes phase-based imaging techniques especially valuable in the high-energy domain.

PBI at high X-ray energies offers several advantages. First, it provides enhanced image contrast for materials with low atomic numbers (low-Z) and those that are weakly absorbing, which are often difficult to visualize with conventional absorption-based methods. Additionally, since PBI relies on phase information rather than attenuation, it enables non-destructive imaging while reducing the required radiation dose, making it suitable for sensitive samples. This technique is also highly versatile, accommodating a wide range of sample sizes and material densities. Most importantly, PBI is particularly effective for revealing fine internal features such as soft tissues, micro-cracks, and delamination zones that are often invisible in standard X-ray images.

In PBI, X-rays are allowed to propagate a certain distance beyond the sample before being

recorded by the detector. During this free-space propagation, interference patterns arising from phase shifts accumulate into detectable intensity variations, revealing edge-enhanced or refractive features of the internal structure.

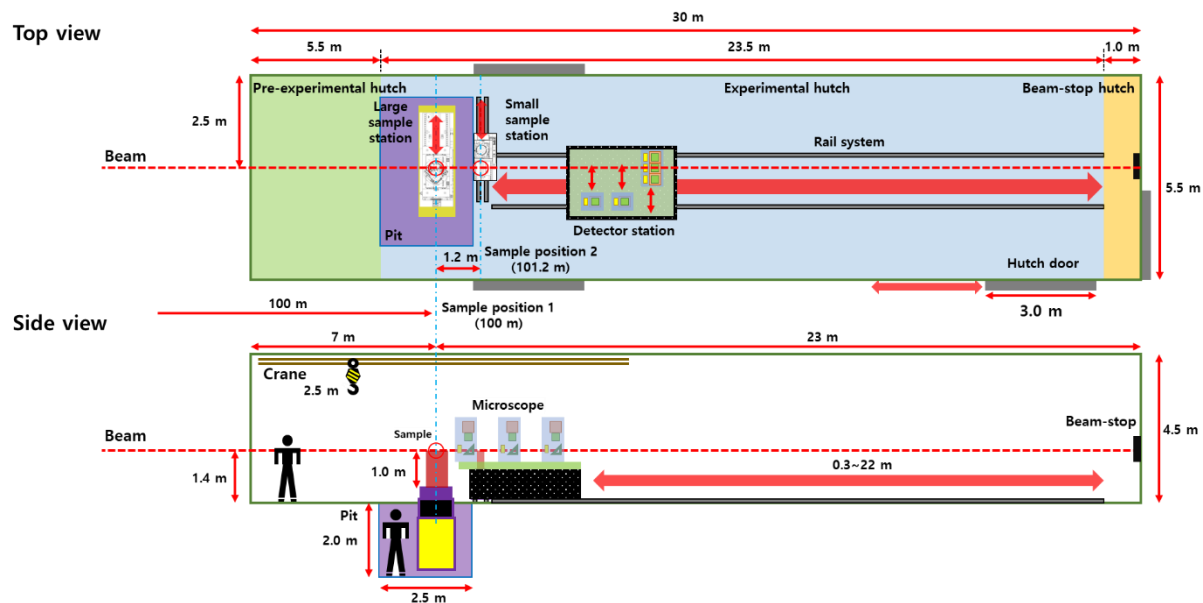
The effectiveness of PBI is primarily governed by two critical geometric parameters. The first is R_1 , the distance from the X-ray source to the sample. A longer R_1 , combined with a smaller source size, leads to lower beam divergence and consequently higher spatial coherence, which is essential for enhancing phase contrast effects. The second parameter is R_2 , the distance from the sample to the detector. By increasing R_2 , the system allows for more pronounced wave-front propagation, thereby improving the visibility of phase contrast in the resulting images.



<Figure 3.2.9.6> Geometrical Configuration for Propagation-Based Phase Contrast Imaging.

(2) Instrument Definitions

The Schematic layout of end station shown in <Figure 3.2.9.7> displays experimental hutch, sample station, detector station, and utility.



<Figure 3.2.9.7> Schematic layout of the end station in the High-Energy Microscopy beamline.

(3) Design Scope

The design scope for the HEM instruments involves integrating nearly all newly designed and purchased components, specifically tailored to meet the outlined scientific objectives. Below is a detailed description of the End-station instruments, their configuration, and functionality.

○ Location & Primary End-Station Design

The HEM instruments are sophisticated systems comprising several critical components. The instrument is positioned as far downstream as possible within the separate building for optimal beam utilization. The experimental hutch will be located 100 meters from the light source and cannot be situated within the storage ring building. Instead, a separate building will be constructed to house it, making it one of the two long beamlines at the Korea-4GSR.

The end station is designed to accommodate diverse experimental needs, providing ample space and dedicated sections for precise experimentation and analysis. Approximately 23 meters along the beam direction, providing ample space for multiple imaging techniques. The crane inside the hatch makes it easy to handle heavy samples.

○ **Sample Manipulation Systems**

Sample manipulation systems are available for handling various sample types and experimental conditions. They accommodate bulky in-situ experiments involving large mechanical loads, extreme temperatures, and other harsh conditions.

The Sample manipulation systems consists of two sample stations. Heavy load large sample station is installed within a 2-meter deep pit, this station is dedicated to handling samples exceeding 100 kg, ensuring a safe and efficient loading process for heavy samples. The small sample station is designed to acquire high-resolution images of small samples.

○ **Detectors and Supporting Motion Systems**

In high-energy X-ray imaging, the primary goal is often to capture a large number of high-resolution images within a limited timeframe. To meet this requirement, detectors used for X-ray microscope must combine fast readout speeds, large-format sensors, and small pixel sizes.

At the HEM beamline, the X-ray microscope is based on indirect detection, which is the preferred approach for high-energy X-rays. Direct detection at these energy levels poses significant challenges, including the risk of radiation damage to camera electronics and optics, as well as reduced sensitivity of the detector itself.

In the indirect detection scheme, a scintillator is placed between the X-ray beam and the camera. The scintillator converts incoming X-ray photons into visible light, which is then captured by an optical sensor such as a CCD or CMOS camera. To achieve high spatial resolution and detection efficiency, the system uses thin single-crystal scintillators. These help minimize light spread and preserve micron-level resolution. A high-resolution optical system typically composed of specialized lenses and mirrors is employed to collect the visible light efficiently while minimizing optical aberrations.

The X-ray microscope is positioned immediately downstream of the sample stage and supports variable magnification by switching optical configurations. This enables the acquisition of datasets at different resolutions under consistent experimental conditions, thereby improving both accuracy and comparability of imaging results.

In propagation-based phase contrast imaging (PBI), phase contrast is significantly enhanced by utilizing small X-ray source sizes and long propagation distances, typically exceeding 100 meters. The strength of the phase contrast effect depends heavily on the sample-to-detector distance (SDD). At the HEM beamline, this parameter is precisely controlled using a motorized rail system, allowing fine adjustments to optimize imaging conditions across a wide range of samples [10].

