次世代放射光施設コアリションビームライン
実施計画に関する国際審査

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Implementation Plan Report of Coalition Beamlines at 3-GeV Next-Generation Synchrotron Radiation Facility

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1. Introduction

1.1 General introduction

Synchrotron radiation (SR) is recognized as an essential research tool for the development of science and technology as well as for industrial applications. A number of advanced SR facilities have been constructed world-wide. This mirrors society's strong demand towards solving energy, environmental, public health problems and achieving sustainable development goals (SDGs). SR facilities around the world now work together to study, understand and solve the COVID-19 pandemic, including new drugs, therapeutic strategies and medical equipment developments, as declared in AOBA Communique 2 [1].

At SR facilities, powerful X-rays with unprecedented brightness are increasingly becoming available because of recent technical advances in storage rings; especially, "multi-bend achromat" magnets. New X-ray sources based on this technology will revolutionize our ability to investigate materials and devices with nanometer spatial resolution, chemical specificity, and dynamic time resolution, which will provide unique analytical capability to industry and academic researchers.

Despite its importance, the SR facility with high brightness especially in the soft X-ray energy region has been lacking in Japan. In 2018, the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan decided to initiate construction of the 3 GeV Next-Generation Synchrotron Radiation (NGSR) facility on the campus of Tohoku University. The construction and operation of the facility will be carried out by a new organization. It is a combined public-private regional partnership, in which the partners are the National Institute of Quantum Radiological Science & Technology (QST), Tohoku University, Miyagi Prefecture, Sendai-City, the Tohoku Economic Federation, and the Photon Science Innovation Center (PhoSIC). Funding comes from private sector investments, local governments, and MEXT through QST.

1.2 Next-generation synchrotron radiation facility and Coalition concept

The prime objective of the NGSR facility is to drive innovation by visualization of materials' function using SR X-rays with unparalleled spatial/temporal resolution and chemical specificity. To achieve open innovation, the NGSR facility should not be limited to SR specialists, but be open to non-SR specialist with unsolved important problems. In other words, the NGSR facility is required to be open to both industry and academia; more importantly, a close collaboration between industry and academia is necessary. Therefore, a new industry-academic alliance scheme, called "coalition concept", is developed at NGSR.

The “coalition concept” is a new research scheme, in which stakeholders from both industries and academia form a strong one-on-one team for the purpose of solving social challenges (Fig. 1.1). Industrial partners often have unsolved problems in their R&D, and require a practical and demand-oriented user-support by the experts. Academic partners often have expertise in measurements and data analysis. Through an interdisciplinary research collaboration in the “coalition concept”, academic researchers can expand the applicability of their expertise to new academic disciplines. This “Coalition Concept” has been attracting industrial users for advanced utilization of the SR facility, which, we believe, will lead to solving the essential problems of industries and will promote the diversity of SR research.

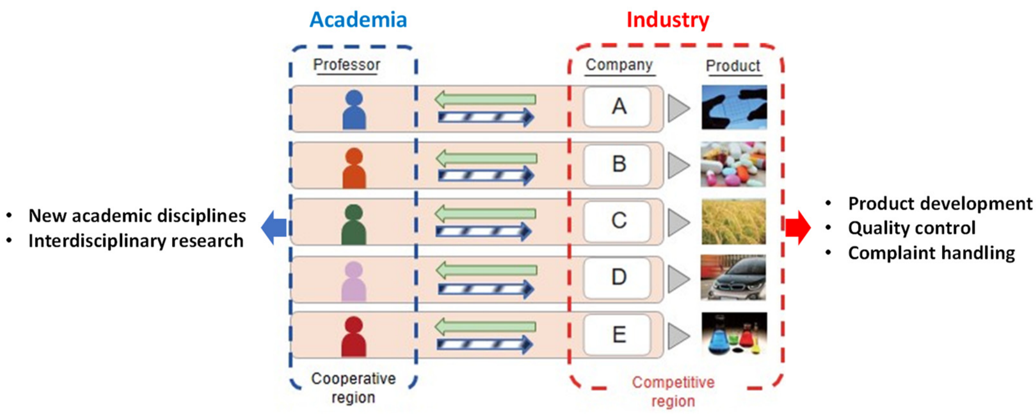

Figure 1.1 “Coalition concept”: A new industry-academic alliance scheme

The “coalition concept” is intended to be an engine to drive the business ecosystem for sustainable growth. We anticipate that a positive spiral will be created in the business ecosystem; excellent strategies and research results are recognized by society, which then attracts talented researchers to join the NGSR facility. Together with these new participants, the host community will build an advanced strategy supported by their knowledge and human resources. Thus, the NGSR facility will be core of the research complex of universities, research institutes, and companies. Tohoku university plans to build research complex “Science Park” at the Aobayama campus, in which the NGSR facility will be constructed. The “coalition concept” shall be the guiding principle of this research complex to create a “research conducting community for innovation”.

1.3 Beamlines at the NGSR facility

The beamlines at the NGSR facility are designed to satisfy the needs of the users from both industry and academia in various disciplines. 10 beamlines will be constructed as the first phase beamlines when the NGSR facility is opened. 7 beamlines will be constructed by the regional partners (Tohoku University, Miyagi Prefecture, Sendai-City, the Tohoku Economic Federation, and PhoSIC) for the use in the "coalition concept" (hereafter, called as Coalition beamlines); the remaining 3 beamlines will be built by QST for shared use (hereafter, called as Shared beamlines). The technological support for the development of the coalition beamlines is given by the International Center for Synchrotron Radiation Innovation Smart of Tohoku university. In the present report, we focus on the 7 coalition beamlines.

The cross-sectional use of 7 coalition beamlines offers the users a one-stop service to collect comprehensive data using a variety of analysis techniques in different photon energy ranges. Typically, the users have to visit different SR facilities to perform experiments using different photon energies. The 7 coalition beamlines cover the whole photon energy range of extreme ultraviolet (EUV), soft X-ray (SX), tender X-ray (TX), and hard X-ray (HX). Figure 1.2 shows the concept of cross-sectional use of 7 coalition beamlines. There are four important keywords among the coalition beamlines: multi-dimensional coherent imaging, all-element operando analysis, mail-in total materials analysis, and plug-and-play technology.

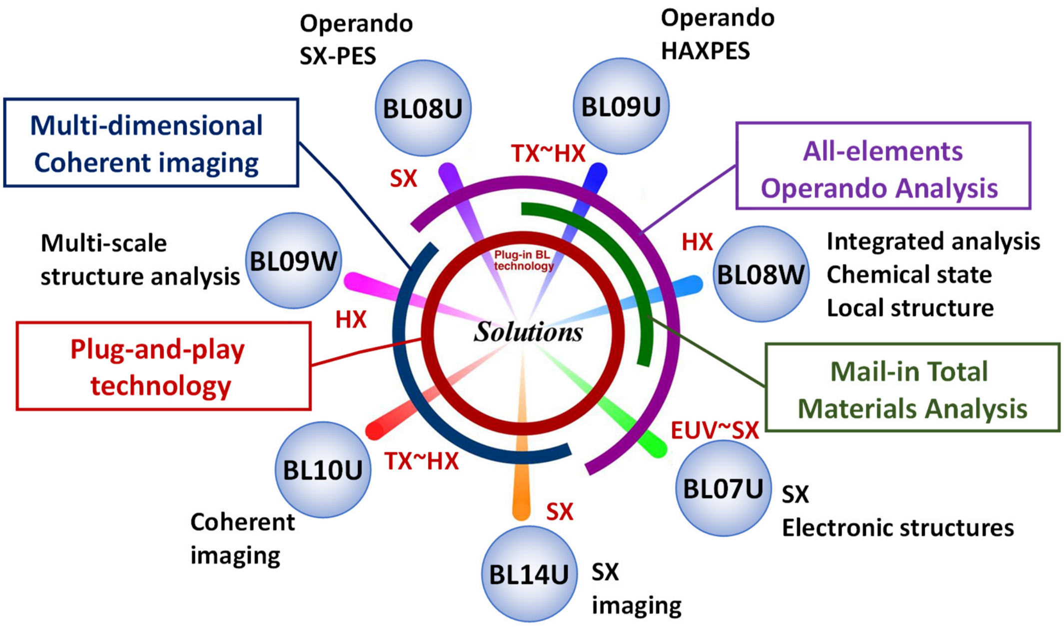

Figure 1.2 Concept of cross-sectional use of the coalition beamlines

The coalition beamlines will have two types of end-station (ES): automated measurement stations and advanced measurement stations. The automated measurement stations enable high-throughput routine measurements by making full use of robot and automation technology along with brilliant X-rays. The advanced measurement stations enable users to make customized measurements under various conditions and environments by installing their own custom-developed instruments in the end-station using a standardized plug-and-play system. Furthermore, the plug-and-play system will allow users to perform measurements utilizing multiple beamlines.

Figure 1.3 Concept of end-stations at the coalition beamlines

In order to take the best advantage of high-brilliance X-rays at the NGSR facility, X-rays beam is split into one main beamline, and one or two branch beamlines. The main beamline hosts advanced measurement stations, which make best use of high-brilliance and coherence of X-rays at the NGSR facility. In contrast, the branch beamline is equipped with automated measurement stations, in which high throughput routine measurements are performed with help of robotics and automation technology.

1.4 History

The history and current status of the NGSR facility project is briefly summarized as follows. The current status of the construction site of the NGSR facility is shown by the aerial picture in Fig. 1.4.

1) The "SLiT-J International Evaluation Committee" for the Conceptual Design Report version 2.1. (CDR 2.1) was held in June 2016 ("SLiT-J" is the former project name of the NGSR).
2) An open design competition for the SLiT-J end-stations was held in July 2017 to gather insights from the experts in Japan.

3) A general incorporation foundation, the "Photon Science Innovation Center" (PhoSIC), was established to receive investments from the private industrial sector for the SLiT-J project in December 21, 2017.
4) The SLiT-J user community was launched in January 7, 2017.
5) PhoSIC requested permission to use a part of Tohoku University's Aobayama campus for SLiT-J.
6) Deliberation on using synchrotron radiation as a source for soft X-rays and its usage began in November 2016 at the committee in MEXT.
7) MEXT initiated construction of the new 3 GeV facility on the campus of Tohoku University in July 2018.
8) The Beamline Review Committee reported the lineup candidates for the first 10 beamlines at the NGSR facility in the "Next Generation Synchrotron Radiation Facility Beamline Review Committee Report" in 2019.
9) Tohoku university has established International Center for Synchrotron Radiation Innovation Smart on October 1, 2019.

Figure 1.4 Aerial picture of the construction site of the NGSR facility as of 28-Jan-2021 (by courtesy of PhoSIC).

1.5 Aim of this report

This report aims to report the implementation plan of coalition beamlines at the NGSR facility, and have review by international experts. Following the review process, we hope to initiate the next step of the Engineering Design Process in the early stage of 2021FY.

This report is organized as follows. In Chapter 1, we introduce the current situation of synchrotron radiation facilities, and the NGSR facility and its new industry-academic alliance scheme called "Coalition concept". In Chapter 2, the brief explanation of insertion devices is given. In Chapter 3, we describe the details of the first-phase 7 coalition beamlines: Science, beamline specifications, beamline optics, and end-stations.

References

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2. Insertion device

At the NGSR facility, 5 types of insertion devices (IDs) will be adopted to cover the whole energy range from EUV to hard X-ray. The specifications of 5 standard IDs are summarized in Table 2.1.

In the region of tender X-ray and hard X-ray (photon energy above 2 keV), two types of IDs are used: in-vacuum undulator (IVU) and multipole wiggler (MPW). IVU provides highly-brilliant coherent X-ray in the photon energy range of 2 to 20 keV; MPW gives continuous white beam in the photon energy range of 2 to 30 keV.

In the region of EUV and soft X-ray (photon energy below 2 keV), APPLE-II undulators [1] and twin helical undulator (THU) are used. The big advantage of the APPLE-II undulator is the capability of polarization control; it can generate linear polarization (horizontal/vertical), and circular polarization. Two types of APPLE-II, APPLE-EUV (periodic length λ_u= 75 mm) and APPLE-SX (λ_u= 56 mm), are built to cover the different photon energy range of EUV and soft X-ray, respectively.

THU consists of two undulator segments which generate circularly-polarized X-ray with opposite helicity. The photon energy of each ID segment can be determined independently, and only one of the two segments is tuned to the photon energy of a monochromator. Therefore, the helicity of X-ray can be switched by changing the energies (undulator gaps) of two segments. This allows faster helicity switching compared to APPLE-II undulator, where the helicity is changed by the mechanical motion of magnet rows. Note that the magnets of THU are same as those for the helical mode of the APPLE-SX undulator.

Brilliances of 5 standard IDs at the NGSR facility are shown in Fig. 2.1. The brilliance was calculated using a code SPECTRA [2].

References

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Table 2.1 Specifications of insertion devices at the next-generation synchrotron radiation facility.

Name	Type of ID	# (pcs)	BL	Periodic Length (mm)	Number of Period	Max. B (T)	Max. K Value
IVU	In-vacuum undulator	2	09U 10U	22	190	1.15 (LHP)	2.36 (LHP)
MPW	Multipole Wiggler	2	08W 09W	120	5	1.91 (LHP)	16.8 (LHP)
APPLE-EUV	APPLE-II	1	07U	75	56	1.08 (LHP) 0.869 (LVP) 0.977 (CP)	7.58 (LHP) 6.09 (LVP) 4.74 (CP)
APPLE-SX	APPLE-II	1	08U	56	75	0.884 (LHP) 0.642 (LVP) 0.521 (CP)	4.62 (LHP) 3.36 (LVP) 2.72 (CP)
THU	Twin Helical Undulator	1	14U	56	35x2	0.521 (CP)	2.72 (CP)

* LHP: Linear Horizontal Polarization, LVP: Linear Vertical Polarization, CP: Circular Polarization
* The parameters in the table might be changed by the detailed design in manufacturing.

