# IAC 2023 Overview of 10 Priority Beamlines for 4GSR and Construction States

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### Outline

**1. Introduction** 

# 2. Present status for beamline construction

- 3. Future Plan
- 4. Summary





### ✤ 3GSR, DBA→4GSR, MBA



 NanoARPES results on HOPG sample obtained with the ANTARES microscope



# Coherent

speckle

~Na 1



 High coherence Low coherence
 High-sensitivity image acquisition through phasecontrast X-ray imaging



### Measurement of 3D lattice, element and strain



### **4GSR Outline**

### Multipurpose Synchrotron Radiation Construction Project

- Period: 2021 July to 2027 June (6yrs)
- Budget: 1.0454 Trillion KRW (≈ USD 750M)
- Land: 540,000 m / Building: 69,400 m
- Location: Ochang, Chungcheongbuk-do

# **Specifications**

- Beam Energy: 4 GeV
- Beam Emittance: less than 100 pm·rad (CDR: 58 pm·rad)
- Circumference: 800m
- Beamlines : more than 40
- Accelerator: Gun, Injector LINAC, 4 GeV Booster
- Lattice: MBA-7 Bend Achromat

# **Beamlines in Phase-I**

(1) BioPharma-BioSAXS
 (2) Material Structure Analysis
 (3) Soft X-ray Nano-probe
 (4) Nanoscale Angle-resolved Photoemission Spectroscopy
 (5) Coherent X-ray Diffraction
 (6) Coherent Small-angle X-ray Scattering
 (7) Real-time X-ray Absorption Fine Structure
 (8) Bio Nano crystallography
 (9) High Energy Microscopy
 (10) Nano-probe



22 <sup>n</sup>	d International Advisory Committee	e Meeting (Novem	ber 13-14, 2023)	Dhoton		
	Beamline	Photon Energy	Resolution	Source	Exp.	Application
Priority	① BioPharma-BioSAXS	5~20 keV	SAXS: 1 Å 이하 ΔΕ/Ε < 10 <sup>-4</sup>	IVU	1 Bio-SAXS	Bio.
support for industries	<ul><li>② Material Structure Analysis</li></ul>	5~40 keV	ΔΕ/Ε < 10 <sup>-4</sup>	Undulator	<ol> <li>1 XRD</li> <li>2 XAFS</li> </ol>	Material Science, Energy material
	③ Soft X-ray Nano-probe	0.1~5.0 keV	sub-micro beam ΔE/E>15×10⁴@1keV	EPU	1 XAS 2 XPS	Semiconductor, Material Science
	<ul> <li>Nanoscale Angle-resolved</li> <li>Photoemission Spectroscopy</li> </ul>	0.1~2 keV	100 nm < ΔΕ/Ε < 10 <sup>-4</sup>	Undulator	① Nano-ARPE S	Semiconductor, Material Science
	⑤ Coherent X-ray Diffraction	3~30 keV	sub-micro beam	Undulator	<ol> <li>1 XRD</li> <li>2 CDI</li> </ol>	Semiconductor, Material Science Geosciences, Chemistry
Support for Academic	⑥ Coherent Small-angle X- ray Scattering	4~40 keV	~ a few nm ~ $\mu$ m $\Delta$ E/E < 2×10 <sup>-4</sup>	IVU	<ol> <li>SAXS/WAXS</li> <li>(GI 기법 포함)</li> <li>XPCS</li> </ol>	Material Science, Chemistry
R&D	<ul> <li>Real-time X-ray Absorption Find</li> <li>ne Structure</li> </ul>	5~40 keV	~ a few µm	Undulator	1 XAFS	Material Science, Environments, Geosciences, Chemistry
	⑧ Bio Nano crystallography	5~20 keV	1Å <	IVU	① MX	Bio.
	I High Energy Microscopy	5 ~ 100 keV	Spatial R. ~ 0.1µm	Superbend	<ol> <li>Projection imaging</li> </ol>	Material Science, Energy material, Bio
	Nano-probe	5~25 keV	~50nm NanoProbe 1~10 µm	IVU	① Ptychograph y/XRF	Semiconductor, Material Science, Geosciences,
			MICIOFIODE			Chemistry, Environments