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3.2.10 ID10 NanoProbe Beamline

A. Introduction

The nanoprobe beamline provides a nano-beam smaller than 50 nm in the hard X-ray energy range of 5 to 25 keV. The nanobeam enables deconvolution microscopy imaging techniques to achieve 20 nm elemental maps with sub-10 nm ptychography. This approach allows quantitative nanoscale analysis of the elemental distribution and quantity of material in a localized region. The energy range of 5 to 25 keV enables quantitative nano-spectroscopy for most transition metals and rare earth metals. Additionally, the high penetration power of this energy range can pass through gas environments and windows for maintaining environments. It allows for the study of materials under In-situ, synthesis and operating conditions. To facilitate such research, the nanoprobe beamline is designed to provide a long working distance of 50 mm despite the small beam size in the tens of nanometer range. This makes it easy to insert devices that offer various conditions, such as high and low temperature, gas environments, liquid environment sample delivery, and the application of electric or magnetic fields, enabling in-situ/operando materials research. The experimental instruments of the Nanoprobe provide various scanning imaging techniques. The primary imaging technique is multi-modal imaging that simultaneously performs 2D/3D XRF and 2D/3D ptychography. Auxiliary imaging techniques include diffraction mapping, ptychography, and Nano-XANES.

The scientific objectives of the nanoprobe beamline are on tracking the reactions and defect growth processes of energy materials and catalyst systems, and the quantitative nanoscale analysis of complex functional materials and material systems in actual manufacturing and operating environments. Also, to accommodate with the trend of scaling up systems by spreading and stacking nano-components for enhanced reactivity and performance, we will introduce high-speed precision nano-stages, allowing us to investigate larger areas at the nanoscale. The signal recording equipment includes X-ray fluorescence detectors and fast speed charge-integrating detectors, providing quantitative simultaneous information on the electron density, strain, and element distribution of the sample, with all experiments designed to be studied in three dimensions. The beamline design focuses on achieving stable beam delivery with a 10% tolerance, considering heat load of optics, horizontal deflection optics, beam position feedback, optimized HVAC for low vibration, and a dedicated experimental hutch for developing new X-ray methods. It also includes an endstation design for new X-ray

experimental methods and future extensions, utilizing in-house developed technologies such as high-speed precision nanostages, high-speed DAQ systems, and mini in-situ cells. The beamline design also includes extra experimental hutch for new X-ray experimental methods and future expansion, including in-house developed technologies such as high-speed precision nanostages, high-speed DAQ systems, and mini-in situ cells.

B. Beamline Requirements for the Insertion Device

The nanoprobe beamline provides an energy range of 5 to 25 keV using an In-Vacuum Undulator(IVU). IDs of Nanoprobe are designed to give the highest brilliance in this range without losing energy continuity. The parameters for the IDs are detailed in <Table 3.2.10.1>. The maximum power represents the maximum beam power passing through a mask with a 2 x 2 mm² opening @ 23 m under the maximum current conditions (400 mA) <Table 3.2.10.1>.

<Table 3.2.10.1> Parameters of insertion device

Undulator	Period (mm)	Length (m)	Location	Max Power	Min. Gap (mm)
In-vacuum	24	3.0	Center of Straight section	0.96 kW	6

C. Beamline Requirements for the Front End

The Front-End(FE) of the nanoprobe beamline is required to 1) handle a 18 kW heat load, 2) beam position diagnostics, and 3) radiation safety. First, the 18 kW total beam power is handled using three masks with water cooled channels. The first mask is a “fixed mask” that has a fixed aperture size in the horizontal direction and can only be adjusted in position, while the other two are “movable masks” that allow the gap size and position to be adjusted. For detailed specifications of the masks, refer to FE chapter [TBA]. Note that although the IDs have a minimum gap of 5 mm, the effective minimum gap required to provide the 5-25 keV range is 6 mm. Consequently, the effective maximum total power of nanoprobe IDs is 12 kW.

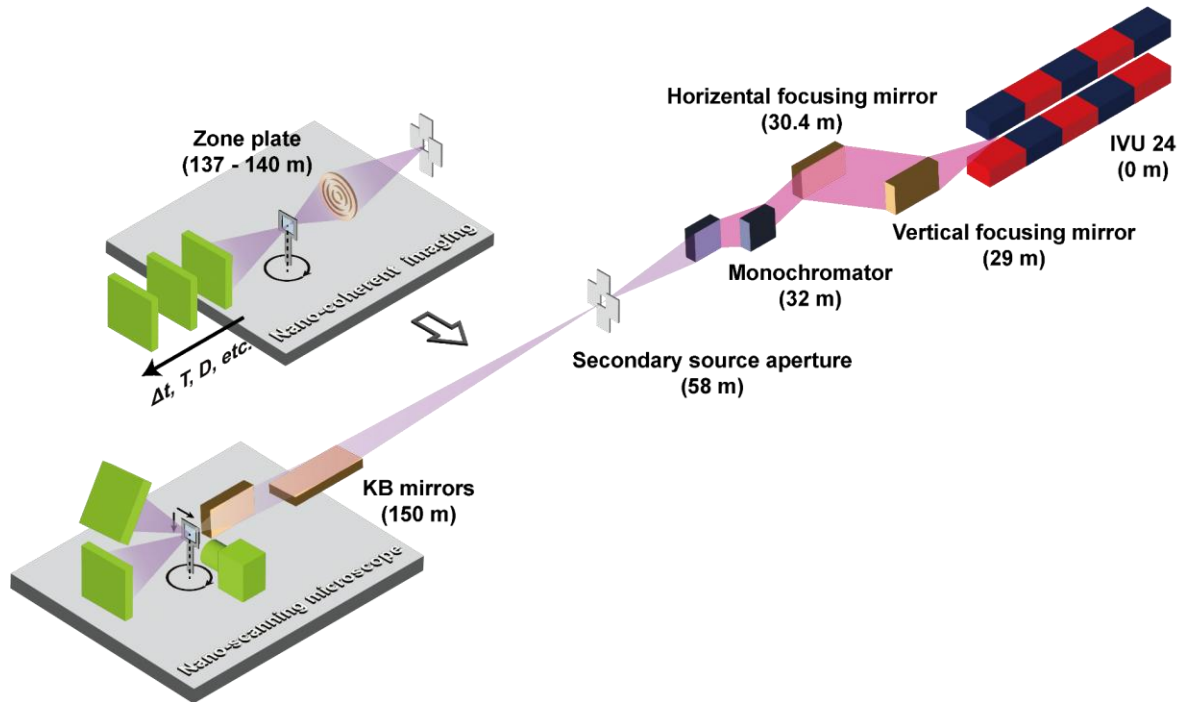
Secondly, the FE includes an X-ray beam position diagnostic device. In the first phase, the diagnostic X-ray beam position will be used to provide feedback for slits position, ensuring the stability of the beam intensity delivered to the sample within 10%. In the mature phase, the

diagnostic X-ray beam position will also be integrated with the electron beam feedback system to enhance performance. For detailed specifications of the diagnostic device, refer to Chapter [TBA].