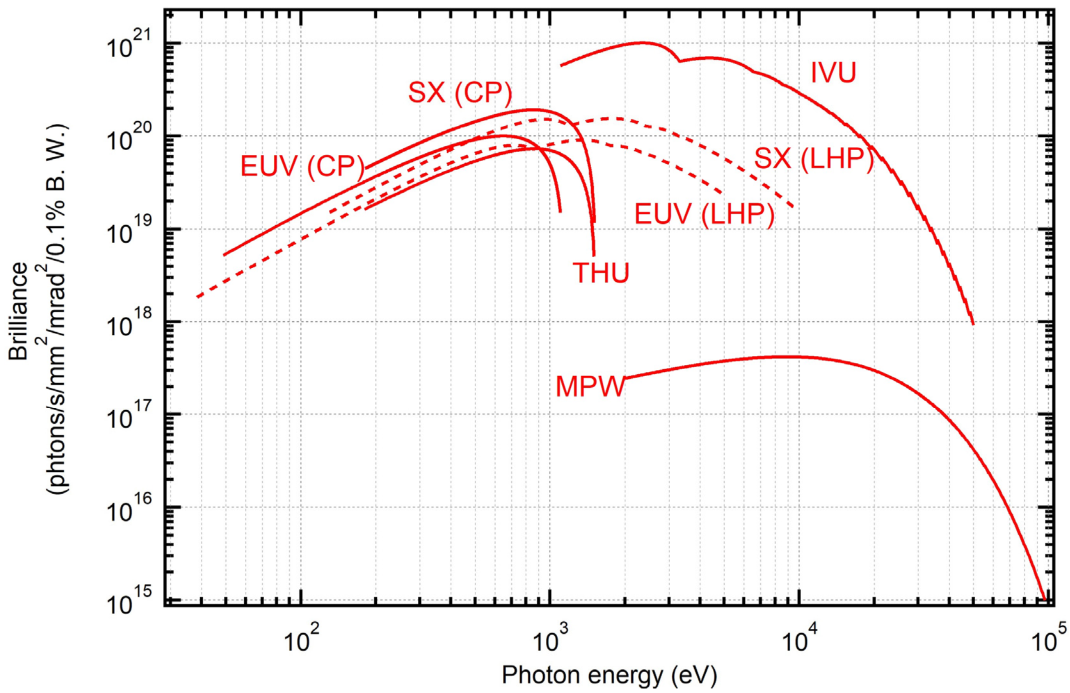

Figure 2.1 Brilliance of insertion devices at the next-generation synchrotron radiation facility

3. Beamline

3.1 Overview of beamlines

The storage ring of the NGSR facility consists of 16 unit cells, each of which has one long straight section and one short straight section. Undulators and MPWs are installed in long straight sections and short straight sections, respectively. Further details of the accelerator can be found elsewhere [1]. The maximum of 28 beamlines can be installed in the storage ring at the NGSR facility. As shown in Fig. 3.1, the beamlines are numbered in the counterclockwise direction in the storage ring. The numbering starts with the beamline located east of an injection beam transport line from a linear accelerator to the storage ring. The alphabet at the end of the beamline name (*e.g.*, BL01U and BL02W) stands for the type of ID: U is undulator, and W is MPW.

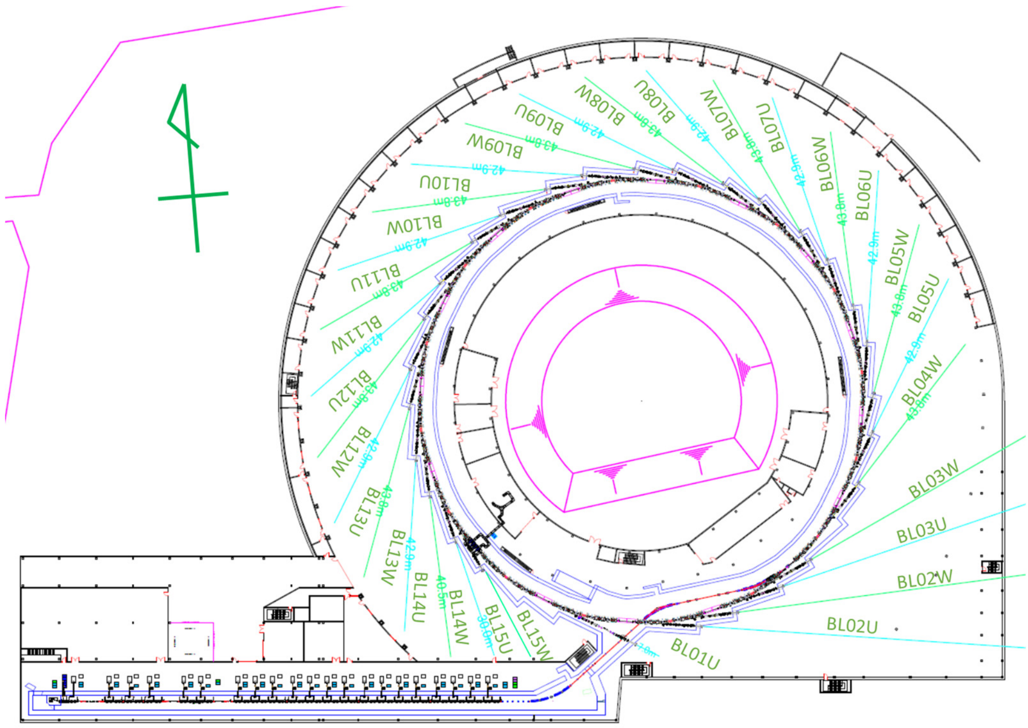

Figure 3.1 Beamline map at the NGSR facility

10 beamlines will be constructed as the first phase beamlines when the NGSR facility is opened: 7 coalition beamlines and 3 shared beamlines. The lineup of the first 10 beamline has been suggested by the QST/PhoSIC Beamline Design Committee to meet the following criteria:

1) effective use of the low-emittance light source
2) the needs of both academia and industry
3) complementary capabilities with other SR facilities in Japan.

Table 3.1 shows a list of the first 7 coalition beamlines; the type of experiments planned at the main beamlines are shown. The details of the branch beamlines will be discussed in Section 3.3.

Table3.1 List of the first 7 coalition beamlines (main beamline)

BL No.	Beamline	Type of experiments
BL07U	Soft X-ray electronic structure analysis	A. nano-photoelectron spectroscopy B. Resonant inelastic scattering spectroscopy
BL08U	Soft X-ray operando spectroscopy	A. Near-ambient pressure X-ray photoelectron spectroscopy B. Near- ambient pressure X-ray absorption fine structure
BL08W	Integrated analysis of chemical state and nano/local structure	A. X-ray absorption fine structure B. X-ray small angle scattering
BL09U	X-ray operando spectroscopy	A. Ambient pressure X-ray photoelectron spectroscopy B. Ambient pressure Extended X-ray absorption fine structure
BL09W	X-ray multiscale structure-analysis	A. Computed tomography B. Absorption/Phase contrast imaging
BL10U	X-ray coherent imaging	A. Coherent diffraction Imaging B. Ptychography
BL14U	Soft X-ray imaging	A. Magnetic imaging B. Soft X-ray Coherent diffraction Imaging

References

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3.2 Coalition beamlines

3.2.1 Soft X-ray electronic structure analysis beamline (BL07U)

3.2.1.1 Science

In the soft X-ray electronic structure analysis beamline, nano-photoelectron spectroscopy and resonant inelastic soft X-ray scattering (RIXS) are performed using high-intensity soft X-rays to visualize the electronic structure of target materials.

In the nano-photoelectron spectroscopy, a monochromatized high-intensity soft X-ray beam is focused by a focusing mirror to observe photoelectrons emitted from a target material, which enables us to analyze the valence band and composition of the "nano-interface" that determines the properties of catalysts, battery electrodes, semiconductor devices and so on. In addition, there is a high demand for the development of a beamline for direct observation of the operating state (operando observation), which is close to the actual device operating environment. As a typical example of research using nano-photoelectron spectroscopy, we can identify the cause of contact resistance in field-effect transistors (FETs) based on the chemical state change in the charge transfer region extending from the channel-metal electrode junction to about 500 nm [1]. In the GaN/AlGaN high-electron-mobility transistor (HEMT), which is expected as a next-generation high-power, high-frequency device, the cause of the "current collapse phenomenon" in which the drain current decreases from the original performance due to high voltage stress was found to be accumulation of electrons trapped at the GaN/AlGaN interface [2]. Here the operando measurement played an essential role in the observation. In the near future, in accordance with the rapid downsizing of the electronic devices, the spatial resolution for the nano-photoelectron spectroscopy should be in the order of 10 nm, which is one order better than the existing 100 nm order. It is expected to be a complementary method to surface microscopy probes such as STM, SEM, and AFM, providing pinpoint element-specific and chemical-state-specific information.

In the RIXS spectroscopy, core electron of a particular element is excited by a monochromatic soft X-ray and subsequent soft X-ray emission occurs by a radiative transition from a valence state to the excited core state. Using the angle-resolved high-energy-resolution soft X-ray spectrometer, we can obtain soft X-ray emission spectra for a series of scattering angles, which can produce an energy dispersion curve against momentum transfer of elementary excitations. In addition to the conventional use, the angle resolved experiment can provide spatial information like the size of nanoparticles or fluctuations in a liquid as observed in small angle X-ray scattering. RIXS is a photon-in and photon-out process and is most compatible with operando observation, has a high degree of freedom in the environment such as solids, liquids, and gases, can accommodate external fields, and has high bulk sensitivity (>100nm) compared to the photoelectron spectroscopy. It is expected to be a novel analytical method that strongly supports water-related science, such as foods, organisms and living organisms that contain water, aqueous solutions, water bubbles, and aqueous interface for functional materials [3,4]. The advantage of high-efficiency measurement makes it possible to perform RIXS measurements under various conditions such as concentration, temperature, external field and so on, which was difficult in the present system due to beamtime constraints.

3.2.1.2 Specifications

The performance of the beamline is summarized in Table 3.2. An APPLE-II EUV undulator will be installed in the long straight section. For the first order light, it is capable of generating light from 50 to 1000 eV (EUV to soft X-rays) with a sufficient flux of 10^{15} photons/sec/0.1% BW. For the use of nano-photoelectron spectroscopy, an energy resolution better than 50 meV can be achieved at 1000 eV. For RIXS, the energy resolution on the source side is set to E/ΔE ~10,000-30,000 in order to surpass the conventional standard resolution E/ΔE ~ 10,000 (the combined energy resolution of the source and spectrometer). The flux on the sample is estimated to be on the order of 10^{13} photons/sec. The beam size on the sample is 50 nm by using a Walter-type focusing mirror, which is characterized by its high transmission efficiency and the fixed focal position over a wide energy range. Although the flux on the sample is

Table 3.2 Beamline specifications

Beamline	Soft X-ray electronic structure analysis
Insertion device	APPLE-II type undulator (APPLE-EUV：75 mm×56 periods)
Photon energy range	50 ~ 1000 eV
Energy resolution（E/ΔE）	10,000 ~ 30,000
Polarization	Horizontal linear polarization (100 ~ 1000 eV) Vertical linear polarization (100 ~ 1000 eV) Right & left circular polarization (50 ~ 1000 eV)
Photon flux (20 m from the light source, 1×1 mm^2 slit)	~10^{15} photons/sec/0.1%BW
Spot size @ sample	50 nm ~ 10 μm@1000 eV

reduced by around half due to the reflection efficiency of the mirror, the obtained EUV and soft X-ray intensity is sufficient for the measurement.

3.2.1.3 Beamline optics

The configuration of this beamline is shown in Fig. 3.2. After being reflected horizontally by the cylindrical mirror M0 to reduce the heat load, the incident light is led to the entrance slit S1 to determine the virtual source size and improve the energy resolution. A curved cylindrical mirror M1 converges the light in the vertical direction, and a plane mirror M2 vertically reflects the light toward the grating, where it is monochromatized by a variable line spacing diffraction grating, which is often used in the EUV and soft X-ray region, and the light of the required wavelength is extracted by the exit slit S2. A soft X-ray chopper, which can extract the necessary bunches from the pulse train of the SR beam, is optionally inserted before the exit slit to enable time-resolved measurements using a single bunch and/or measurements of biological samples and catalysts that are susceptible to irradiation damage. The monochromatic light through the exit slit is directed to the tandemly aligned nano-photoelectron spectroscopy and RIXS endstations. When the RIXS station is used, the sample holder of the upstream nano-photoelectron spectroscopy station is retracted to pass the beam to the RIXS station. The focusing mirror placed just before each end-station is planned to be a Walter-type focusing mirror that can be easily adjusted and can be retracted when it is not in use.

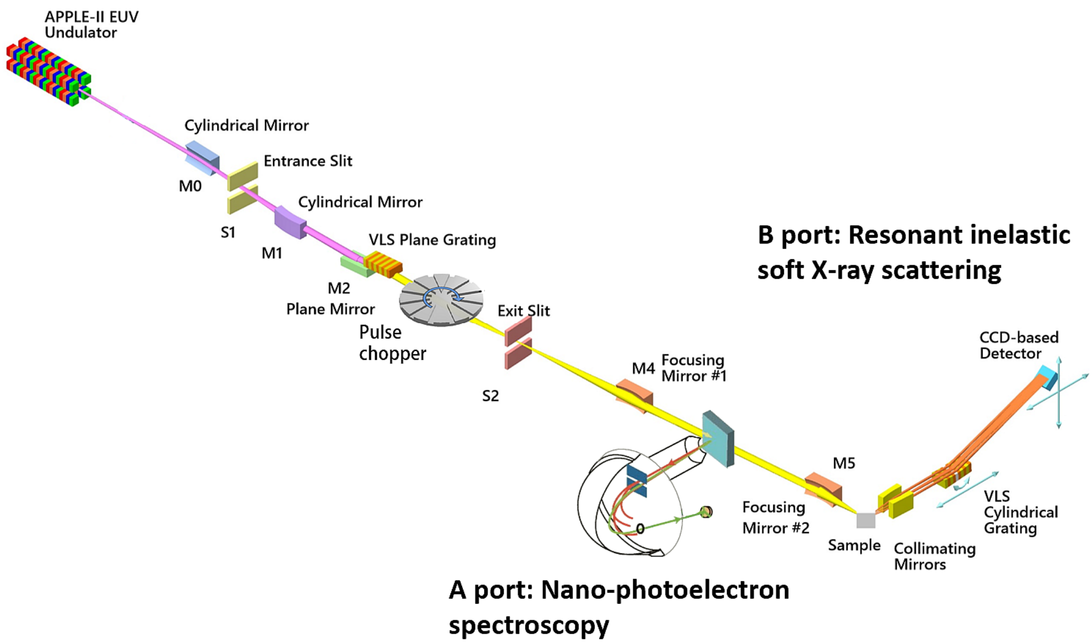

Figure 3.2 Overview of soft X-ray electronic structure analysis beamline (BL07U)

3.2.1.4 End-station

3.2.1.4.1 A port: Nano-photoelectron spectroscopy station

An overview of the nano-photoelectron spectroscopy system is shown in Fig. 3.3. Monochromatized EUV/soft X-ray beam is focused on a sample at φ50-100 nm, and the emitted photoelectrons are detected by an energy-dispersive and angle-dispersive electron analyzer. This enables not only angle-resolved photoemission spectroscopy of conventional and small-sized (< 1μm diameter) single-crystal samples, but also depth-resolved measurements of devices and buried interfaces down to around 3 nm. The sample can be scanned by a piezo-driven x-y stage, which enables two-dimensional mapping of photoelectrons. The system is equipped with a sample exchange mechanism and electrodes as well as a multi-probe head for operando measurements. A spatial resolution of 50 nm both in horizontal and vertical direction will be achieved by using the Walter-type focusing mirror. Thanks to the high photon flux of the incident beam and the high transmission of the focusing optics, it is possible to conduct both combinatorial mode experiments where measurements are made under various (operando) conditions, and the other mode where two-dimensional mapping measurements with high spatial resolution (φ50 nm) are made over a large area of the sample. In addition, the high energy resolution of the incident beam will enable detailed electronic structure analysis.