Storage Ring for 4GSR

다목적방사광가속기구축사업단



# ✤ 4GSR Storage Ring Specification

Parameter	4GSR	PLS-II
Beam energy[GeV]	4	3
Beam current[mA]	400 Top-up mode	250( Max. 400), Top-up mode
Circumference[m]	798.8	281.82
Lattice structure	Multi-Bend	Double-Bend
Super-period	28	12
Emittance	62 pmrad	5800 pmrad
RF frequency	499.877 MHz	499.96 MHz
Bunch length[ps]	10.68 (without HC)	20
	53.43 (with HC)	
Number of Bunches	1065	300
Energy spread	0.12%	0.1 %





[출처, 다목적방사광가속기 구축사업 기반시설 공모안, (주)형림종합건축사사무소]

# Supercell Structure > 28 supercell(12.85°/cell)



22<sup>nd</sup> International Advisory Committee Meeting (November 12,14, 2023) Monochromator Type



**Beamline Design** 

- Deliver the required X-ray beam to the experiment:
  - ✓ Energy and bandwidth
  - ✓ Spot size
  - ✓ Divergence/convergence
- Preserve source characteristics ; intensity, brightness, coherence...
- Handle the <u>heat load of the beam</u>
- Optimize signal / background
- Be very stable and reproducible, in position, intensity and energy
- Be safe to operate
- Be user friendly to operate
- Achieve all the above within a reasonable budget !

Photon Source Optical system Heat Load Simulation Stabilization Safety(personal & Instrument) User friendly Budget...

# **Photon Sources**

Photon Source	Ту.	Periods length [mm]	Total Length [m]	Photon Energy(keV)	#	Applicable BL	Beam Port
Bending Magnet	BM			5 ~ 100	1	#09. HEMicroscopy	BM10
Out-vacuum	EPU	78	2	0.1 ~ 3.2	1	#03. Soft X-ray NanoProbe	ID26-1
Undulator		98	3.6	0.05 ~ 2	1	#04. NanoARPES	ID25
In-Vacuum	IVU	IVU 20 24	3	5 ~ 40	2 # #	#06. CoSXAS	ID20
Undulator						#08. BioNX	ID22
			3	3 ~ 40	5	#01. BioPharma.	ID21
						#02. Mat. Structure	ID24
						#05. CoXRS(CDI)	ID19
						#07. Realtime XAFS	ID23
						#10. NanoProbe	ID10
			1.5	2 ~7	1	#03. Soft X-ray NanoProbe	ID26-2

# **Properties of Photon Source**

Undulator	(Unit.)	IVU20	IVU22	IVU24	EPU78	EPU98	ВМ	PLS-II (IVU20)
Period Length	[mm]	20	22	24	78	98	-	20
Periods		148	134	123	23	34	-	68
Device Length	[m]	3	3	3	2	3.62	0.186	1.4
K <sub>max</sub> value		1.90481	2.3007	2.7458	K <sub>v</sub> 6.95 K <sub>c</sub> 4.39 K <sub>H</sub> 5.65	К <sub>v</sub> 9.24 К <sub>с</sub> 6.07 К <sub>н</sub> 8.05	-	1.811
B <sub>max</sub>	[T]	1.02	1.12	1.22	B <sub>∨</sub> 0.95 B <sub>c</sub> 0.60 B <sub>H</sub> 0.77	B <sub>V</sub> 1.01 B <sub>c</sub> 0.66 B <sub>H</sub> 0.87	2	0.969
Gap <sub>min</sub>	[mm]	5	5	5	15	15	-	5
٤ <sub>1st</sub>	[eV]	2699.6	1893.9	1327.3	77.48 / 97.28 / 114.84	35.48 / 46.41 / 40.96	[E] 21280.8	1618.78
Total Power	[kW]	12.47	14.97	17.94	6.61 / 4.37 / 5.21	13.75 /10.44 / 11.87	1357.83	2.91
Max.Power Density	[W/mrad <sup>2</sup> ]	164.1	164.1	165.5	24.31	38.06	Lin. Pow. Density (kW/mrad) 0.216	22.5
Max.central cone	[mrad]	Σ <sub>x'</sub> 0.0093 Σ <sub>y'</sub> 0.0089	Σ <sub>x'</sub> 0.0109 Σ <sub>y'</sub> 0.0106	Σ <sub>x'</sub> 0.0129 Σ <sub>y'</sub> 0.0126	Σ <sub>x</sub> <sup>,</sup> 0.0854 Σ <sub>y</sub> <sup>,</sup> 0.0854	Σ <sub>x</sub> , 0.0956 Σ <sub>y</sub> , 0.0955		Σ <sub>x'</sub> 0.0341 Σ <sub>y'</sub> 0.0171