Lastly, the FE is equipped with safety devices to protect against bremsstrahlung radiation and electron beam insertion in FE. Specifically, a safety magnet with 0.5 T is installed to handle scenarios where the electron beam enters the FE. This ensures that an electron beam inserted into the FE is deflected horizontally and prevented from reaching the optical hutch.

D. Beamline Layout

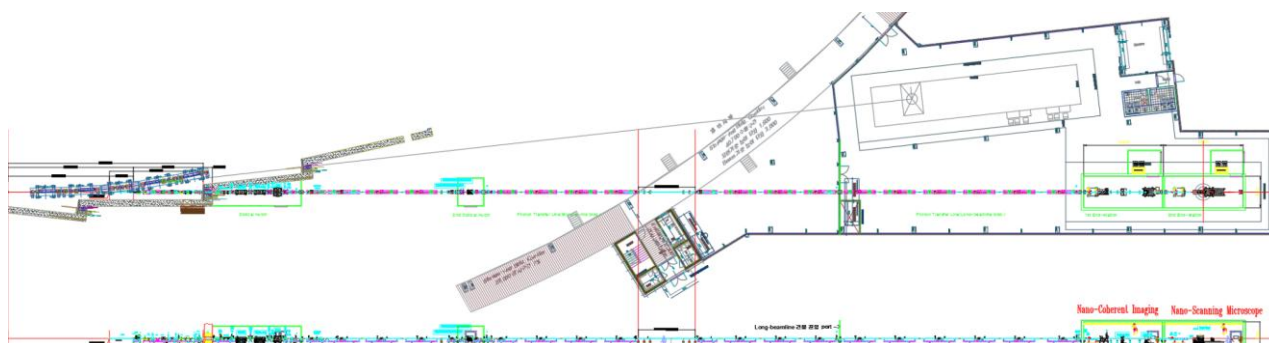
(1) Beamline overview



<Figure 3.2.10.1> Beamline schematic of Nanoprobe beamline.

<Figure 3.2.10.1> shown in the nanoprobe beamline schematic. Two horizontal deflection mirrors focus the beam in both the vertical and horizontal directions to the SSA. The SSA is then appropriately adjusted according to the required experimental characteristics and directs the beam to the two end stations.

(2) Beamline floor plan



<Figure 3.2.10.2> Beamline drawing of Nanoprobe beamline.

<Table 3.2.10.2> Main component list of Nanoprobe beamline. HHML: High heat load mirror, DBPM: Diamond beam position monitor. NBPM: Nano-Beam Position Monitor. SSA: Secondary source aperture.

Distance (m)	Location	Component name	Description
0	Front-End	In-Vacuum Undulator	Period 24 mm, Device length: 3 m
28.0	Optical Hutch 1	White beam slit	Up to 4 kW heat load
28.8		Diamond monitor	Resolution < 1 μ m, Diamond thickness 100 μ m
29.0		HHML	Spherical cylinder, 3-strip coating (Pt, Rh, Si), Sagittal focusing
29.8		Diamond monitor	Resolution < 1 μ m, Diamond thickness 30 μ m
30.4		Horizontal mirror	Elliptical cylinder Bendable, 3-strip coating (Pt, Rh, Si)
31.0		White beam DBPM	Resolution beam size < 0.1%, Beam position feedback
32.0		HDCM	Offset: 10 mm
35.0		DBPM	Resolution beam size < 0.1%, Beam position feedback
57.0	Optical Hutch 2	NBPM	Resolution 100 nm, Target angle resolution < 50 nrad
58.0		SSA	Aperture resolution ~ 500 nm, Aperture size: 2 to 50 μ m
137.0	Experimental Hutch	Beam monitor	Diamond screen monitor, 1 μ m resolution, Removable
138.0		Endstation 1	Flexible set up
147.0		Beam monitor	Diamond screen monitor, 1 μ m resolution, Removable
148.0		Ion gas chamber	I_0 monitor
149.5		KB mirror and chamber	H: 300 mm, V: 100 mm, 3-strip coating (Pt, Rh, Si)
150.0		Endstation 2	Fixed set up

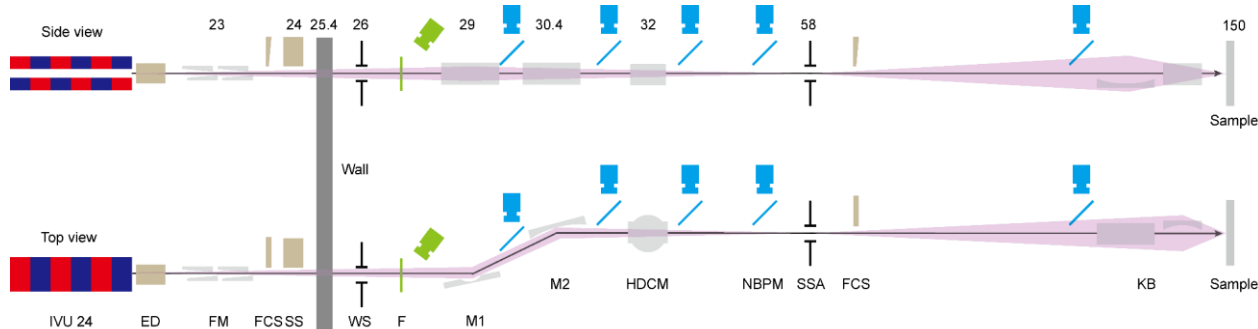
The Nanoprobe beamline is one of the two “long beamlines” for the Korea-4GSR construction. The experimental hutch for the Nanoprobe Beamline will be installed in a satellite building that extends from the storage ring. The experimental equipment for the nanoprobe beamline will be installed in separated concrete hutches and the slab of the experimental hutch are separated from the experimental hall <Figure 3.2.10.2>. The concrete experimental hutches (the concrete is 300 mm thick) provide temperature stabilization, and the isolated slabs of the experimental hutches are designed to minimize vibration.

E. Optics overview

(1) Optics simulation

In this section, we describe the optics and beam specifications of the nanoprobe beamline. For parameters related to the electron beam, refer to the chapter [TBA]. All optical simulations were performed in Shadow3 with the OASYS environment [1,2]. The simulations for the optical components were primarily conducted at 10 keV, which is expected to be frequently used, and also at 20 keV for comparison. Note that the X-ray beam source parameters provided by the OASYS environment do not take into account the electron energy dispersion. This means that the divergence angle of the beam presented by the OASYS is less than twice as small at high X-ray energies (High harmonics). Thus, we use the source parameters provided by SPECTRA as a Geometry source app in OASYS. Also, the BDA gap size and photon flux calculations were conducted using in-house script in the Matlab environment.