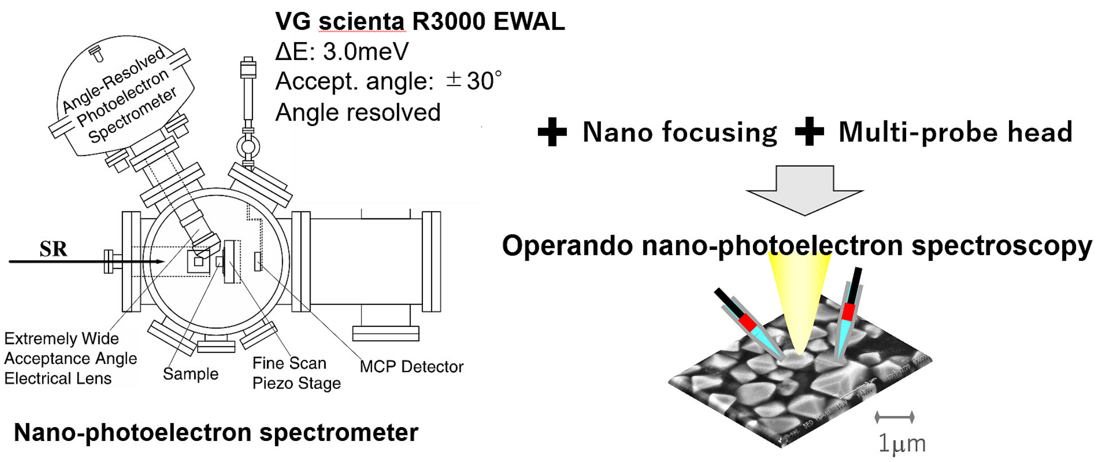

Figure 3.3 Schematic diagram of the nano-photoelectron spectrometer.

3.2.1.4.2 B port: Resonant inelastic soft X-ray scattering station

An overview of the resonant inelastic soft X-ray scattering measurement system is shown in Table 3.3 and Fig. 3.4. The system is equipped with an angle-resolved soft X-ray emission spectrometer with a 2.5 m arm from the sample to the detector that includes three valid-line-spacing gratings with an improved slope-error for broadband spectroscopy in the range of 50-1000 eV and high spatial resolution soft X-ray CCD detector with its resolution better than 5 μm. Combining the soft X-ray spectrometer with the state-of-the-art Walter-type mirror that can focus the incident beam smaller than φ 0.5 μm on the sample, the total energy resolution will be E/ΔE~20,000 (26 meV @ O 1s edge). Depending on the irradiation damage the focus size can be tuned from 0.5 μm to 5 μm. RIXS is one of the spectroscopic methods that requires the highest incident photon flux. To avoid the irradiation damage of fragile samples, we will develop and introduce an operando spectroscopy system (temperature, humidity, electric field, magnetic field, etc.) that enables fast sample position scanning and/or liquid jet system with total sample recovery. According to requests from users and by scientific needs, the system will be upgraded to accommodate real ambient pressure measurement without window materials but with differential pumping.

Table 3.3 Specifications of Resonant inelastic soft X-ray scattering equipment

Photon energy range	50～1000 eV
Total Energy resolution（E/ΔE）	10,000～20,000
Spot size @ sample	500 nm～5 μm
Temperature range	6～500 K
Scattering angle range & angular resolution	45～135° & 0.1°

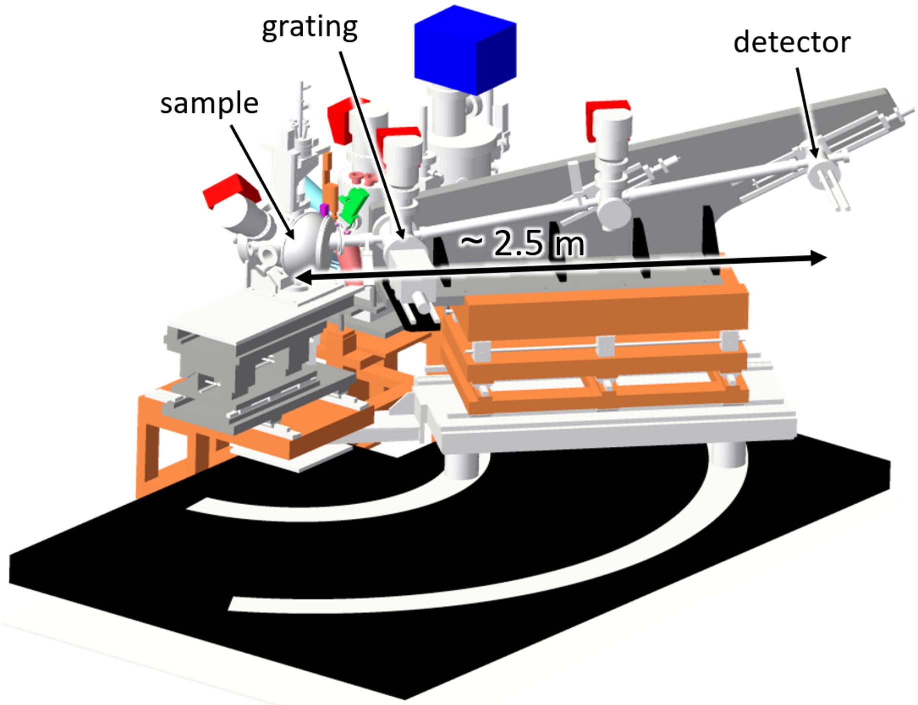

Figure 3.4 Schematic diagram of a high-efficiency, high-resolution RIXS station.

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3.2.2 Soft X-ray operando spectroscopy beamline (BL08U)

3.2.2.1 Science

Soft X-ray spectroscopies, such as photoemission or absorption, have been used to investigate electronic states in matters. Recently, there have been needs to directly trace them in materials during operation and to unveil their functionalities. Such experiments, so-called "operando observation", have been developed vigorously in both academic and industrial fields. Giving an example of catalytic reaction, operando observation with soft X-ray beam has an advantage to probe in situ chemical states of both heavy metal atoms in catalysts and light elements, such as C, N. and O, in reacting molecules. The technique allows us to understand the whole picture of the reaction.

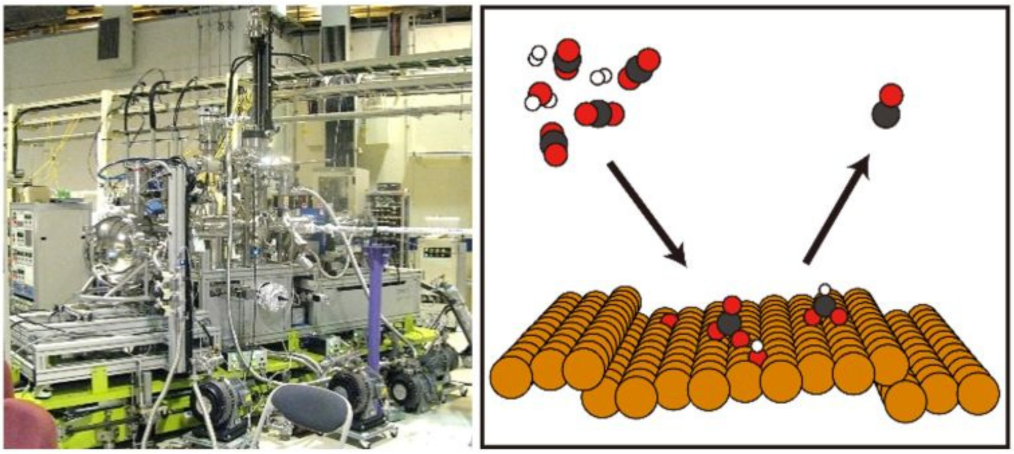

Figure 3.5 AP-XPS system and science at soft X-ray operando spectroscopy [1,2]

The soft X-ray operando beamline, BL08U, offers advanced instrumentation of Ambient Pressure X-ray Photoelectron Spectroscopy, AP-XPS. The beamline is designed primarily for operando chemical analysis of interfaces/surfaces under reaction or working conditions and it is aimed to reveal the detailed mechanisms. Research at the beamline covers catalysts, battery, and bio-materials, for examples. Measurements of AP-XPS allow users to examine chemical states of their samples with element selectivity, with precise quantitative evaluation, and under the actual environments. Gas pressure in AP-XPS will reach 1 atm (760 Torr), which is large enough to link gas pressure of reaction experiments in users' laboratories. These instruments at the beamline make it possible to track varieties of catalytic reactions, such as methanol synthesis on CuZn, that have not been realized in conventional systems of near-ambient pressures XPS (NAP-XPS), typically at 1-20 Torr. In addition, the beamline will be also equipped with nano-beam optics to spatially visualize chemical states or to track local functions in non-uniform samples. The beamline BL08U will be a research base to examine energy materials to sustain our societies and also to be a platform to study cutting-edge nanomaterials, such as nanopatterned catalysts.

3.2.2.2 Specifications

Table 3.4 Beamline specifications

Beamline	Soft X-ray Operando Spectroscopy
Insertion device	APPLE-II undulator （APPLE-SX：56 mm×75 periods）
Photon energy range	130～2,000 eV
Energy resolution（E/ΔE）	> 10,000
Polarization	Horizontal linear polarization（130～2000 eV） Vertical linear polarization（230～2000 eV） Right & left circular polarization（180～1400 eV）
Photon flux @ sample	>1×10^{12} photons/sec/0.01%BW
Spot size @ sample	50 nm～3 µm

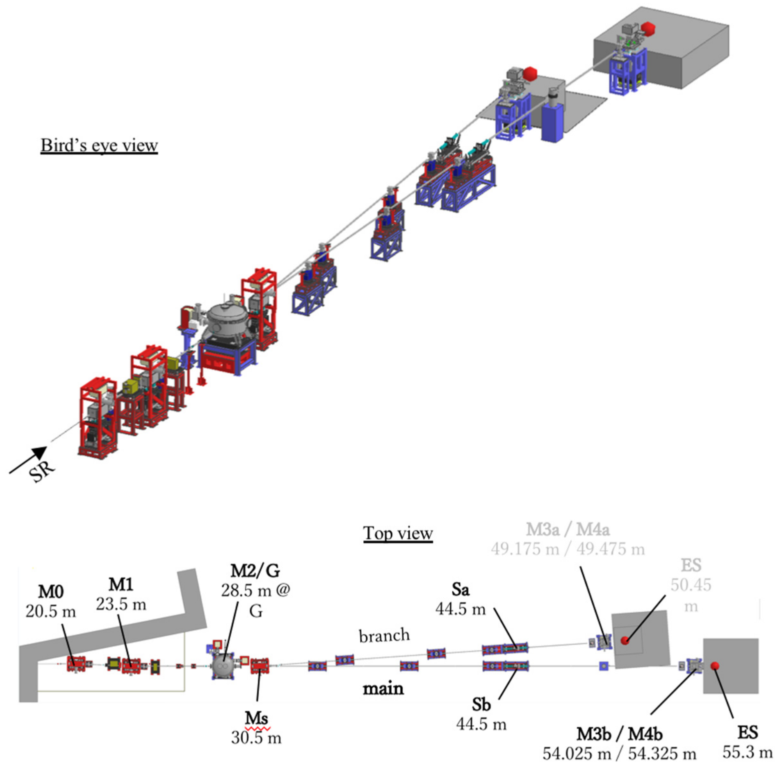

Figure 3.6 Overview of soft X-ray operando spectroscopy beamline (BL08U). M and G stands for a mirror and a grating, respectively, while S represents a slit. The main and branch beamlines are individually installed with end stations (ES's).

3.2.2.3 Beamline optics

The beamline BL08U employs an entrance-slitless variable-included-angle Monk–Gillieson mounting monochromator with a varied-line-spacing plane grating (G), as shown in Fig. 3.6. Two types of the diffraction gratings, graving densities of 600 lines/mm and 1200 line/mm, will be installed. The entrance-slitless layout effectively restricts the magnification of the monochromator and facilitates high transmission. Beam focusing will be operated with a combination of a KB mirror and a Wolter mirror. A soft X-ray beam will be divided into the main and branch beamlines by a mirror (Ms) at the downstream of the grating.

3.2.2.4 Endstation

A soft X-ray AP-XPS system will be installed at the main beamline. The instrument is equipped with a mass spectrometer and with an electron analyzer that has a multi-differential pumping unit in the electrostatic lens. The system will allow users to make measurement of AP-XPS as well as AP-NEXAFS (Near-edge X-ray absorption fine structure) in the gas pressure, tuned up to 1 atm. Nanobeam with a beam size of 50 nm will also be ready at the station.

In the branch beamline, we plan to install a measurement system of XPS and NEXAFS that makes remote experiments by users or automatic measurements of mail-in samples.

References

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3.2.3 Integrated analysis of chemical state and nano/local structure beamline (BL08W)

3.2.3.1 Science

Integrated analysis of chemical state and nano/local structure beamline (BL08W) can obtain information on the chemical state and the structure using X-rays of 2.1 to 17.4 keV. The main beamline aims for X-ray absorption fine structure (XAFS) and Small-Angle X-ray Scattering (SAXS) measurements using X-rays from 2.1 to 13 keV. In XAFS measurement, the electronic structure (valence, chemical species) and coordination structure of the specific element can be analyzed from the spectrum near the absorption edge (X-ray absorption near-edge structure: XANES). Furthermore, information on the local structure (interatomic distance, coordination number) around a specific element can be analyzed from the region away from the absorption edge (extended X-ray absorption fine structure: EXAFS). On the other hand, SAXS measurement can obtain information on nanoscale density difference in a sample, which means the structure of scatters (size, shape, distribution, higher-order structure, surface structure) from several nm to several hundred nm. This beamline uses complementarily these measurement methods to evaluate the correlation between changes in the electronic structure of specific atoms and macroscopic structural changes under dynamic conditions in polymers, metals, battery materials, etc. (Figure 3.7).

In this beamline, since continuous energy scanning can be easily performed with energies lower than 3.5 keV, the K-edges of phosphorus and sulfur and the L-edge of palladium, which play important roles in functional materials and biomaterials, are the objects of measurements. Furthermore, dynamic anomalous small-angle X-ray scattering (ASAXS) using the anomalous effect in near absorption edge can visualize the time-space distribution of specific atoms.

The use of this beamline in combination with the X-ray operando spectroscopic beamline (BL09U), X-ray multiscale structure-analysis beamline (BL09W), and X-ray coherent imaging beamline (BL10U) advance hierarchical structure analysis, which is important for materials science and engineering. Besides, two branch beamlines for multipurpose X-ray diffraction and general-purpose SAXS measurement will be prepared by taking advantage of the wide beam in the horizontal direction from MPW. The flux of the branch beamlines is larger than that of the SPring-8 bending magnet beamline. Furthermore, we are planning to introduce soft X-rays from the adjacent soft X-ray operando spectroscopic beamline (BL08U) into this beamline and build a system that irradiates the sample with both soft X-rays and hard X-rays as the next phase development in the future.