**Brilliance and Photon Flux** 



# Coherence







# 01. BioPharma-BioSAXS

Variable *q*-range vacuum chamber

### ✤ 3D structure of therapeutic biological molecules

- ✓ Overall structure of therapeutic molecules
- $\checkmark$  Overall status of biological molecule/drug complex
- ✓ Docking model of protein-protein complex



# Dia Kinat al Natura Comm

D. n. Kimet. al., Nature Comm . 2020, 11, 148

### Beamline Goal

 구 분	내용
Light Source	IVU22 (L=3.0 m)
Photon energy	5-20 keV (optimized at 8-25 keV)
Energy resolution	∆E/E ~ 2 x 10 <sup>-4</sup>
Beam size	< 10 $\mu$ m at the detector
Length scale	~ 3 - 4480 Å
Time resolution	~ 10 Hz
Beam flux	10 <sup>12</sup> ~10 <sup>13</sup> ph/s @ 16.02 keV
Sample to Detector Distance	0.5 ~ 6 m
Techniques	(Solution) SAXS/WAXS



### Sample environment

- ✓ Automatic sample changer robot ✓ S
- ARINAX, BIO-SAXS
- Minimum sample volume (5ul)
- Standard 96 well plate
- Static & flow mode
- Temperature control (4°C 60°C)



Control Software Control Electronics Rack Fluid Management Unit (FMU)

### ✓ SEC-SAXS system

End-station layout for high throughput Bio-SAXS technique

- Agilent infinity 1260 system, RI, UV, MALS, & DLS
- Separation and Analysis of polydisperse species or mixture

@WXALT

WYATT

### > Variable q-range vacuum chamber

✓ Detector is placed in the vacuum chamber to facilitate SDD change





Example; 12 ID-B, APS

# 02. Material Structure Analysis



\* Flight beam path and the stage for in-situ experiment (orange box) should be aligned together

Photon Source	IVU24(L=3.0 m)
Photon energy (hv)	5 ~ 40 keV [Main : 20 keV for HRPD]
Energy resolution (△E/E)	~ 1.3 x 10 <sup>-4</sup> (Si (111) ~ 2.7 ×10 <sup>-5</sup> (Si (311)
Beam size (FWHM)	~ 600 (h) × 230 (v) μm <sup>2</sup> @sample (69m for XAFS) ~ 670 (h) × 230 (v) μm <sup>2</sup> @sample (75m for HRPD)
Beam flux	~ 1 ×10 <sup>13</sup> ph/s @sample
Techniques	XAFS: Step scan mode HRPD: Multi-analyzer detector system

X-ray Absorption Fine Structure (XAFS)



Gas auto-exchange system required \* Fluorescence detector \*\* Hexapod sample stage

Multi sample holder Sample stage to configure various experiments High-Resolution Powder Diffraction (HRPD)



# 03. Soft X-ray Nano-probe



- ✤ Nano-XPS/XAS for Branch 1
  - Scanning Photoemission Microscopy
  - Dynamic beam size incl. zone-plate

### focusing

Binding energy (et





	EPU78(L=2 m)	IVU24(L=1.5 m)
E <sub>1st</sub>	77.45 ~114.73 eV	1336.4 eV
Energy range	90 – 3,200 eV	2000 ~ 5000 eV
Beam size at Sample	70 nm × 140 nm by FZP	10.8 µm x 8.4 µm
Brilliance [photons.s –1 mrad -1 .	1.18 × 10 <sup>19</sup> at 15 mm gap	1.11925 × 10 <sup>21</sup> at 5 mm gap
mm -2 (0.1%B.W)]		

- Tender XPS/XAS for Branch 2
- Tender X-ray Phtoemission Spectroscopy & XAS
- Non-destructive bulk property probe.