(2) Consideration for optical layout



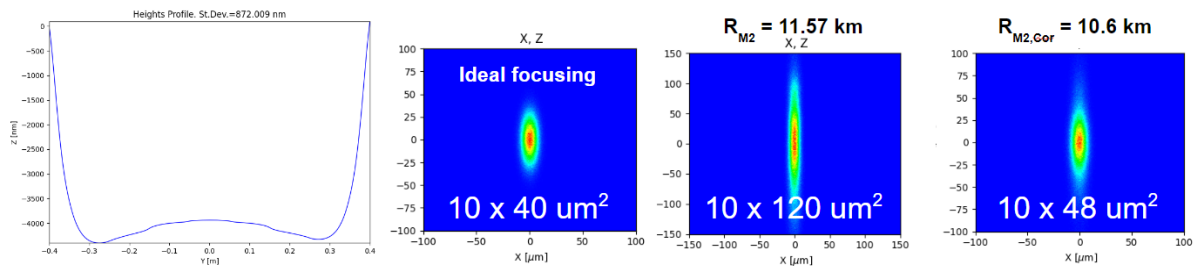
<Figure 3.2.10.3> Optical layout of Nanoprobe beamline. M1(Sagittal focusing) and M2(Meridional focusing) are horizontally reflecting mirrors. HDCM is Horizontal deflecting Double Crystal Monochromator. SSA is a secondary source aperture, also called a beam defining aperture (BDA). ED: Electron deflector, FM: Fixed mask, FCS: Fast close shutter, SS: Safety shutter, WS: White beam slit, F: Diamond Filter, HDCM: Horizontal double crystal monochromator, NBPM: Nano-beam position monitor, SSA: Secondary source aperture, KB: Kirkpatrick–Baez mirror.

<Figure 3.2.10.3> shows the optical layout of the nanoprobe beamline. The ultimate goal in designing the layout and specifications of the optical components is to keep the beam size, intensity and position instability delivered to the sample below 10%. To achieve this, we are considering two main aspects. First, the beamline layout of the nanoprobe beamline incorporates a secondary source focusing method that enables a flux-versus-coherency trade-off using the SSA. This design utilizes SSA to properly trade the required transverse coherence for beam flux. It also converts positional instability to intensity instability. While intensity instabilities can be easily compensated for with diagnostic devices such as an ion chamber, positional instabilities require high computational power to compensate for. This design is suitable for nanoprobe beamlines that primarily utilize scanning microscopy.

Second, the design ensures that the peak power density on the DCM is kept below 40 W/mm^2 [11-13]. This is to prevent thermal bumps and damage from the first crystal and is a value that distorts the rocking curve of Si <333> to $<1 \mu\text{rad}$ [11, 12]. To reduce the peak power density, Korea-4GSR beamlines are taking one of two strategies. The first strategy is to locate the DCM more than 50 m away from the source. This approach minimizes the number of optical components. Also, this strategy prevents wavefront distortion caused by imperfections(slope error, surface roughness, etc.) of mirror surface and beam instability caused by optics vibrations.

However, this strategy cannot optimize the beam flux. Because it can only accept a limited beam flux that does not cause thermal bumps.

The second is using a High Heat Load Mirror (HHLM) with notch design. By absorbing heat through the HHLM, this strategy allows for increased flux while reducing the heat load on the DCM. However, the trade-off is that it requires additional manipulation to correct thermal bumps of HHLM (More detailed heat power estimations are provided in the “(3) Heat Load Consideration” section). <Figure 3.2.10.4, (Left)> shows the slope error profile of M1 with the maximum heat absorption power conditions ($W_{abs} = 134\text{ W}$). Here, the M1 mirror has a notch design. It broadened the beam by more than three times at the SSA. <Figure 3.2.10.4, (Right)> shows the simulation result of bending the M2 mirror to compensate for this. Thermal bump correction strategy using a bending pre-focusing mirror can provide a high mono-beam flux above 10^{12} ph/s (Coherent flux: $>10^{11}$ ph/s @ 10 keV). One of the objectives of a nanoprobe beamline is to rapidly investigate a large sample in nanoscale resolution, as mentioned in the scientific objective section. To achieve this, beam flux maximization is necessary. Thus, we have chosen the second strategy.



<Figure 3.2.10.4> Mirror surface profile resulting from the thermal bump on the M1 mirror and the expected beam profile (VxH) at the SSA. The mirror slope error graph shows the thermal bump profile when the maximum total power is delivered to the HHLM with the notch design applied. Bend M2 to correct the focused beam size at the BDA to be closer to the ideal size.

(3)Heat Load Consideration

<Table 3.2.10.3> shows the calculation of the thermal energy absorbed by the optics with a 50 um diamond filter applied. <Table 3.2.10.4> shows the results without applying the diamond filter for comparison. Absorption heat load is calculated using SRCalc [6, 7]. M1 mirrors are Pt-coated, M2 mirror is Si-coated from 5 to 10 keV, Rh-coated from 11 to 22 keV, and Pt-coated above that. <Table 3.2.10.3> and <Table 3.2.10.4> shows that the acceptance angle is 37 urad (Open 1 x 1 mm² @ 27 m).

<Table 3.2.10.3> Calculated the heat load of an optical component with a 50 um diamond filter

Energy	5 keV	7 keV	10 keV	15 keV	20 keV	23 keV
K	0.73	1.85	1.34	1.98	2.23	2.27
M1: Peak power density (W mm ⁻²)	7.3E-3	5.6E-2	2.2E-2	6.2E-2	8.0E-2	9.1E-2
M1: Absorbed power (W)	3.1	24.4	9.5	27.8	35.4	40.8
M2: Peak power density (W mm ⁻²)	2.1E-2	1.3E-1	7.5E-2	4.4E-2	3.3E-2	3.3E-2
M2: Absorbed power (W)	8.5	54.6	31.4	18.8	13.9	15.0
1st cry.: Peak power density (W mm ⁻²)	12.4	13.5	7.9	10.4	10.5	9.3
1st cry.: Absorbed power (W)	29.5	44.1	37.0	89.4	106.1	107.3

<Table 3.2.10.4> Calculated the heat load of an optical component without a diamond filter