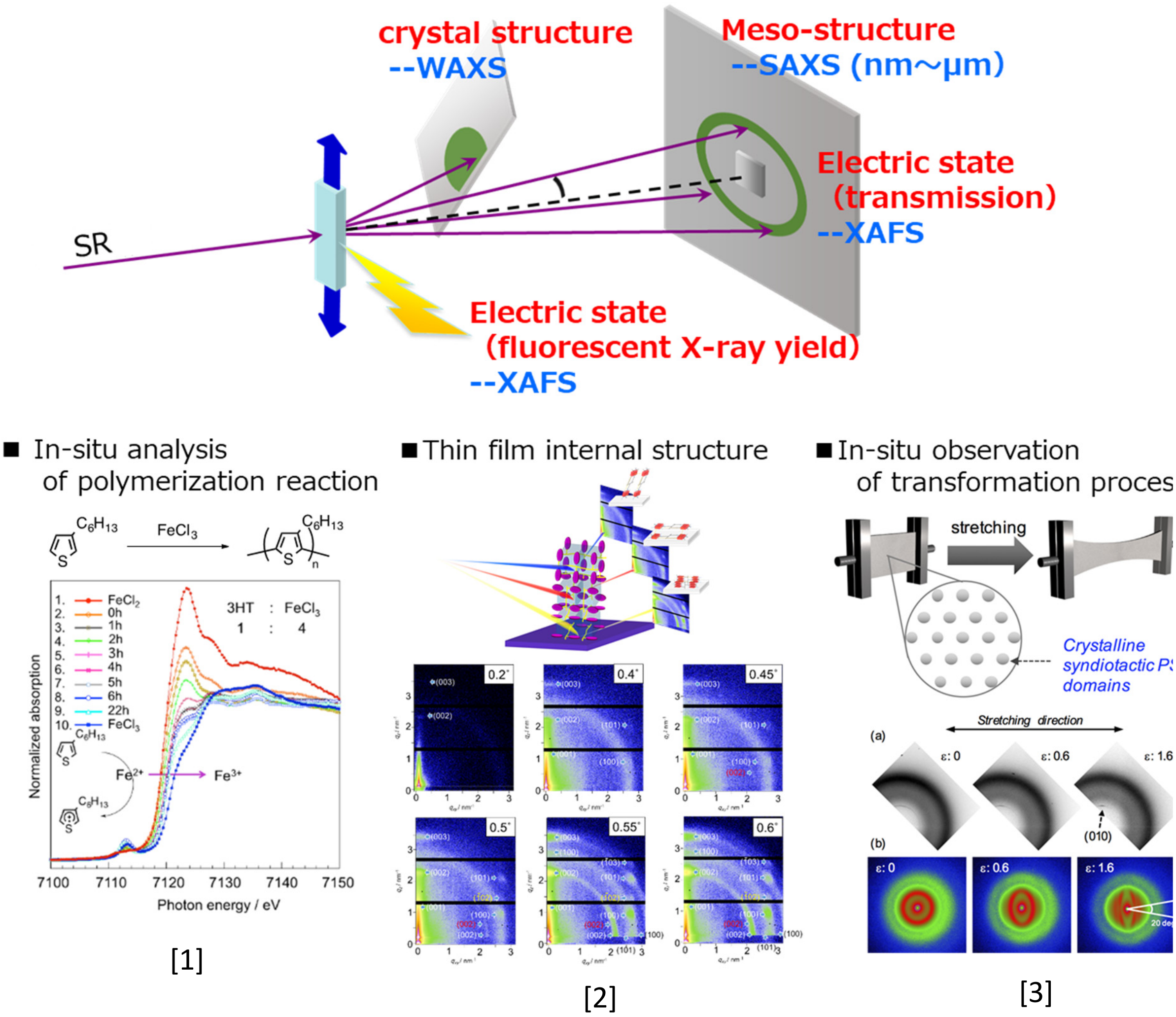

Figure 3.7 Measurement methods for the beamline and applications [1-3].

3.2.3.2 Specifications

Table 3.5 Beamline specifications

Beamline	Integrated analysis of chemical state and nano/local structure
Insertion device	MPW (120 mm×5 periods)
Photon energy range	Master beamline: 2.1～13 keV Branch beamline: 8～17.4 keV
Energy resolution（E/ΔE）	1,600~13,000
Polarization	Horizontal linear polarization
Photon flux (20 m from the light source, 1×1 mm^2 aperture)	2×10^{11}～2×10^{12} photons/sec/0.1% b.w.
Spot size @ sample	150 μm×50 μm

3.2.3.3 Beamline optics

Figure 3.8 shows the bird's eye and top views of the Integrated analysis of chemical state and nano/local structure beamline. The beam emitted from the MPW is incident on the Si (111) double crystal monochromator (DCM), and an X-ray beam of arbitrary energy reflected from the energy range of 2.1 to 13 keV is emitted at a fixed position. The chamber of the DCM will be miniaturized by setting the offset distance between the optical axes of the incident X-ray beam and the outgoing X-ray beam to 50 mm and limiting the upper limit of the energy used to 13 keV. A toroidal mirror coated with Pt is installed downstream of DCM so that two-dimensional focusing of 150 μm in horizontal and 50 μm in vertical can be achieved at the focal point at 45 m from the light source. In the upstream area of the experimental hatch, boron carbide (B_4C), Ni-coated, and Pt-coated plane mirrors are installed and can be used to remove higher harmonics.

3.2.3.4 Endstation

The size of the experimental hatch of the master beamline is 4 m in width × 12.5 m in length × 4 m in height. An optical bench (1.5 m in width and 3 m in length) for installing a sample stage, detector, exposure shutter, absorbers will be installed in the middle area of the experimental hatch. Besides, slits for reducing parasitic scattering can be installed where needed. When conducting SAXS measurements, the sample is placed in a vacuum chamber and the chamber is connected to the detector by a vacuum path.

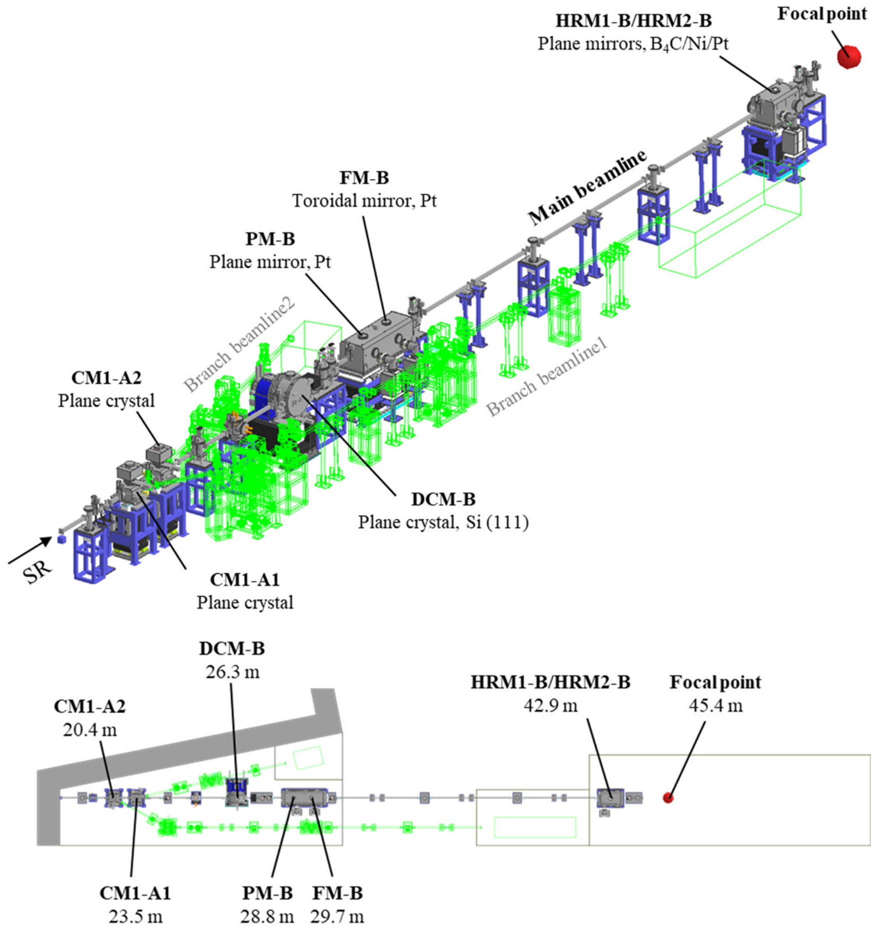

Figure 3.8 Overview of integrated analysis of chemical state and nano/local structure beamline (BL08W)

SAXS measurements up to a camera length of 13 m can be performed in the main beamline. The light path from the sample to the detector positions is connected with a vacuum pipe. Assuming that the energy used is 6 keV, the *q* range that can be covered is 10^{-3} nm^{-1} at the camera length of 13 m. Furthermore, the main beamline is supposed in situ SAXS measurement using a large apparatus provided by the user.

XAFS measurements can be conducted by the conversion electron yield method, fluorescent X-ray yield method, and transmission method. The time resolution during XAFS measurement is 10 s. Furthermore, the measurement arrangement for transmission mode allows simultaneous measurements of XAFS and SAXS on the same sample. When conducting XAFS and SAXS measurements at the energy of less than 4 keV or less, it is necessary to replace the sample surroundings with a vacuum (for solids) or He atmosphere (for solutions) to suppress the effect of decreased transmissivity of X-rays due to the atmosphere.

A high-temperature furnace and a cooling/heating stage can be attached to the sample stage on the optical bench placed in the experimental hatch, and operando/in situ observation can be conducted both XAFS and SAXS under variable temperature conditions. Gas supply equipment will be installed to enable measurements under reaction conditions. In addition, the downstream of the experimental hatch can be equipped with a user-carrying device up to 1.5 m in width and 2 m in length.

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3.2.4 X-ray operando spectroscopy beamline (BL09U)

3.2.4.1 Science

X-ray operando spectroscopy beamline (BL09U) is a beamline in which the bulk electronic structure and geometric structure of materials can be studied by hard X-rays with a bulk sensitivity. More specifically, hard X-ray Photoemission Spectroscopy (HAXPES) and X-ray absorption fine structure (XAFS) spectroscopy will be used to investigate the bulk electronic structures and geometric structure of materials under operando conditions.

Utilizing the high brilliance of IVU undulator, the XAFS system will allow measuring trace elements, 2D scanning microscopy XAFS with a spatial resolution of 100 nm, and quick XAFS (QXAFS). The HAXPES system will start with measurements in high vacuum, and will be upgraded to measurements under atmospheric pressure (Ambient pressure HAXPES, AP-HAXPES). This beamline will be able to visualize reactions in a wide range of materials, which include catalysts, batteries, power devices, steels, and biomaterials.

By the complementary use of soft X-ray operando spectroscopy beamline (BL08U), one can obtain information on the electronic structure and structure from the surface to the bulk.

3.2.4.2 Specifications

Table 3.6 Beamline specifications

Beamline	X-ray operando spectroscopy
Insertion device	IVU（22 mm×190 periods）
Photon energy	6 keV（HAXPES, AP-HAXPES） 2.1 ~ 15 keV（XAFS）
Energy resolution（E/ΔE）	> 20,000 @6 keV（HAXPES、AP-HAXPES） >5,000（XAFS）
Polarization	Horizontal linear polarization（2.1 ~ 15 keV）
Photon flux @ sample	~7×10^{12} photons/sec (E/ΔE > 20,000, spot size 6.0 μm (H) × 0.2 μm (V), 6 keV) ~1.5×10^{11} photons/sec (E/ΔE > 20,000, spot size 0.16 μm (H) × 0.2 μm (V), 6 keV)
Spot size @ sample	100 nm ~ 10 μm @ 6 keV（HAXPES, AP-HAXPES） 100 nm @ 8 keV（XAFS）

3.2.4.3 Beamline optics

Figure 3.9 shows an overview of this beamline. Brilliant hard X-rays from the IVU are first monochromatized by the Si(111) double crystal monochromator (DCM) in the optical hutch. A high-precision 4-way slit (4WS), placed at the downstream of the optical hutch, controls the size of the X-ray beam, which works as a virtual source of X-ray nano-focusing optics. In the experimental hutch, high-reflection mirrors (HRM), channel-cut monochromator (CCM), and X-ray nano-focusing optics are installed. High-order X-rays can be cut off by choosing the coating materials of HRM. The CCM is used for HAXPES experiments that require higher energy resolution; for XAFS experiments, the CCM is not used and retracted from the beam path. The energy resolving power E/ΔE of > 20,000 can be achieved by using DCM (Si(111)) and CCM (Si(311)). The X-ray nano-focusing optics consists of KB mirrors. In order to achieve the beam size of 100 nm at a sample position, the size of the virtual source needs to be reduced to ~10 μm by the 4WS at the sacrifice of photon flux.

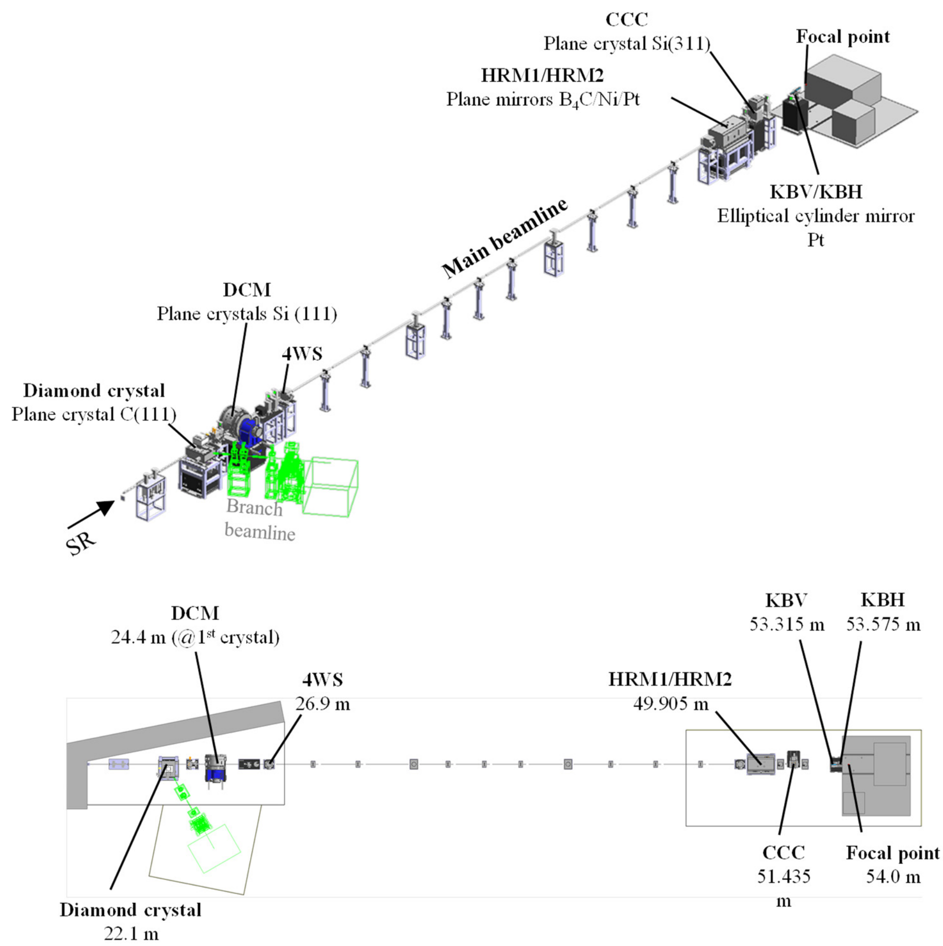

Figure 3.9 Overview of X-ray *operando* spectroscopy beamline (BL09U)

3.2.4.4 Endstation

There are two endstations in the experimental hutch: HAXPES and XAFS endstations. At the HAXPES endstation, the HAXPES measurements in high vacuum are allowed at the start-up phase; the upgrade of the system by introducing a differentially-pumped electron analyzer will enable the HAXPES measurements in a gas atmosphere above atmospheric pressure. The HAXPES system is designed to be movable with respect to a focal point of KB mirrors so that the beam size can be adjusted, and the beam size can be optimized for each sample to avoid beam damage. At the XAFS endstation, one can perform 2D scanning microscopy XAFS using the focused X-ray beam with a spatial resolution of 100 nm. In addition, the temporal resolution of s~ms in EAXAFS measurements will be achieved by QXAFS. Note that these two endstations can be switched against the same focal point of X-rays.