(a)

Si 4+ (SiO2



(b)

(e)



(c)

(f)







22<sup>nd</sup> International Advisory Committee Meeting (November 13-14, 2023) 04. Nanoscale Angle-resolved Photoemission Spectroscopy(NanoARPES)

Light Source	EPU98(L=3.6 m)
Photon energy(hv)	0.1 – 2 keV [Optimize: 50 ~200 eV]
Energy resolution (△E/E)	20,000
Beam size	100 x100 nm <sup>2</sup> by FZP
Beam flux	<ul> <li>10<sup>12</sup> - 10<sup>13</sup> ph/s</li> <li>90eV ~ 2,000eV</li> <li>10<sup>10</sup> - 10<sup>12</sup> ph/s</li> <li>2,000eV ~ 3,200eV</li> </ul>

nd-stations	nano-ARPES	<ul> <li>nano-focusing optics: Zone plate @ Capillary mirror</li> <li>Hemisphere electron analyzer</li> <li>Photon energy range: 100-200 eV</li> <li>Energy Resolution: &lt; 10 meV @ 100eV</li> <li>Photon flux: ~ 10<sup>11</sup> phs with ZP @ 100eV</li> </ul>
	µ-ARPES	<ul> <li>micro-focusing optics: K-B Mirrors or Capillary Mirror</li> <li>Hemisphere electron analyzer with spin detectors</li> <li>Photon energy range: 100 - 2000 eV</li> <li>Energy Resolution: &lt; 5meV @ 100 eV</li> <li>Photon flux: &gt; 10<sup>12</sup> phs @ 100eV</li> </ul>
nge: 10 – 100 grating : ~ 50 nm wi power: 50eV, > 3000	00 eV th FZP 00@ whole energy	range



# 05. Coherent X-ray Diffraction(CXD)

IAC( Nov. 13-14, 2023)

		BCDI Bragg ptychog
Light Source	IVU24(L=3.0m)	
Photon energy	3 – 30 keV	
Energy resolution( △E/E)	< 2 x 10 <sup>-4</sup>	Sample Cham
Beam size	< 500 nm ~ few micron at the sample	
Beam flux	~10 <sup>13</sup> ph/s at the sample	Aray .
Techniques	CDI, (time-resolved) Nanobeam X-ray Diffraction	
Experimental hutch	EH1) 6-circle diffractometer(Kappa)	
instrument	EH2) CDI chamber, Flight path	
Detector	Lambda 250k, Eiger2 X 1M, Eiger2 X 4M, 7-channel SDD	
Undulator	M2 (36 m) (22 m) M1 (30 m) DCM (34 m)	KB Mirror (65 m) Sample (67.5 m)
Front-e	nd Optical hutch	Experimental hutch 1



< Transmission Ptychography >





IAC( Nov. 13-14, 2023)

# 06. Coherent Small-angle X-ray Scattering



X, Y, Z direction and Tilt around Y

22<sup>nd</sup> International Advisory Committee Meeting (November 13-14, 2023) Real-time X-ray Absorption Fine Structure

Beamline Goal



- Multi-crystal

von Hamos spectrometer

→ Si(200), Si(200), Si(220)

Ge(111), Ge(200, Ge(220)

### End-station layout

### - Main experiment

Absorption spectroscopy: XAFS, QXAFS Emission spectroscopy: XES, HERFD-XAS

### - Design goal

Wide energy range: 4 ~ 40 keV High photon flux: ~  $10^{14}$  ph s<sup>-1</sup> Small beam size: ~ 21 (H) x 7 (V)  $\mu$ m<sup>2</sup>