Energy	5 keV	7 keV	10 keV	15 keV	20 keV	23 keV
K	0.73	1.85	1.34	1.98	2.23	2.27
M1: Peak power density (W mm ⁻²)	8.9E-3	6.2E-2	2.68E-2	7.6E-2	8.2E-2	9.3E-2
M1: Absorbed power (W)	3.9	26.8	33.2	31.2	36.5	41.8
M2: Peak power density (W mm ⁻²)	2.2E-2	1.3E-1	7.9E-2	4.5E-2	3.5E-2	3.5E-2
M2: Absorbed power (W)	9.2	56.8	61.7	19.5	14.9	15.9
1st cry.: Peak power density (W mm ⁻²)	16.7	19.4	12.6	15.0	12.3	10.9
1st cry.: Absorbed power (W)	40.8	65.7	61.7	111.9	123.1	126.6

With a notch design and cooling on the mirrors, the beam size is estimated to be only 2-3 times larger than ideal focusing on the calculated heat load. We have confirmed that mirror notch design and cooling mitigate beam size broadening due to thermal bump. Further investigations about mirror notch and cooling system design are ongoing, and some mirror specifications may be modified based on these results. The nanoprobe beamline uses M1 and M2 mirrors with notch design and cooling. Since the M1 mirror absorbs 2 to 10 times higher

heat load than the M2 mirror, M1 applied a cooling strategy using a gallium bath <Table 3.2.10.7> and <Table 3.2.10.8>. The M2 mirror uses side cooling and a mirror bender to correct the beam broadening at SSA. To ensure the stability of both mirror systems, they are sufficiently separated, and diagnostic and slit devices are placed between them to allow machine studies.

(4) Specification and strategy of beam delivery to BDA

The beamline layout is designed to provide a reliably controllable SSA aperture size for consistent X-ray experiments. <Table 3.2.10.5> shows the SSA opening size under the condition that the normalized degree of coherence($\mathcal{J}$) is 0.91 ($A\theta = \lambda/4$) [3,4]. Here, θ is the half angular acceptance of KB mirrors and A is SSA opening size. Under these conditions, ptychography images in single probe mode have a resolution degradation of less than 10% [5]. In particular, the nanoprobe beamline is planned to provide wide sample area scanning with fly-scan at a few kHz frame rate. Under these high degree of coherence conditions, image reconstruction can be achieved with reasonable computation power.

<Table 3.2.10.5> SSA opening size that makes coherent illumination of the KB mirrors

Energy	SSA-H (um)	SSA-V (um)
5 keV	37.98	12.63
10 keV	18.99	6.32
15 keV	12.66	4.21
20 keV	9.50	3.16
25 keV	7.60	2.53

On the other hand, an optical design with a high magnification ratio of M1, M2 at the BDA allows for a shorter beamline with lower construction costs. However, the engineering challenge lies in making well controllable apertures smaller than a few tens of micrometers. <Table 3.2.10.6> shows RMS beam size at the SSA for different magnification ratios. A magnification ratio of 1:1 provides a reasonable aperture size compared to SSA opening size for coherence mode($\mathcal{J} = 0.91$) and RMS beam size. Thus, the first optics after the shielding wall is 29 m from the source, and thus BDA optimal position is 58 m.

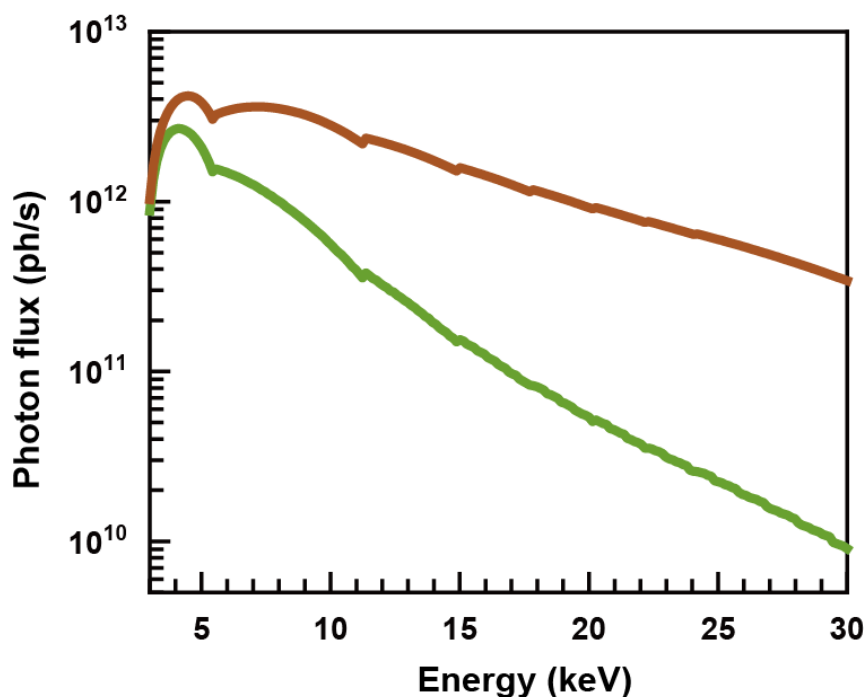
<Table 3.2.10.6> The RMS beam size at the SSA for different magnification ratios

Energy	Beam size	Magnification 3:1	Magnification 1:1	Magnification 1:2
10 keV	H x V, RMS (um)	9.5 x 2.3	19.0 x 4.5	29.4 x 7.0
20 keV	H x V, RMS (um)	9.5 x 2.1	18.9 x 4.2	29.3 x 6.5

<Table 3.2.10.7> shows the coherence fraction, which is the ratio of the total flux to the coherent flux in a mono beam. Coherent flux is the flux passing through the BDA when it is opened to the coherence length in <Table 3.2.10.5>. <Figure 3.2.10.5> shows the expected coherent flux delivered to the sample, taking into account mirror reflection coefficient, number of mirror reflections, BDA size, angular acceptance of the nanofocusing optics(KB mirror), and the polarization effect of the HDCM.

<Table 3.2.10.7> Flux and coherent fraction

Energy	Coherent flux (ph/s)	Total flux (ph/s)	Coherent fraction
10 keV	1.47×10^{13}	7.42×10^{13}	19.8 %
20 keV	1.67×10^{12}	2.85×10^{13}	5.9 %



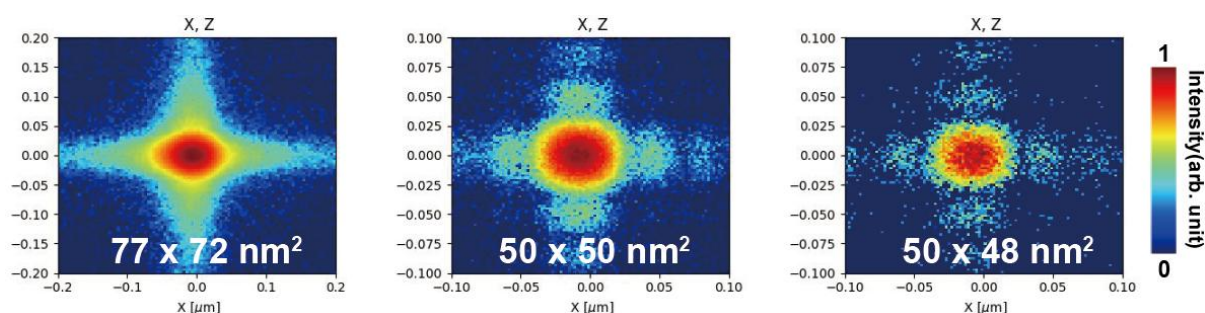
<Table 3.2.10.5> Focused photon flux(brown) and coherence mode flux(green) at sample position.