3.2.5 X-ray multiscale structure-analysis beamline (BL09W)

3.2.5.1 Science

The MPW source of the NGSR facility can provide an X-ray beam having features that cannot be attained at existing SR facilities in Japan, which have potential to develop a new science frontier in the scheme of coalition concept. The beam has a large area, a wide bandwidth, and a flux that cannot be achieved with a bending magnet source at SPring-8 for X-ray energies less than 30 keV. The X-ray multiscale structure-analysis beamline (BL09W) takes advantage of these features to realize sub µs temporal-resolution X-ray imaging, sub ms temporal-resolution X-ray tomography (high-speed-rotation [1] and multi-beam X-ray tomographies [2]), ms temporal-resolution dispersive XAFS (DXAFS), and dispersive surface X-ray diffraction

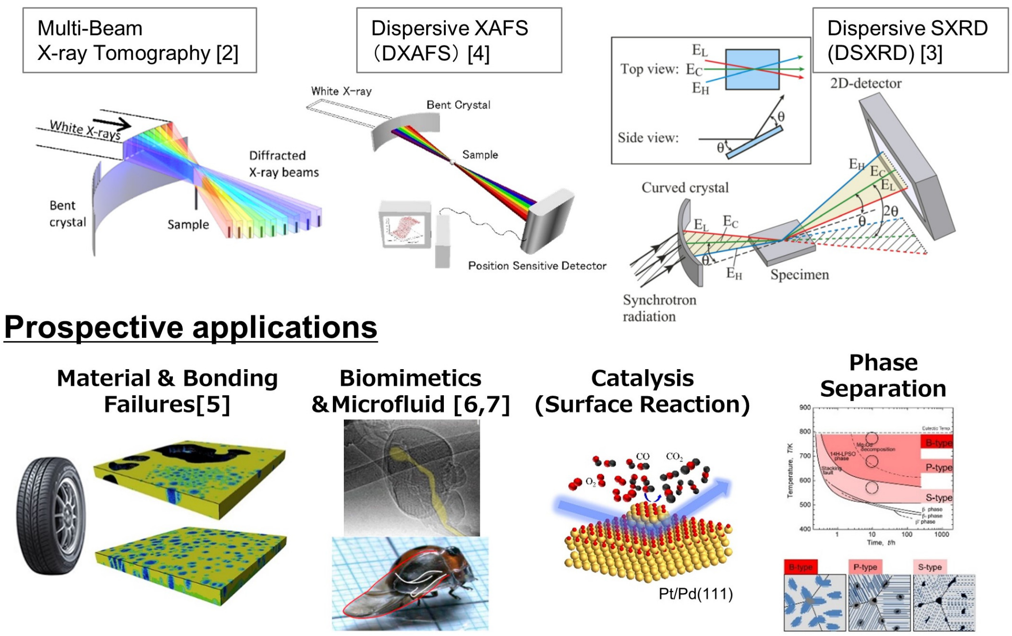

Figure 3.10 Measurement methods and their prospective applications.

Table 3.7 Specifications of measurement methods and perspective applications.

Methods	Max. time resolution	Spatial Resolution (μm)	Application examples
X-ray imaging	0.1 μs	0.2～20	Material & bonding failures Biomimetics Microfluidics Phase separation
X-ray tomography	0.1 ms	0.2～20	
Dispersive XAFS	1 ms	10	Catalytic reaction
Dispersive SXRD	1 ms	10	Surface reaction
X-ray diffraction			Inorganic materials Organic materials Practical materials
Residual stress measurement		50	Practical materials
Fluorescent X-ray imaging		50	Agricultural & marine products Practical materials cultural properties
X-ray fluorescence holography		50	Single crystalline (short- and middle-range-order structure)

(DSXRD [3]) that can make it possible to realize in-vivo, in-situ, and operando observation of dynamic phenomena with high temporal resolutions and high throughputs. By complementarily using other BLs such as the integrated analysis of chemical state and nano/local structure beamline (BL08W) and the X-ray coherent imaging beamline (BL10U), it will unveil unprecedented spatiotemporal region in materials and life sciences.

In addition, the wide beam in the horizontal direction enables us to install two other branch beamlines, where general-purpose X-ray diffraction experiments (powder, single-crystalline, thin-film, multilayer-film structure analysis, and residual stress measurement) can be performed with a larger flux than that of the bending magnet beamlines in SPring-8. Furthermore, in the future, an optionally insertable two-dimensional focusing mirror will make it possible to realize scanning residual stress measurement, scanning fluorescent X-ray imaging, and X-ray fluorescence holography, which are important for industrial applications. Figure 3.10 and Table 3.7 summarize the measurement methods (specs) and their perspective applications realized at BL09W.

3.2.5.2 Specifications

Table 3.8 Beamline specifications

Beamline	X-ray multiscale structure analysis
Insertion device	MPW (120 mm×5 periods)
Photon energy range	5～30 keV
Energy resolution（E/ΔE）	～1 (white beam)
Polarization	Horizontal polarization
Photon flux @ sample	2×10^{11}～2×10^{12} photons/sec/0.1%BW
Spot size @ sample	Non-focusing ： 50 mm (horizontal)×5 mm (vertical) (50 m position from the source) Focusing：50 μm×50 μm (55 m position from the source)

3.2.5.3 Beamline optics

Figure 3.11 shows an overview of this beamline. A large area beam from MPW is reflected by a water-cooled planar mirror HRM-B (low energy-pass filter) for the main endstation. The planar mirror is Pt-coated and used at glancing angles ranging from 3 to 8 mrad, corresponding to maximum energies of the reflected X-ray beam, approximately, from 10 to 30 keV. A vertical offset of 15 mm for the reflected beam is kept for a gamma stopper (GS) located downstream of the mirror. The mirror enables us not only to control of the spectrum of the reflected beam for the white X-ray imaging experiments but also to effectively suppress higher harmonics in the experiments of monochromatic X-ray imaging and DXAFS. The lower limit of the X-ray energy (5 keV) is determined by the absorption by the water-cooled beryllium windows for the vacuum beam path to the main endstation. Note that the L absorption edges of Pt makes it difficult to perform DXAFS experiments from 10 to 15 keV. It is therefore desired that the mirror has Pt and Rh-coated areas with a stripe shape and they are switchable by a translational stage. In addition, it will

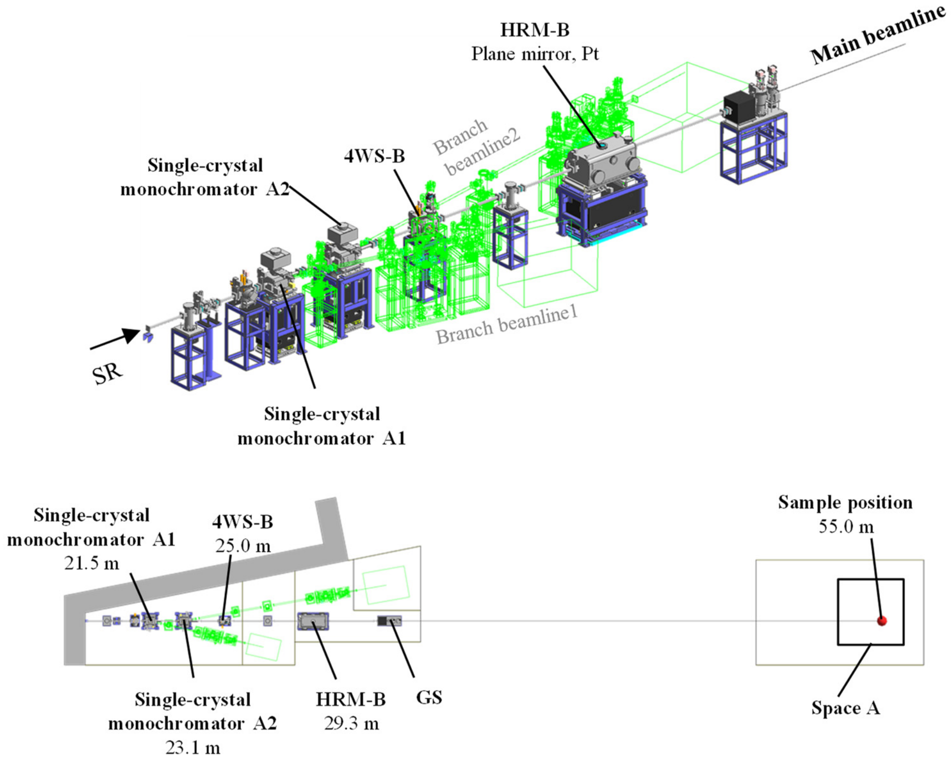

Figure 3.11 Overview of X-ray multiscale structure-analysis beamline (BL09W)

be possible in the future to optionally replace the mirror with a Pt-coated toroidal focusing mirror which provides a two-dimensionally focused beam with a size of 50 μm (1: 1 focusing) at a position 55 m from the source.

3.2.5.4 Endstation

In the main endstation, experiments of monochromatic and white X-ray imaging, DXAFS, and DSXRD will be implemented for increasing demand of high-speed and/or high-throughput measurements. Monochromatic X-ray imaging can be performed using a channel-cut crystal, while DXAFS and DSXRD can be done using a polychrometer. Both the channel-cut crystal and polychrometer will be installed on an optical table in the upstream side of the endstation. In its downstream side, a large area space (space A) is kept for user's apparatuses with a size up to a 3 m x 3 m area and a 3.5 m height to perform these measurements. A high-speed rotation of a sample in the user's apparatus allows for up to sub ms temporal-resolution X-ray tomography. A multi-beam imaging system [2] can also be installed in this space. The latter will make it possible to realize sub ms temporal-resolution 4D X-ray tomography without rotation of a sample, and therefore enables us not only to observe living creatures and deformable materials (e.g., liquid, viscoelastic materials) but also to introduce a complicated environment around a sample. Because such a 4D X-ray tomography measurement is normally completed in a few seconds, it is desired that an automatic sample changer is installed in the endstation, which can contribute to effective manpower management and high-throughput measurements. The shutter and absorber at the entrance of the endstation should have a sufficiently high response speed to reduce radiation damage of the samples in the high-speed and/or high-throughput measurements. Note that highly sensitive and quantitative X-ray phase-contrast imaging is also possible by an X-ray grating interferometer, which can be easily installed in both upstream and downstream sides of the endstation. The multimodality of this X-ray grating interferometry is also worth being noted. It provides three independent images: absorption, phase-contrast, and small-angle-X-ray-scattering (SAXS)-contrast images. The former two can makes it possible to realize element-selective X-ray tomography, while the latter can provide information on unresolvable microstructures.

After installing the toroidal focusing mirror, scanning residual stress measurement, fluorescent X-ray imaging, and X-ray fluorescence holography will be possible with the two-dimensionally focused beam with a size of 50 μm at the position 55 m from the source. In these measurements, samples are located on a diffractometer in the space A.

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3.2.6 X-ray coherent imaging beamline (BL10U)

3.2.6.1. Science

Coherent X-ray imaging, such as coherent diffraction imaging and ptychography, can provide imaging with high spatial resolution at the nanoscale. These methods allow us to quantitatively visualize the spatial distribution of electron density and lattice distortion of a sample by capturing them as phase shift of X-rays. In other words, coherent X-ray imaging is an extremely useful imaging technique for visualizing the spatial distribution of microstructures at the mesoscale, which lies between the atomic and macroscopic scales. In this beamline (BL10U), meso-scale structure visualization by coherent X-ray imaging [1] is the cornerstone, and local atomic imaging by X-ray fluorescence holography [2], holotomography [3], and full-field imaging by imaging microscopy [4] are used in a complementary manner to seamlessly visualize structures from atoms to sub-millimeters. In addition, a variety of information on elements and chemical states is obtained by combining scanning X-ray fluorescence microscopy for mapping trace elements [5] and X-ray absorption spectroscopy [6, 7] (Fig 3.12).

Many functional materials have spatial hierarchical structures ranging from atomic to macro scales, and the mesoscale microstructures formed by various processing techniques are heterogeneous and are the source of functional expression. On the other hand, in living organisms, the mesoscale is also a spatial scale dominated by higher-order structures of biological macromolecules and cellular organelles, and its visualization is essential for understanding cellular functions [8]. The use of this beamline will enable us to pioneer materials science and biology at the mesoscale. In addition, the imaging technology provided by this beamline is expected to be applied not only to academia but also to industry. For example, solving various manufacturing problems in industry, such as the cross-linked heterogeneous structure of tire rubber, the elution and decomposition process of platinum catalysts in fuel cells, and the diffusion path of lithium ions in the cathode active material of storage batteries, is

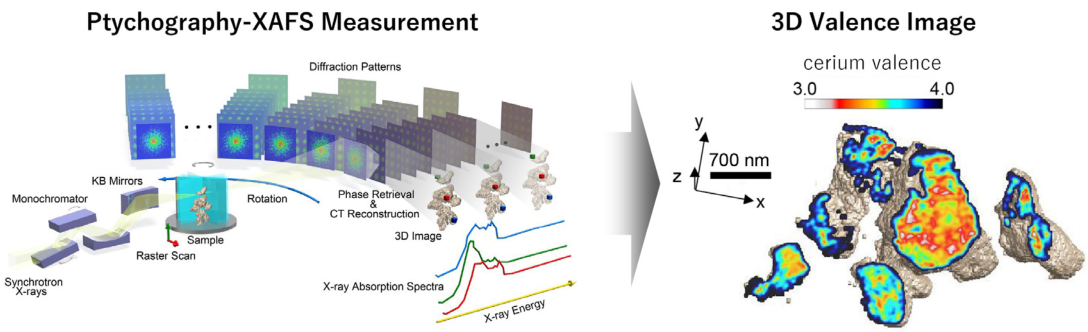

Figure 3.12 Three-dimensional valence imaging by ptychography-XAFS

expected to lead to the optimization of processing technology and the creation of new functional materials.

3.2.6.2. Specifications

Table 3.9 Beamline specifications

Beamline	X-ray coherent imaging
Insertion device	IVU (22 mm×190 periods)
Photon energy range	2.1~15 keV
Energy resolution（E/ΔE）	7,000
Polarization	Horizontal linear polarization（2.1 ~ 15 keV）
Photon flux @ sample	~ 10^{13} photons/sec (@5keV） ~ 10^{11} photons/sec (@5keV, coherent illumination)
Spot size @ sample	~ 1 μm (@5keV, Experimental hatch 1 @focusing) ~ 50 μm (@5keV, Experimental hatch1 @non-focusing) ~ 200 nm (@5keV, Experimental hatch2 @focusing)

3.2.6.3. Beamline optics

In this beamline, as shown in Fig. 3.13, high-brightness SR emitted from the undulator is monochromatized by a liquid nitrogen-cooled Si double-crystal monochromator and mirror optics, and 2.1 keV to 15 keV X-rays are supplied to a fixed position at the end station. The mirror optics consists of three planar mirrors, and by adjusting the grazing incidence angle of each mirror, the height of the optical axis just after the mirror optics is kept constant during insertion and retraction. The plane mirror has three surfaces on a single-crystal silicon substrate: silicon mirror surface, Ni-coated mirror surface, and Rh-coated mirror surface, and the surface can be selected according to the energy used. In addition, a high-precision four-quadrant slit is placed downstream of the optical hutch and its aperture size is adjusted to control the spatial coherence and flux of X-rays required for each measurement.