# **\*XES & HERFD-XAS**





- 2D detector

Detector

Dimension

Pixel size

Count rate

(ph/s/mm<sup>2</sup>)

Readout

rate

LAMBDA

(X-Spectrum)

85 x 28 mm<sup>2</sup> (750k)

170 x 170 mm<sup>2</sup> (2M)

55 x 55 μm<sup>2</sup>

~3 x 10<sup>8</sup>

1 kHz - 24 kHz

### **\*XAFS & QXAFS**



- Multi-sample - Fluorescence detector - Grided gas ionization holder & Hexapod chamber stage







### Equipment for In-situ measurement (examples)

Linkam heating cell

(~ 1000 °C)

Flat capillary heating cell (~ 400 °C)

- Optical table



In-situ electrochemical cells & Potentio-/Galvanostat





- In situ XAFS & XES



 $\checkmark$ 

 $\checkmark$ 

 $\checkmark$ 

### ✤ Beamline goals

Light Source	IVU20(L=3.0m)
Photon energy(hv)	5 ~ 20 keV [Optimize :6.5 ~ 20 keV]
Energy resolution (△E/E)	~ 1 x 10 <sup>-4</sup> (Si (111)
Beam size	~16 (h) ×4 (v) $\mu$ m <sup>2</sup> at sample
Beam flux	~10 <sup>13</sup> ~ 10 <sup>14</sup> phs/s @ sample
Techniques	Experimental Hutch : X-ray crystallography Wet Laboratory: crystallization facility

### Crystal Cry

# Biomacromolecule crystal structure

High resolution (~1 Å) Understanding life science at the molecular level Chemical drug design support Antibody Drug study support

# 08. Bio Nano crystallography (BioNX)

### Structure-based drug design

- High-throughput structure analysis
- ✓ Identification Fragment Definition
- ✓ Accelerated Sculpture Design
- ✓ 500 data/day



# 09. High Energy Microscopy (HEM)

# Design goals

Imaging spatial resolution	a few µm (1 µm)
Photon energy	10-130 keV
Beam size	200 mm
CT scan taking time	Minutes
Phase contrast effect (Refraction detection limit)	< 0.1 µrad
Sample position	100 m
In-situ/operando sample space	a few m
Max sample weight	300 kg

# Experimental Equipment



### X-ray High aspect ratio High resolution microscope Field of View 200 x 25 mm<sup>2</sup> 1.3 x 1.3 mm<sup>2</sup> Pixel size 5 µm 0.25 µm Pixel number 200 million 25 million Data size 400 MByte/img 50 MByte/img 1 TByte/set 3D data size 16 TByte/set

### **Heavy Load Sample Station**



### > Multiscale Imaging



Walsh, C. L., et al. (2021). *Nature methods*, *18*(12), 1532-1541. Images taken at BM05, a predecessor beamline, at 60-80 keV



Lang et al. (2023), e-Journal of Nondestructive Testing 28(3). Multiscale Phase-Contrast Tomography at BM18

### In-situ/operando tester

**Dimension (LxWxH)** : 820 mm x 630 mm x 180 mm

Weight : 216 kg

Max. Capacity : 10 kN

Stroke Space : 1400 mm

# A. T. elc. KB mirror KB mirror

# 10. Nano-probe beamline

Beamline Goal

	Nano-Coherent imaging	Nano-Scanning microscopy					
Energy	5-25 keV						
Beam size	~ 100 nm	~ 50 nm					
Exp.	In-situ Coherent imaging	Ptychography Nano-XRF Multimodal imaging					
Resolution	< 50 nm (XRF), < 5 nm (Imaging)						
Photon flux	10 <sup>9</sup> -10 <sup>11</sup> phs/s @ Sample						





Xu, Yahong, et al. *ACS Energy Letters* 2.5 (2017): 1240-1245. Tsai, Esther HR, et al. *IScience* 11 (2019): 356-365.