(5) Optics specification and tolerance

<Table 3.2.10.6> Optical component specification

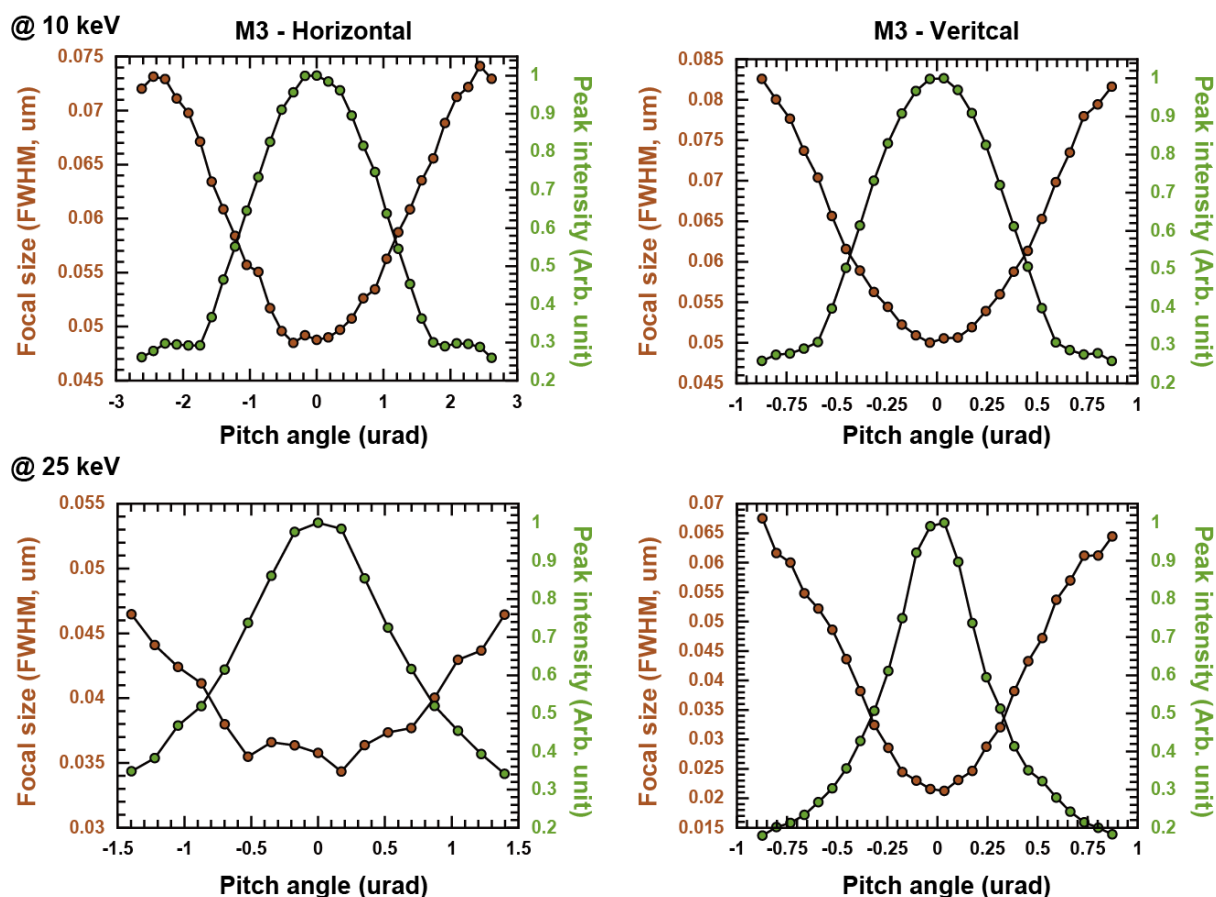
	M1	M2	DCM	M3 V	M3 H
Distance (m)	29	30.4	32	149.69	149.9
Incident Angle	2.5 mrad	2.5 mrad	3 to 45 degree	3.0 mrad	3.0 mrad
Shape	Fixed spherical cylinder	Bendable spherical cylinder	Plane	Elliptical cylinder	Elliptical cylinder
Source distance	29.0 m	30.4 m	-	91.69 m	91.9 m
Image distance	29.0 m	27.6 m	-	0.31 m	0.1 m
Type	Sagittal focusing	Tangential focusing	Horizontal deflection	Tangential focusing	Tangential focusing
Coating material	Pt (50 nm)	Si, Rh, Pt (50 nm)	-	Pt (50 nm)	Pt (50 nm)
Mirror size (L x W x T, mm ³)	600 x 50 x 55	600 x 50 x 55	1st: 60 x 25 x 50 2nd: 140 x 25 x 30	300 x 50 x 50	100 x 50 x 50
Figure error (nm, RMS)	< 0.3	< 0.3	< 1	< 0.15	< 0.15
Slope error (μrad, RMS)	< 10.0	< 0.5	< 1	< 0.10	< 0.10

<Table 3.2.10.6> lists the specifications of the mirrors used in the nanoprobe beamline. The specifications of the mirror system are designed to focus the beam on the BDA located at 58 m. The slope and figure error tolerance is set to ensure that the beam broadens below 10% and peak intensity decreases below 20% (Maréchal criterion). The M3 mirror is a Nano-KB mirror designed to produce a beam of < 50 nm at energies above 8 keV. <Figure 3.2.10.6> shows the results of a beam simulation delivered to the sample when these tolerances are met.



<Figure 3.2.10.6> Beam simulation results at the sample position with included mirror figure and slope error. Here, X-ray energy is 10 keV. (Left) SSA full open, (Middle) 19.0 x 6.3 μm² open, (Right) 5.0 x 5.0 μm² open. Colormap scale is logarithmic.

To investigate the tolerance for angular vibration errors (or pitch alignment errors) of the M3 mirror, we simulated the focal size and peak intensity based on the pitch tilt angle. The simulation results are shown in <Figure 3.2.10.7>. To keep the variations in focal size and peak intensity below 10%, the range of pitch angular vibrations is smaller than $2.0 \mu\text{rad} \times 0.68 \mu\text{rad}$ at 10 keV and $0.4 \mu\text{rad} \times 0.2 \mu\text{rad}$ at 25 keV.