3.2.6.4 Endstation

The end station consists of two experimental hutches arranged in tandem: experimental hutch 1, 29 m away from the source, and experimental hutch 2, 47 m away from the source. The size of the experimental hutch 1 is 6 (optical axis direction) × 4 (W) × 3.3 (H) m^3. On the other hand, the size of the experimental hutch 2 is 10 (optical axis direction) × 4 (W) × 3.3 (H) m^3. Total-reflection focusing mirrors (focusing size ~1 µm @ 5 keV) are installed upstream of the experimental hutch 1, and various imaging experiments (e.g., coherent diffraction imaging, ptychography, X-ray fluorescence holography, Bragg coherent diffraction imaging [9], cryogenic coherent diffraction imaging [10], and full-field imaging with total reflection imaging mirrors. In the experimental hutch 2, total reflection focusing mirrors (focusing size ~200 nm @ 5 keV) and a multimodal imaging system are installed for high-resolution imaging by ptychography, wide-field imaging by holotomography, and imaging XAFS measurements. In the user space upstream of the experimental hutch 2, for example, trace element mapping and XAFS measurements are performed using a scanning X-ray fluorescence microscope. Coherent diffraction imaging and X-ray photon correlation spectroscopy experiments requiring a camera length of more than 10 m can also be performed by placing samples in experimental hutch 1 and image detectors in experimental hutch 2. As the image detectors, high-count rate image detectors such as CITIUS being developed at RIKEN, and visible light conversion image detectors with a high resolution of several microns will be available.

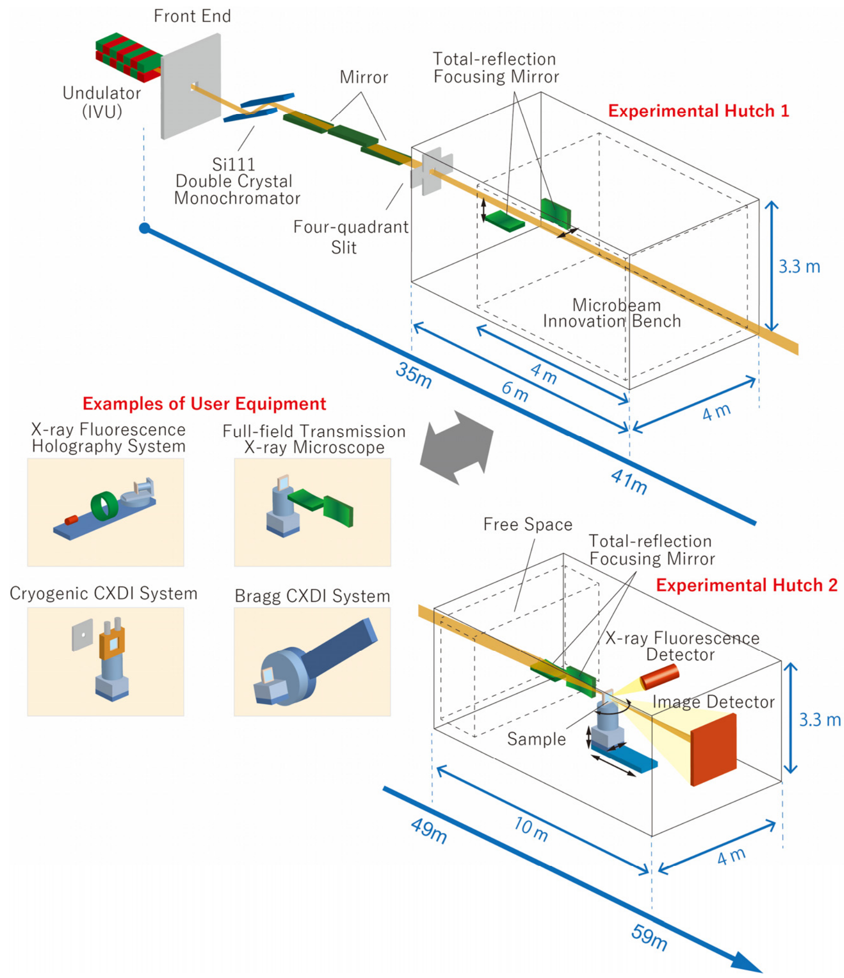

Figure 3.13 Overview of X-ray coherent imaging beamline (BL10U)

□ Experimental hatch 1

Permanent installation

- Total-reflection focusing mirrors

Examples of user equipment

- Cryogenic coherent X-ray diffraction imaging system
- X-ray fluorescence holography system
- Coherent X-ray diffraction imaging system with Bragg geometry
- Full-field Transmission X-ray microscope

□ Experimental hatch 2

Permanent installation

- Total reflection focusing mirrors
- X-ray ptychography apparatus

Examples of user equipment

- Scanning X-ray fluorescence microscope

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3.2.7 Soft X-ray imaging beamline (BL14U)

3.2.7.1 Science

Soft X-ray absorption spectroscopy (SXAS) provides element-specific information about the electronic and magnetic states of materials through core-electron excitation at the absorption edge of each element. In modern materials science, it is widely known that inhomogeneities in the microstructure on the nm to µm scale greatly affects the function of the materials. This fact implies that material properties can be improved through appropriately controlling the microstructure. However, until very recently it has been difficult to visualize the chemically and magnetically inhomogeneous distributions superimposed on the microstructure using conventional observation techniques. Fortunately, with the advent of SXAS microscopy techniques, quantitative visualizations of the inhomogeneous distributions have been realized, which has facilitated analysis of the local electronic and magnetic properties in materials with nm-scale microstructures. The acquired "large-scale-data" describing the locally varying properties contains information which could ultimately lead to discoveries of hidden and essential properties of these materials by making full use of modern data science techniques.

The SXAS microscope has a variety of applications. Electrode materials in energy devices are using transition metal compounds, carbon materials, and oxide materials, in which the nm-scale structures relate to the chemical states that affect the performance of the devices. Furthermore, chemical and electronic states at the nm-scale need to be understood in many complex materials of interest to both fundamental science and advanced material technologies: for example, the bio-elements and other trace elements in biological samples, microscopic samples derived from asteroids, environmental materials such as microplastics, and organic materials used in many products such as rubber, plastics, and polymers. Magnetic circular dichroism (MCD) of SXAS, in which circularly polarized soft X-rays are used, is the most popular way to evaluate the element-specific magnetic properties of materials. The SX-MCD measurement technique has found applications in studies of permanent magnets, spintronics materials, and other novel magnetic materials, which are the key materials for energy products and information technologies. As with SXAS, SX-MCD microscopy observations are crucial for understanding the local magnetic interactions between magnetic grains and will be an important tool for elucidating the microstructure-dependent coercivity mechanism. The BL14U beamline is mainly dedicated to the SXAS and the MCD microscopies and will be constructed at the BL14U port in which soft X-ray radiation is generated using a twin helical undulator. In the twin helical undulator, the upstream and downstream helical undulators are arranged in tandem and generate left- and right-circularly polarized soft X-rays, respectively. The helicity of the soft X-ray is switched by only changing the undulator gaps to minimize the effect of polarization changes on the electron orbits of the storage ring without modulation of the electron orbits.

From a technical point of view, various types of SX microscopy techniques have been developed in many synchrotron facilities all over the world, so far, including scanning, imaging, and coherent diffraction. A great advantage of the NGSR facility, which is a low emittance light source of 1.1 nm·rad, is to use the high coherent flux which makes it possible to record coherent diffraction images with high-speed and high-quality. Besides, the small electron beam size increases practically the intensity of the focused X-ray beam illuminating the sample surface. The BL14U beamline has advantage of the nm scale information of materials and contributes to the development of "nm scale science and technologies".

3.2.7.2 Specifications

Table 3.10 Beamline specifications

Beamline	Soft X-ray Imaging
Insertion device	Twin helical undulator (THU) (56 mm×35 periods×2 sets) Right circular polarization 1 set Left circular polarization 1 set
Photon energy range	250 ~ 1400 eV
Energy resolution （E/ΔE）	3000 ~10000
Polarization	Right & Left circular polarization (250 ~ 1400 eV)
Photon flux (exit slit = 25μm)	5.0×10^{12} ~ 3.9×10^{13} photons/sec
Spot size @ sample	50 nm～10 μm

3.2.7.3 Beamline optics

Figure 3.14 shows the optical layout of the BL14U. The soft X-rays emitted from THU are introduced into the entrance slit of the monochromator through the M0 mirror, the beam splitter, and the M1 mirror. The monochromator is a constant-angle-of-deviation type using a varied-line-spacing plane grating. Two diffraction gratings are set in the monochromator; the line densities of the diffraction grating are 600 and 1200 lines/mm. A high-precision 4-way slit is placed in front of the focusing mirror system to control the spatial coherence and flux of X-rays required for each measurement. The focusing mirror system is a combination of a KB mirror and a rotational Walter mirror, which is currently under development to make the beam size variable from 50 nm to 10 µm. The optical layout by applying a variable-angle-of-deviation type monochromator is also discussed as an alternative design.

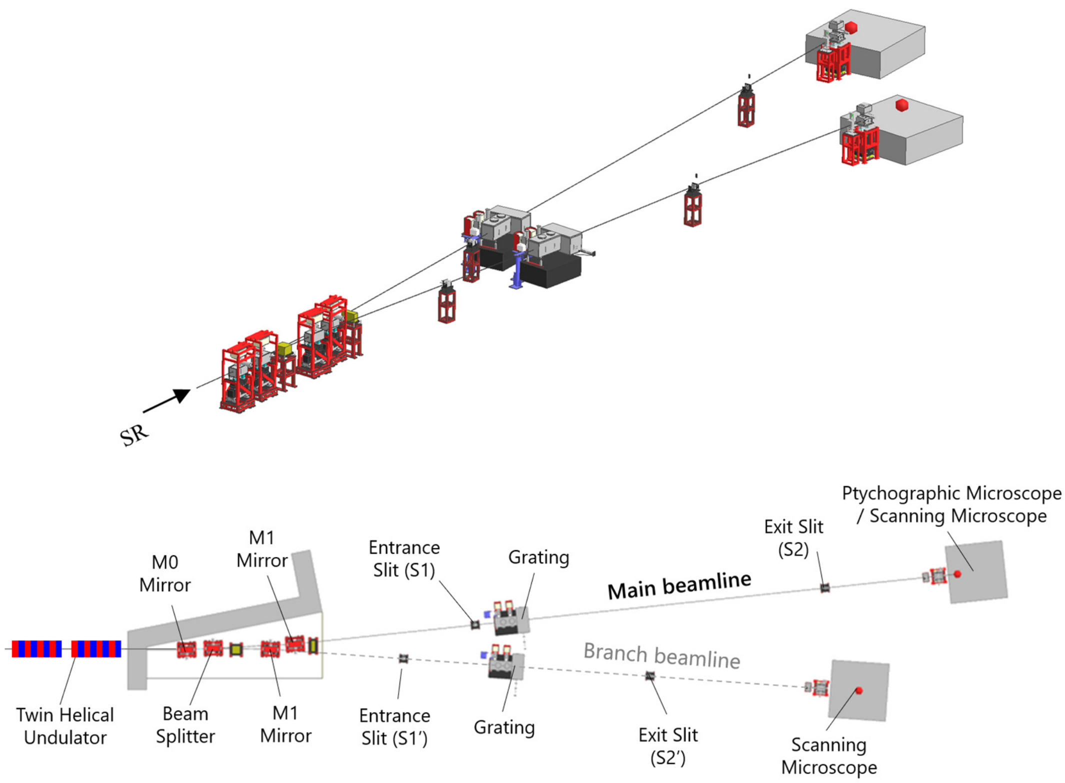


Figure 3.14 Overview of soft X-ray imaging beamline (BL14U)

3.2.7.4 Endstation

At the end stations of the BL14U, two types of imaging systems will be installed. One is a ptychographic spectro-microscopy based on the coherent diffraction technique with a spatial resolution of less than 10 nm. The other is a scanning microscope with a focusing optical system that produces a several 10nm-scale beam spot, where both transmission and electron/fluorescence yield detection are planned. The two imaging systems will be switched by moving the whole apparatus using guide rails installed on the floor. A preferable application in the branch beamline that is under consideration is a scanning transmission microscope because the high beam intensity is unnecessary when using a photon-counting detector to record the transmitted soft X-ray. As an attractive usage of the beamlines, simultaneous measurements at both the main and branch beamlines with different energy regions could possibly be performed by setting the relevant undulator gaps accordingly for each measurement. Of course, interference and/or contamination between two distinct color soft X-rays should be investigated in advance.

3.3 Branch beamlines

3.3.1 Concept of branch beamlines

A beamline at the NGSR facility consists of a main beamline and branch beamlines. At SR facilities, it is common to have multiple branch beamlines to accommodate different endstations to meet the demands by the users for various measurements. However, X-ray beam is usually delivered to only one of the main/branch beamlines and the users can perform experiments at only one endstation at the same time. The users' beamtime is limited by the operation hours of the storage ring.

In order to maximize the users' opportunity to use the high-brilliance X-rays at the NGSR facility, X-rays beam is split into main beamline and branch beamlines. The users can operate multiple systems working in parallel. This is called as a simultaneous branching method. The main beamline hosts advanced measurement stations, which make best use of high-brilliance and coherence of X-rays at the NGSR facility. In contrast, the branch beamline is equipped with automated measurement stations, in which high throughput routine measurements are performed with help of robotics and automation technology. In addition, the research and developments for the future measurement methods and optics will be performed at the branch beamlines. This allows the NGSR facility to increase the productivity and the competitiveness in the cutting-edge SR science.

3.3.2 Methods for beam branching

The simultaneous branching methods at the NGSR facility are summarized in a matrix format in Fig. 3.15. We consider the wavefront splitting by an edge mirror for soft X-rays, and the amplitude/wavefront splitting by crystal (Si and diamond) for tender/hard X-rays. The applicability of the methods for each X-ray energy range is shown in the matrix. For the soft X-ray region, sufficient reflectance is available with sufficiently large angle of reflection to separate the branched beams. The wavefront splitting by edge mirror will be used for the branching of the soft x-ray beamlines. For the hard X-ray region, both Si crystal and diamond crystal provide suitable Bragg reflections for the branching. We plan to adopt the amplitude splitting by the thin diamond crystal for the narrow beam from the hard x-ray undulator (IVU), while adopt the wavefront splitting by the Si crystal for the relatively wide beam from MPW, as shown in Fig. 3.16.

3.3.3 Branch beamline list

The branch beamlines at the first phase are summarized in Table 3.11. With the simultaneous branching methods, there will be 15 beamlines in total at the first 7 coalition beamlines that can be operated in parallel.

As shown in Fig. 3.16, MPW beamlines (BL08W and BL09W) will be branched into three beamlines using the wavefront splitting by two Si crystals. BL09U (IVU beamline) will be branched into main beamline and one branch beamline using the amplitude splitting (transmitted beam and reflection beam) by thin diamond crystal. Since a large coherent flux is required for coherent diffraction imaging, BL10U (IVU beamline) will not be branched.