# ✤ Long BL

- 09. HE Microscopy BL(L=100 m)
- 10. NanoPrpbe BL(L=150 m)
- ➤ Key point
- Vibration
- Radiation Safety
- Thermal stability



BM10: #09 HE microscope(100 m)

- Slab for Vibration Damping
  - I m Slab structure
  - Similar to Petra-III, ALBA, ESRF-EBS.



- ➢ Radiation Safety : PTL and Exp. Hutch Concrete
  - HE Micriscopy : 5 ~ 100 keV
  - NanoProbe : 5 ~ 25 keV
- House in house hutch structure

# Canted BL Available (for Phase-II)

1 mrad canted study for 4GSR

# $\rightarrow$ Apply to design

Undulator Configuration



Example)

APS 2-ID BEAMLINE, UPGRADE TO CANTED CONFIGURATION

**0.4 mrad canted** Two U33(L=2.4 m)



https://accelconf.web.cern.ch/medsi2016/posters/wepe18\_poster.pdf

# **Considering Timing Structure (for Phase-II)**



22<sup>nd</sup> International Advisory Committee Meeting (November 13-14, 2023)

	Beamline	Photon Energy	Resolution	Photon Source	Exp.	Application
Priority support for industries	1 BioPharma-BioSAXS	5~25 keV	SAXS: 1 Å 이하 ΔΕ/Ε < 10 <sup>-4</sup>	IVU24	1 Bio-SAXS	Bio.
	② Material Structure Analysis	5~40 keV	ΔΕ/Ε < 10 <sup>-4</sup>	IVU24	<ol> <li>HRPD, XRD</li> <li>XAFS</li> </ol>	Material Science, Energy material
	3 Soft X-ray Nano-probe	0.1~5.0 keV	sub-micro beam ΔE/E>15×10 <sup>-4</sup> @1keV	EPU78 +IVU24	<ol> <li>XAS</li> <li>XPS</li> </ol>	Semiconductor, Material Science <u>* Tandem U., Two Branched Beamline</u>
	<ul> <li>Nanoscale Angle-resolved</li> <li>Photoemission Spectroscopy</li> </ul>	0.1~2 keV Optimize: 50 ~200 eV	100 nm < ΔΕ/Ε < 10 <sup>-4</sup>	EPU98	1 Nano-ARPES	Semiconductor, Material Science *Two Branched Beamline
	<b>5</b> Coherent X-ray Diffraction	3~30 keV	sub-micro beam	IVU24	1 XRD 2 CDI	Semiconductor, Material Science Geosciences, Chemistry
Support for Academic R&D	⑥Coherent Small-angle X-ray Scattering	4~40 keV Optimize: 8-17 keV	~ a few nm ~ μm ΔΕ/Ε < 2×10 <sup>-4</sup>	IVU20	<ol> <li>SAXS/WAXS</li> <li>(GI 기법 포함)</li> <li>XPCS</li> </ol>	Material Science, Chemistry
	<ul> <li>⑦ Real-time X-ray Absorption Fine Structure</li> </ul>	5~40 keV	~ a few µm	IVU24	1 XAFS	Material Science, Environments, Geosciences, Chemistry
	⑧ Bio Nano crystallography	5~20 keV	1Å <	IVU20	① MX	Bio.
	④ High Energy Microscopy	5 ~ 100 keV	Spatial R. ~ 0.1µm	Centerbend	<ol> <li>Projection imaging</li> </ol>	Material Science, Energy material, Bio * Spatial Resolution : 0.1 µm→0.3-0.5 µm
	10 Nano-probe	5~25 keV	~50nm NanoProbe	IVU24	① Ptychography /XRF	Semiconductor, Material Science, Geosciences,

# Summary Goal : Prepare Another Successful Playground for Science

- > Overview of beamline construction status.
- > High Heat Load devices(PBPM, Mask, DCM) need study & developing.
- > Human resources training and planning.
- > Need to adapt and introduce for contemporary experimental method.







### From Naturejobs Blog

# Thanks to:

# All 4GSR Project Supporting Division