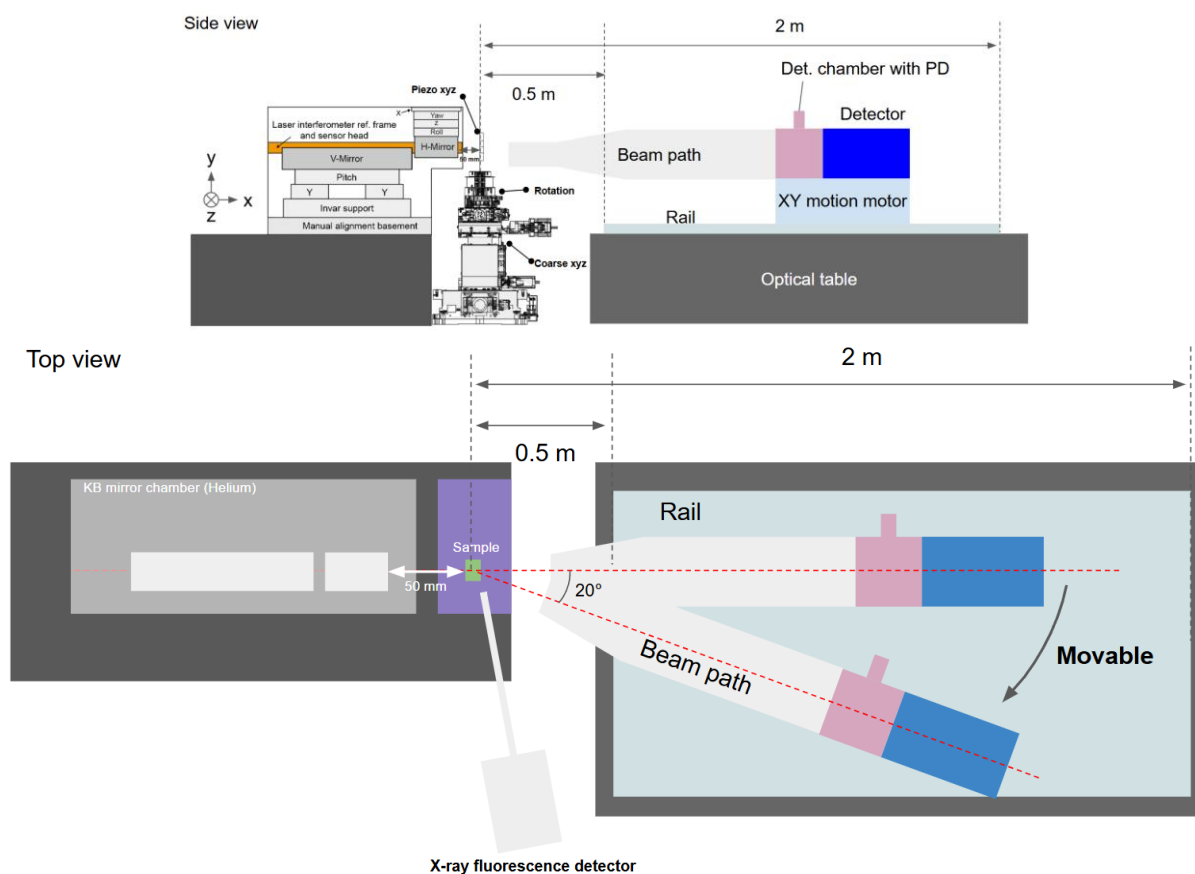
<Figure 3.2.10.7> Pitch angular vibration of M3 mirrors.

F. Instrument overview

(1) Experimental method

The experimental instruments of the Nanoprobe provide various scanning imaging techniques. The primary imaging technique is multi-modal imaging that simultaneously performs 2D/3D XRF and 2D/3D ptychography. Auxiliary imaging techniques include diffraction mapping, ptychography, and XANES. The nanoprobe beamline has two operation modes. The first mode supports multi-modal imaging, providing a nanobeam using a KB mirror

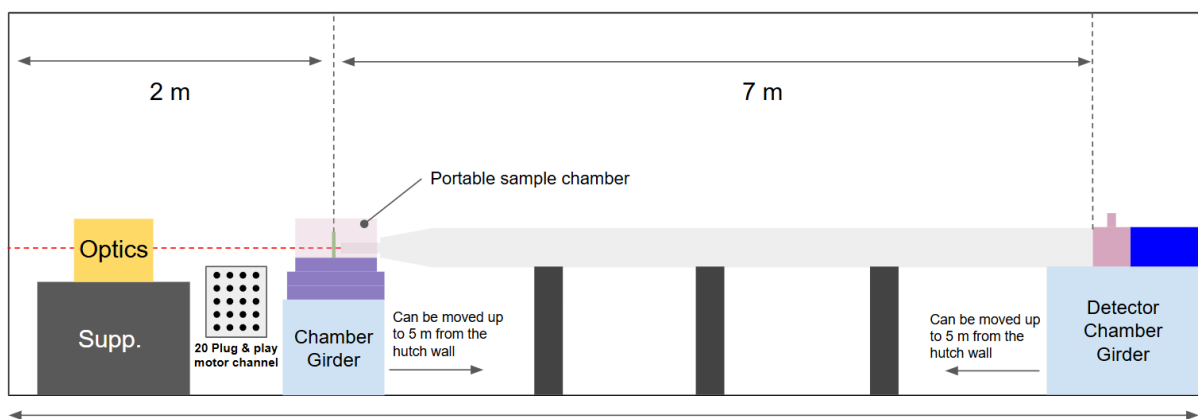
(working distance 50 mm) with the sample in a fixed position (150 m from the source). This operating mode is designed for general users, with high demand expected in research fields such as energy materials, catalyst and semiconductors etc. It will provide high-resolution 2D/3D element maps and electron density images using XRF and ptychography in in-situ/operando conditions. Additionally, to support high-speed piezo systems, a sample stage compatible with lightweight in-situ cells (Target weight $\ll 100$ g) will be provided [9,10]. The high-speed motor features a close-loop system using a piezo motor with an operation rate exceeding 20 kHz and is designed to maintain a consistent footprint during fly-scan. Initially, the machine study for the scan system will focus on optimizing the close-loop frequency, motor trajectory, and parameters. The ultimate goal of the machine study is to achieve a stable enough system to conduct multimodal imaging in turn off close-loop feedback.



<Figure 3.2.10.8> A schematic of instrument and motor motion of a Nano-Scanning Microscope hutch in a nanoprobe beamline. 18 axes of control motion(including granite yz motion and Detector chamber y motion) and 3 axes of manual motion are required. The laser interferometer head for sample position metrology and its support are not shown. Experiment with samples from a fixed location (150 meters from the source).