In the case of the SX beamline, a part of the X-ray beam will be reflected by the edge mirror into the branch beamline with a reflection angle of about 4°. Note that measurements at the branched beamline are restricted by the undulator gap determined by the main beamline. Therefore, the operation column of the undulator beamline is described as "semi-simultaneous" in the table. This problem can be mitigated by pre-adjusting the allocation of the users' beamtime.

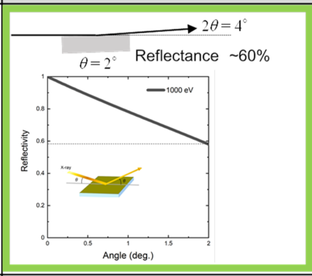
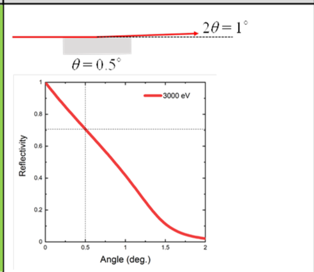
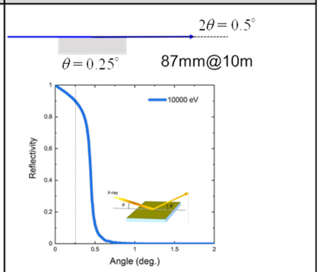
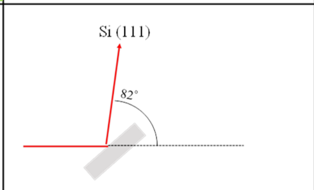
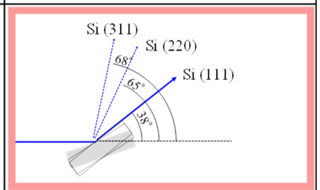
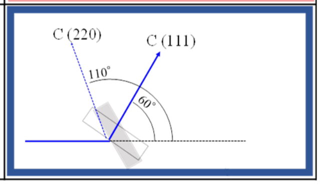
Method	E = 1 keV (Soft X-ray)	E = 3 keV (Tender X-ray)	E = 6 keV (Hard X-ray)
Splitting by edge mirror			
Splitting by Si crystal (Reflection)	No suitable Bragg reflection		
Splitting by Diamond (Transmission)	No suitable Bragg reflection	No suitable Bragg reflection	

Figure 3.15 Beam splitting methods.

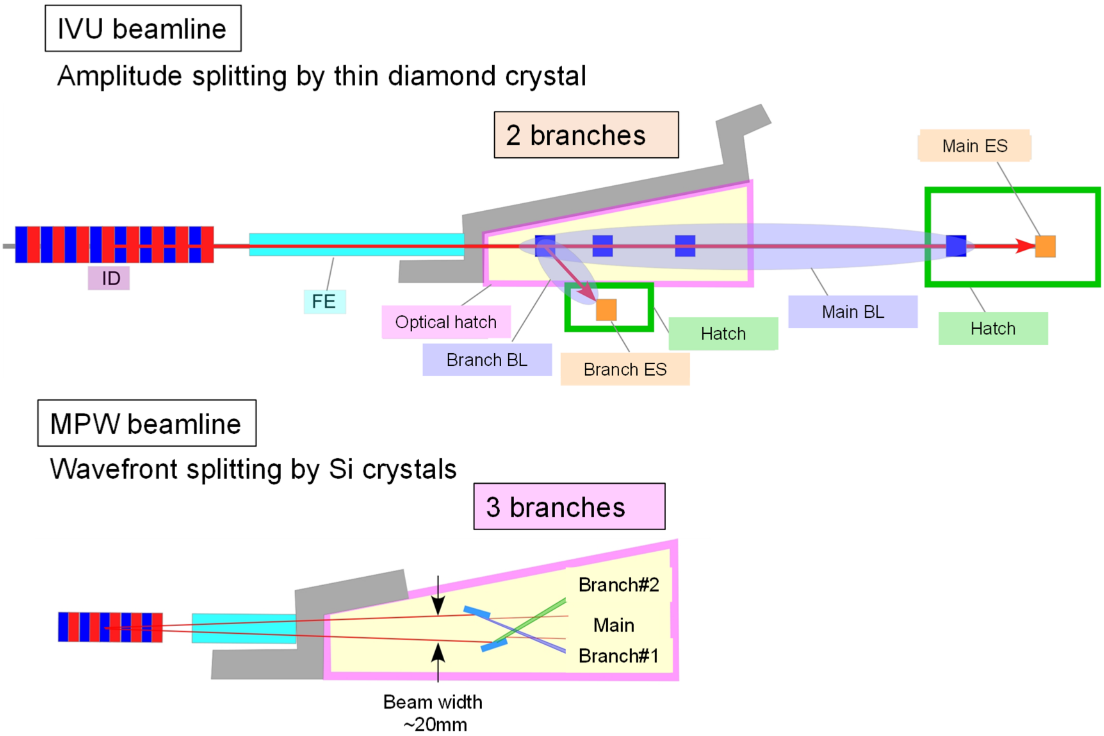


Figure 3.16 Schematic views of the beam splitting by thin diamond crystal (upper) and by Si crystals (lower).

Table 3.11 Branch beamlines in the first stage

BL No.	(ID) Range	BL name	Branch method	Branches	End stations	operation
BL07U	(APPLE-EUV) EUV, SX	Soft X-ray Electronic Structure Analysis	under consideration	Main	RIXS, nano-PES	primary
				Branch#1	High-speed SX imaging （Tentative）	semi-simultaneous
BL08U	(APPLE-SX) SX	Soft X-ray operando spectroscopy	Wavefront splitting by edge mirror	Main	Near Ambient Pressure XPS, and XAFS	primary
				Branch#1	MM-PES (Tentative)	semi-simultaneous
BL08W	(MPW) TX, HX	Integrated analysis of chemical state and nano/local structure	Wavefront splitting by Si crystal	Main	XAFS, SAXS	primary
				Branch#1	Smart-SAXS (Tentative) 8.0 / 13.1 keV	simultaneous
				Branch#2	XRF (Tentative) 17.5 / 28.5 keV	simultaneous
BL09U	(IVU) TX	X-ray operando spectroscopy	Amplitude splitting by thin diamond	Main	Ambient Pressure HAXPES, EXAFS	primary
				Branch#1	HAXPES, XRD	semi-simultaneous
B09W	(MPW) TX, HX	X-ray multiscale structural analysis	Wavefront splitting by Si crystal	Main	XCT, Absorption/Phase contrast imaging	primary
				Branch#1	Smart-XRD (Tentative) 17.5 keV / 28.5 keV	simultaneous
				Branch#2	Smart-XRD (Tentative) 22.7 keV	simultaneous
BL10U	(IVU) TX	X-ray coherent imaging	-	Main	CDI, Ptychography	primary
BL14U	(THU) SX	Soft X-ray Imaging	Wavefront splitting by edge mirror	Main	SX-CDI, Magnetic Imaging,	primary
				Branch#1	STXM, PEEM (Tentative)	semi-simultaneous

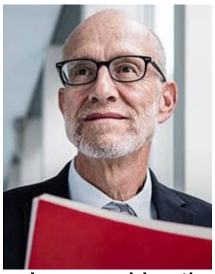
Feb. 10, 2021

International Review of Coalition Beamlines Implementation

International Center for Synchrotron Radiation Innovation Smart
Tohoku University
Director, Prof. Atsushi Muramatsu

Tohoku University launched the International Center for Synchrotron Radiation Innovation Smart (SRIS) on Oct. 2019 to lead the Next Generation 3GeV Synchrotron Radiation Facility project as one of the project partners which include QST, MEXT, Miyagi Prefecture, Sendai City, Tohoku Economic Federation, Tohoku University and the Photon Science Innovation Center. SRIS is in charge of the Science and Technology of the 7 beamlines organized by industry and academia coalitions, referred to as Coalition beamlines.
SRIS is organizing a review of the 7 Coalition beamlines in order to obtain an independent scientific evaluation of the plan for their implementation. In addition, we would like to solicit suggestions for future scientific and technical developments of the beamlines. The panel will be composed of experts in SR beamline science and technology from leading international facilities.

Review Panel



Dr. Jerome Hastings
Professor of SLAC
Stanford University(US)
(Chair)

Dr. Shunji Goto
Division Director of
Light Source
JASRI/SPring-8

Dr. Steven Hulbert
R&D Manager
NSLS-II
BNL(US)

Dr. Andreas Scholl
Deputy for Science
ALS(US)

Dr.Thomas Schmidt
Group Leader
PSI/SLS (Swiss)

Schedule(Important date) 2021

Technical Report	Feb. 15
Terms of Reference	Feb. 16
Mail Review	Feb. 16-Mar. 1
Review Report (draft)	Mar. 8
Final Report	Mar. 15

March 15th 2021

Executive summary

The NGSR is a state-of-the-art near diffraction limited storage ring that will provide a broad photon energy range and provide user access in a unique and innovative way: the "Coalition Concept". The ring design is aimed at robust operation from the beginning and is based on the experience at SPring-8. The innovative "Coalition Concept" aims to create an environment that is most conducive to a collaborative approach to addressing scientific and technical challenges that benefit society. It goes beyond access to a single beamline but rather to a suite of capabilities using the latest x-ray techniques. Not only has industry joined the coalition but universities and national research institutes as well.

The potential for the "coalition concept" to contribute to the most challenging problems facing society today is clear. The scientific environment that the NGSR will create will bring together industry and academia in a way that the breadth of the scientific and technical questions that are investigated broadly with x-rays in both industrial and basic research environments can be advanced.

The designs of the x-ray sources, the undulators and wigglers, are based on experience from SPring-8. In some aspects the undulator design is ambitious and may only be fully realised when the NGSR is in mature operation. It is noted that in the very unlikely event that there are challenges to meet the beamline needs there are solutions that can be implemented.

The suite of the initial 7 beamlines addresses a broad range of capabilities that are matched to the scientific needs today. There are of course opportunities beyond those discussed in the report, for example aspects of energy science and environmental science. It is noted that as the facility comes on-line there is room for growth and further development of new x-ray capabilities to address both existing areas of research as well as emerging scientific and technical challenges. The initial suite is already impressive and future development should be based on the evaluation of the operation of the first 7 beamlines.

In summary the proposed development of the NGSR is well founded on known technologies and provides an environment, the "coalition concept", that will stimulate the development of solutions to important questions that will benefit society.

Shunji Goto, Japan Synchrotron Radiation Research Institute
Jerome Hastings, SLAC National Accelerator Laboratory, Chair
Steven Hulbert, Brookhaven National Laboratory
Thomas Schmidt, Paul Scherrer Institute
Andreas Scholl, Lawrence Berkeley Laboratory

I. Benefits of the Coalition BL system

X-rays are a unique analytical tool. The advent of accelerator based x-ray sources has pushed the capabilities to the point where spatial resolution on 3d objects can reach voxel sizes of 10x10x10 nm^3 over mm scale objects, imaging structure and elemental maps. Protein crystallography has become routine. Diffraction techniques have advanced our understanding of a breadth of materials. The majority of this development has been driven by basic researchers found predominantly in academic institutions. The challenge has always been how to provide these unique capabilities to the breadth of the R&D community with special emphasis on industry with the specific aim to drive innovative solutions to the ongoing societal challenges. Ultimately, for this to be successful there is a need for an environment that promotes collaboration between industry and academia bringing the strengths of both to bear.

To address this need NGSR has developed the “coalition concept”, a new research scheme in which stakeholders from both industry and academia form a strong one-on-one team for the purpose of solving societal challenges). Industrial partners have unsolved problems that could benefit from access to state of the art tools and demand-oriented user-support by the experts. Academic partners often have the expertise in measurement and data analysis. Through an interdisciplinary research collaboration in the “coalition concept” academic researchers can expand the applicability of their expertise to new disciplines.

The “Coalition Concept” is a natural extension of the participating research team system (PRT) developed at NSLS now more than 40 years ago. But it goes qualitatively beyond that first step. It is a format that on the one hand gives access not just to one x-ray technique but rather to many specialized capabilities and on the other forms a natural environment to create partnerships between industry and academia. It does even more. It creates the opportunity for collaboration amongst the science communities at the academic partners as well. There are many academic research efforts within university communities that would directly benefit from collaboration between x-ray specialists and subject matter specialists. These collaborations are enabled by the coalition concept.

This “Coalition Concept” has been attracting industrial users interested in utilizing the latest x-ray techniques made possible by the NGSR facility. This approach will almost certainly lead to solutions for challenges that are critical to society that are being attacked by industry today.

One can think of the “coalition concept” in terms of an ecosystem for sustainable growth. The hope and expectation are that a positive spiral will be created in the business ecosystem; strategies and research results are recognized by society, which then attracts talented researchers to join the NGSR facility. Together with these new participants, the host community will build an advanced strategy supported by their knowledge and human resources. The NGSR facility will be the core of a research complex of universities, research institutes, and companies. It should be noted Tohoku university plans to build a "Science Park" at the Aobayama campus, the site of the NGSR facility. The "coalition concept" shall be the guiding principle of this research complex to create a "community for innovation".

NGSR should be applauded for launching the "Coalition Concept" and its importance is demonstrated by the strong commitments from industry and academia.

II. Scientific and technological value of the project for development of interdisciplinary research and industry-academia collaboration.

X-ray techniques are unique analytical tools. They provide direct information about the structure of matter whether crystalline, liquid, even amorphous as well as information on heterogeneity on length scales from sub-nanometer to microns to millimeters and even larger distances. The information one gleans informs basic questions in materials, chemical and biological sciences as well answers to questions that help industrial progress and the development of solutions to important problems that impact society. The challenge that is faced by the facilities that provide these unique tools is how to couple problem solvers to problems. That is, there are experts, found mostly in academia, who develop methods and instrumentation while in both the academic world as well as industry there are problems begging for results. The “Coalition Concept” is an outgrowth of the very successful soft matter ‘alliance’ that was established at SPring-8. It is the next step at a much larger scale and with both academic institutional members as well as industrial members it has the potential to overcome the ‘divide’ between x-ray science experts and the broader research community. With access not just to one ‘technique’ but a breadth of experimental tools the “coalition Concept” has the right combination of partners and methods. The challenge will be stimulating this research ecosystem. The direct involvement of Tohoku University is a key step. The construction of an office/lab complex on the NGSR facility site is also an important aspect that should be considered. Physical proximity of researchers has always driven collaboration and it would almost certainly do so at the NGSR facility.

Noteworthy is the academic institution membership. Cross disciplinary studies at these institutions almost certainly will be nurtured through the “Coalition Concept”. The community at large will be looking carefully at the development of the “Coalition Concept” eager for its success.

III. Comment on the general scientific/technical merits of the design for the individual beamlines.

a. Undulator development

Using variable polarization APPLE-II undulators for the soft x-ray beamlines and in-vacuum undulators for the hard x-ray beamlines follows the design strategies of the established medium energy storage rings. In addition, the hard x-ray undulators shall also serve the tender x-ray regime.