The second mode supports a more flexible experimental setup. The experimental hutch we will provide is 20 meters long and is located from 135 meters to 155 meters from the light source. The first mode described above will primarily utilize the space from 150 m to 155 m. The second mode can support sample to detector distances of up to 18 m by bypassing the KB mirror and endstation utilized in the first mode. It offers 20 plug&play motor channels to seamlessly support custom chambers built to meet the needs of various user communities. For user convenience, the connected motors can be freely named in the user interface. A floor rail system has been installed to safely move various types of supports on the floor. The beam path can provide sample to detector distance of 18 m at 0° and up to 6 m at 45°.

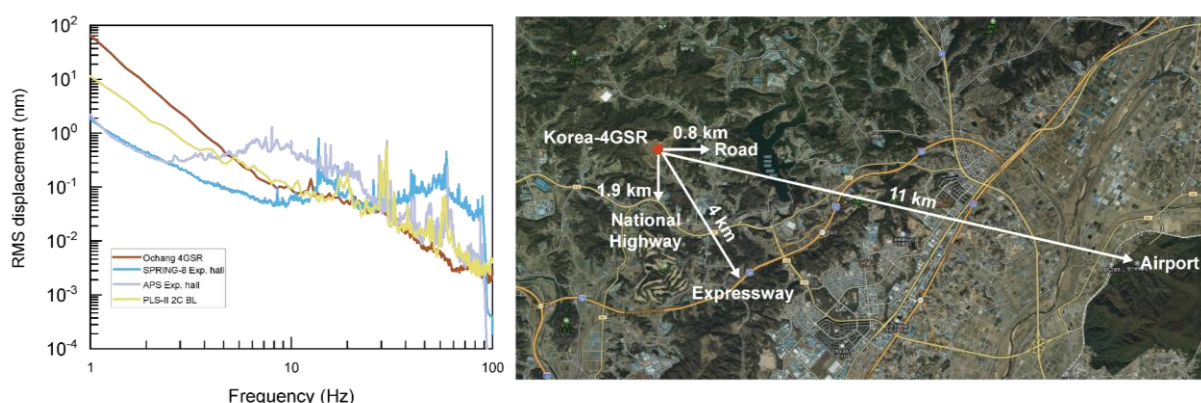
Additionally, granite supports that can move on the floor rails allow the sample stage to be installed at the desired position within the hutch. This granite supports an air bearing stage to minimize vibration effects and provide alignment for the user's equipment. Also, we prepare an extra movable granite stage. This is to accommodate users who need different types of experimental chambers or new sample setups. This extra stage will allow for sample environment setup and parameter adjustments to be completed before being moved into the experimental hutch. This approach is designed to reduce time wasted in user switching, minimize variability in instrument setup locations, and provide better prepared experimental parameters.



<Figure 3.2.10.9> A schematic of instrument and motor motion of a Nano-Coherent Imaging hutch in a nanoprobe beamline. 11 axes of control motion(including granite yz motion and Detector chamber y motion) and 20 plug&play motor channels are required. The experimental chamber and detector stage can move up to 5 m from the hutch wall. Experiment with samples from a fixed location (140 meters from the source).

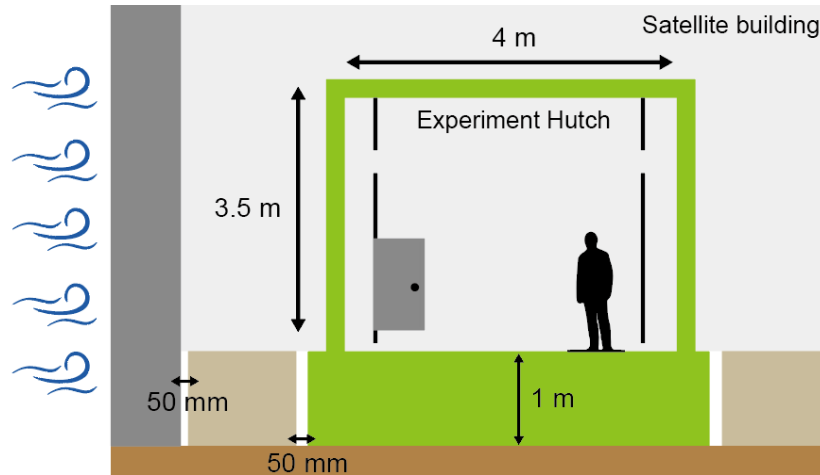
(2) Experimental floor and hutch design

In designing the mechanical specifications for nanoprobe, the golden rule is to keep the instability of the beam delivered to the sample to less than 10%. This means ensuring beam stability of less than $0.2\ \mu\text{m}$ in the Optical Hutch II (Secondary aperture position) and less than 5 nm in the Experimental Hutch area. To achieve this, we focused on reducing natural, cultural vibrations and thermal instability.



<Figure 3.2.10.10> (Left) Vibration level of synchrotron facilities [8] (Right) Floor vibration source.

First, we'll introduce natural vibrations in the Korea-4GSR facility. <Figure 3.2.10.10, (Left)> shows the amplitude of floor vibrations by frequency for synchrotron facilities. The measurements for Korea-4GSR were taken at the construction site. The Korea-4GSR site has floor vibrations similar to those of other synchrotron facilities and even shows lower vibration above 30 Hz. <Figure 3.2.10.10, (Right)> briefly outlines the surrounding cultural vibration sources. To isolate the experimental hutch from the mentioned vibration sources, the Nanoprobe adopted two strategies. The first strategy involved isolating the experimental hutch slab from the surrounding slabs, as illustrated in <Figure 3.2.10.11>. Here, the slab length is 21 m. The second strategy involves using alternatives to cultural vibration sources such as vacuum pumps and cooling fans. For example, the experimental chamber will use helium flow instead of a vacuum environment, and most electronic equipment using cooling fans is replaced with water-cooled systems.



<Figure 3.2.10.11> Stellite building and hutch structure of Nanoprobe beamline.

To reduce thermal drift by hutch temperature deviations, the experimental equipment is thermally isolated in two stages. The first stage involves constructing the hutch with 300 mm thick concrete and implementing an HVAC system inside. Concrete hutch has a thermal conductivity 360 times lower than that of a steel-lead-steel hutch, making it less sensitive to temperature changes around the experimental hutch. The HVAC system is designed to maintain the temperature within the hutch at $< 0.1\text{ }^{\circ}\text{C}$. The second stage is installing the KB mirror and experimental sample stage inside a $2.0 \times 1.5 \times 2.0\text{ m}^3$ thermal insulation enclosure. This enclosure is equipped with water-cooled panels to control the internal temperature to $< 0.02\text{ }^{\circ}\text{C/h}$. Here, $0.02\text{ }^{\circ}\text{C/h}$ is the condition under which a 1 m granite block experiences thermal movement of less than 5 nm. This enclosure is a compact version of the enclosure introduced in Ref. [10]. The decision to install this enclosure will depend on the performance of the HVAC system, and it will be installed after undergoing machine study.

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