Combining tender x-rays with hard x-rays out of one source requires a rather high K-value to have an overlap between the first and third harmonics. In order to accomplish this the proposed U22 undulator needs to reach a minimum gap of 5mm to provide the K-value of 2.36 with the latest grade of NdFeB magnets to guarantee the needed overlap. The gap is a result of the scaling of SPring-8 in-vacuum undulator operation to the NGSR parameters. However, compared to the existing mid-range storage ring facilities this is very ambitious. For example, SLS2.0 aims to achieve a 4.2mm gap with 3m long U18 undulators with the same small acceptance $A = (gap/2)^2/\beta_{L/2} = 1.45$ with $\beta_{L/2} = \beta_0 + (L/2)^2/\beta_0$ as the U22. We note the user specifications in terms of photon energy range can be met already at a larger gap with either a U18: 5.2mm or a CPMU16: 4.5mm. Thus, the U22 can be exchanged for a CPMU or longer period undulator at a later date, if required.

For the soft x-ray undulators the APPLE II undulators are used due to the adopted off-axis injection. The chosen parameters for the VUV seem to be a reasonable compromise between lowest photon energies and power load, which is already close to 11kW and with the soft x-ray UE56 undulators the Carbon edge can be covered in all polarizations states.

Fast helicity switching with the twin helical undulator (THU) concept and the monochromator with small gap changes results in small orbit distortions and in addition to much faster switching compared to shifting of the magnet arrays. The parameters for the THU given in table 2.1 suggest that only helical light will be used. However, in the beamline description it is stated that BL14U is **mainly** dedicated to SAXS and MCD microscopies. Just in case it is not planned, adding a simple phase-matcher between the two APPLE X undulators could expand the capabilities of the beamline to the other polarization states and higher energies. In addition,the flux can be increased by using both undulators even with circular light. With the high stability of modern synchrotrons MCD spectra can be taken also by successive scans of the two helicities. Finally using the third harmonic with elliptical light the energy range above 1400 eV could be addressed.

b. Soft X-ray electronic structure analysis beamline (BL07U)

Science target and appropriateness of the technical approach:

The beamline is designed to use the high brightness of the source to study the nanoscale chemistry and electronic structure of electronic materials and devices and relies on sophisticated Wolter focusing optics. Core-level PES will be used to interrogate local band-bending effects in devices, and the complementary RIXS technique will be used to study bulk electronic effects. This is an interesting combination of techniques that should find usage in the electronic characterization of quantum materials, novel storage media, and electronics. Core-level PES will make excellent use of the nano focus and is less demanding than RIXS. RIXS studieswill be challenging using a nano focus because of the low data rates and the risk of sample degradation and heating. It is not clear whether ARPES is available at the beamline. If available, academic and industrial users might be interested in studying the electronic band structure of novel topological materials and devices under operando conditions.

Source:

The APPLE-II EPU75 is a good choice to cover the 50 - 1000 eV photon energy range. Since polarization control is an important parameter for this beamline, a polarization analyzer diagnostic should be included downstream of the exit slit.

Optics:

Consider using the focusing VLS-PGM beamline design from Reininger and de Castro (2005), if that isn’t the current plan. The advantages of this design include a simple method of focusing the beam at the exit slit and being able to correct for first order (“spherical”) deformations of resolution-determining optical elements such as M2 and the grating. Furthermore, the variable focusing capability could permit independent vertical sources for the refocusing Wolter-type mirrors for the two endstations by being able to focus at either of two exit slits with locations chosen to optimize the focusing performance at the two endstation positions.

We endorse the following optics design aspects: (1) provision of a pulse chopper for time-resolved studies, and (2) use of sophisticated Wolter-type refocusing mirrors, which provide the possibility of providing superior focusing performance compared to standard solutions such as Kirkpatrick-Baez mirror pairs.

We provide two warnings regarding the optics design: (1) focusing to < 100 nm at EUV photon energies (< 100 eV) can be limited by diffraction properties, and (2) focusing high-flux EUV/SX photon beams to < 100 nm spot sizes can result in undesirable heating of the sample.

Endstations:

NanoARPES and nanoRIXS techniques are both state-of-the-art. Combining those with operando sample conditions and identified scanning/imaging modes will provide unique experimental capabilities.

Comments:

- Navigating on the sample and finding a region of interest will be challenging when using inefficient probes like XPS and especially RIXS. Methods should be developed to fiducialize regions of interest using optical microscopy or SEM and then transfer the coordinate system to the x-ray endstation.
- Manipulation of the sample with nanometer precision and stability will be challenging, especially for angle-dependent RIXS when the sample and spectrometer need to be rotated synchronously while maintaining a common focus on the sample.
- Diffraction-limited focusing at the lower energies will require a very large numerical aperture. Reaching the required optical specifications will be challenging.
- Focusing the projected beamline flux to a sub 100 nm scale focus will likely cause heating and sample damage issues that will be difficult to mitigate since each individual x-ray pulse deposits a large amount of energy, causing instant heating of the sample that can’t be outrun by translation.

c. Soft X-ray operando spectroscopy beamline (BL08U)

Source:

The APPLE-II EPU56 is a good choice to cover the 130 - 2000 eV photon energy range. Since polarization control is an important parameter for this beamline, a polarization analyzer diagnostic should be included downstream of the exit slit. The photon flux value at the sample (10^{12} ph/sec/0.01% bw = 10^{13} ph/sec/0.1% bw) looks reasonable.

Optics:

If you are not planning to do so already, consider using the focusing VLS-PGM beamline design from Reininger and de Castro (2005). The advantages of this design include a simple method of focusing the beam at the exit slit and being able to correct for first order ("spherical") deformations of resolution-determining optical elements such as M2 and the grating. Furthermore, the variable focusing capability would permit independent vertical sources for the refocusing Wolter-type mirrors for the two endstations by being able to focus at either of two exit slits with locations chosen to optimize the focusing performance at the two endstation positions.

Endorsement of refocusing optics design: while very few details are provided regarding refocusing, the use of sophisticated Wolter-type refocusing mirrors, apparently in conjunction with KB mirror pairs, will offer the possibility of providing superior focusing performance.

Sample heating by highly focused soft X-ray beams: focusing a high-flux soft X-ray photon beam to ~50 nm spot size can result in undesirable heating of the sample, certainly under vacuum conditions. Modeling of the convective cooling provided by the atmospheric sample condition would be important in addressing the sample heating issue for this beamline.

Endstations:

Nano AP-XPS and nano AP-NEXAFS techniques operated at up to 1 atmosphere gas pressure will be state-of-the-art. Good experience in both techniques exists in Japan, which forms a solid basis for proceeding with this beamline.

Suggestion regarding scanning capability: We wonder if it is intended to include sample (or beam) scanning capability to provide spatial XPS and NEXAFS maps under ambient pressure conditions. Adding scanning capability would make this beamline and endstations even more unique in the world.

d. Integrated analysis of chemical state and nano/local structure beamline (BL08W)

The beamline capabilities to combine spectroscopy and scattering to obtain information on the chemical state and the structure using X-rays of 2.1 to 17.4 keV gives access to elements in the periodic table from the K edge of phosphorus to the L_{III} edge of uranium. The use of X-ray absorption fine structure (XAFS) will give simultaneous information about the electronic structure (valence, chemical species) and coordination of the specific element and information on the local structure (interatomic distance, coordination number) around a specific element. The SAXS measurements provide information on the nanoscale inhomogeneity in a sample, size, shape, distribution, higher-order structure, surface structure on lengths scales from several nm to several hundred nm. This beamline uses these measurement methods to evaluate the correlation between changes in the electronic structure of specific atoms and macroscopic structural changes under dynamic conditions in polymers, metals, battery materials, etc. The access to photon energies from 2.1 keV from a wiggler source permits straight forward energy scanning easily reaching the K-edges of phosphorus and sulfur and the L-edge of palladium as well as the L_{III} edge of uranium. These elements, phosphorus and sulfur, play important roles in functional materials and biomaterials. Furthermore, dynamic anomalous small-angle X-ray scattering (ASAXS) can visualize the time-space distribution of specific atoms on the second time scale.

Source:

A wiggler meets the needs defined for this beamline and the ‘wide’ horizontal fan intrinsic to wiggler sources enables branch line capabilities which are proposed for future development. Because the focal spot size is modest the use of an undulator source is not required.

Optics:

Here it is important to ensure that the energy resolution of the monochromator is better than the core-hole lifetime for the full range of x-ray edges that can be accessed. Best would be to have the ability to switch between the Si(220) reflection and the Si(111) reflections in the DCM. The increased resolution (x2 approximately) will not result in a significant loss in intensity. When reaching the lower end of the spectral range the Si(111) is required.

Experimental equipment:

The 13 m maximum camera distance for SAXS is important for many systems with nm scale density fluctuations and is noted. As well, the capability for simultaneous SAXS and XAFS is an important attribute.

e. X-ray operando spectroscopy beamline (BL09U)

Science target and appropriateness of the technical approach:

X-ray spectroscopies are unique in their ability to be elementally specific. The most widely used of these spectroscopies X-ray Absorption Spectroscopy (XAS) in it's two forms, X-ray absorption near-edge structure (XANES) and extended (EXAFS) access both the electronic structure (XANES) and the atomic structure (EXAFS). When combined with hard x-ray photoemission spectroscopy (HAXPES) with nanometer scale beams these spectroscopies are important tools for the investigation of materials ranging from catalysts to batteries, from steel to biomaterials. BL09U aims to provide these spectroscopic capabilities. It will almost certainly have extremely high demand.

Source:

The aim of this beamline is tunable x-rays beams with scale 100 nm foci. The nano-focus 'demands' an undulator source to maximize the flux which translates directly to the minimum concentration of minor constituents that can be studied in 'bulk' materials. Thus, the proposedsource is well matched to the experimental techniques that will be available on this beam line.

Optics:

There are two important requirements that drive the optical solutions: (1) focal spot size, here aimed at 100 nm and (2) energy resolution here defined as resolving power ($R=E/\Delta E$). For HAXPES the stated requirement is R=20,000 and for XAFS R=5000. The focal spot size requirement is good. However, the 5000 resolving power is a bit low for XAFS. Here you want to be sure that the instrumental resolution is better than the core-hole lifetime and as a rule of thumb better would be to have $R \geqq 10{,}000$. This is easily achieved by, for example, using the Si(220) reflection rather than Si(111) in the DCM.

The other concern is throughput for the nano-focus. Here the 100 nm beam size is achieved by imaging the slit placed just after the upstream DCM. To maximize the flux the 'standard' approach is a 1:1 mirror system that focuses the source onto the beam defining slit. This approach should be considered for this beamline.

There is also the desire to be able to 'tune' the spot size for HAXPES and almost certainly as well, for XAFS. The proposal is to operate downstream of the focus. There should be consideration of developing bendable KB mirrors and/or studying the impact focal spot size with a large upstream slit opening.

Comments:

It is strongly suggested to implement the capability to do 'simultaneous' HAXPES and XAFS. By simultaneous what is meant on the same sample position keeping in mind the 100 nm focal spot size. Also, sample environment and sample positioning at the sub 100 nm level is critical to reach the full potential of the beamline capabilities.

f. X-ray multiscale structure-analysis beamline (BL09W)

Energy dispersive XAFS, surface XRD, and multi-beam x-ray tomography will provide unique solutions of the high-throughput measurements for the coalition users, particularly users from industry. The wiggler source, providing sufficient photon flux of broadband x-rays, is suitable for the purposes. The energy dispersive optics will enable reasonable measurements with proper spatial-temporal resolution. Beam splitting is a very effective way at this beamline to obtain sufficient beam-time for coalition users, starting with a limited number of coalition beamlines. Branch lines will be designed and used mostly for the general purpose high-throughput measurements.

Beam splitting using the single-bounce Si monochromator seems to be feasible. Fixed photon energy use is very helpful for the simple design of the monochromator under stable operation. Heat load at the optics will be up to 100 W for the main line, and several tens of watts at the branch lines. They should move to critical engineering consideration/design for the beam splitting system with proper water cooling soon. Spatial interference between the main beam and branch beams must be carefully avoided. High-heat-load energy dispersive optics should also be into a technical design phase soon.

They propose several different techniques at the beamline. End stations should be commissioned and opened, based on the priority determined by availability of equipment and also by user demands.

g. X-ray coherent imaging beamline (BL10U)

Tender to hard x-ray coherent imaging beamline is one of the state-of-the-art beamlines of the NGSR. It will be a very attractive one for coalition users, who need the meso-scale material information using various imaging techniques.

Source:

An IVU is the best choice for this beamline covering the energy from tender to hard x-ray region.

Optics:

Stable operation of the optics is very crucial for a coherent imaging beamline. There are so many optical components including a DCM, harmonic rejection mirrors, and focusing K-B mirrors. Each must be carefully designed for the beam stability. Experience at SPring-8, for example, will be helpful. Cryogenic cooling of the Si(111) DCM is essential for the beamline. The energy range limited up to 15 keV seems to be reasonable. Again, for imaging, stable operation of the DCM is critical. This is best achieved by limiting the number of stages required for fixed exit operation. Also, if possible, minimize the range of motion for the stages. In order to insure a high quality coherent beam for the main line a branch line has quite low priority. However, studying wavefront preservation with a single crystal diamond Bragg reflector to send radiation to a side branch is encouraged. The in-line three-mirror higher-order rejection system is a good choice for the operation of the tandem end stations. The mirror surface finish must be specified carefully, avoiding unwanted speckle and wave-front distortion for coherent imaging.

Endstations

Aside from the main CDI and Ptychography station, other imaging techniques: x-ray fluorescence holography, holotomography and full-field microscopy will also play important roles for the various user demands. Several imaging techniques coexist at the beamline with time-sharing operation. End stations should be commissioned and opened, based on the priority determined by availability of equipment and also by user demands.

h. Soft X-ray imaging beamline (BL14U)

Science target and appropriateness of the technical approach:

Scanning probes will be of significant interest to a range of industry and academic communities, e.g., studying battery materials, porous materials for capture and catalysis or filtration, quantummaterials for computing and data storage purposes, structural materials such as concrete, biological and bioinspired materials, soil samples from industrial clean-ups.

The two endstations appear to be differentiated by the data acquisition process, ptychographic in one case, point detector in the other. Running a diverse set of experiments will require very different sample environments, e.g., cooling, high fields, possibly vacuum for quantum and magnetic materials; operando cells for energy materials; introduction of frozen samples for cell studies. Consider offering point detection and ptychography on both endstations and differentiate by the sample environment they offer.

Source:

The choice of Twin Helical Undulators (THU56) is appropriate to cover the 250 - 1400 eV range with fast-switching circular polarization accomplished by varying the THU gaps as described in the insertion device section (section 2 of the Coalition BL Report). Even though the sources have fixed polarization, the beamline optics will alter it, so including a polarization analyzer diagnostic downstream of the exit slit is recommended.

The tandem undulators can also be set to the same gap and polarization values and used as a single, intense source for fixed-polarization techniques. In such cases, the brightness and coherence of the combined insertion device can be optimized by introducing a phasing magnet between the two undulators, as pointed out in the undulator section of this report.

The photon flux range at the sample (presumably at that location, not stated) of 5×10^{12} to 4×10^{13} photons/sec for 25 microns exit slit appears reasonable, but it would be easier for comparison to other beamlines to state this flux in units of ph/sec/% bw.

Optics:

We suggest adoption of the variable-included-angle VLS PGM optics design proposed by Reininger and de Castro (2005). The advantages of this design include a simple method of focusing the beam at the exit slit and being able to correct for first order ("spherical") deformations of resolution-determining optical elements such as M2 and the grating. Furthermore, the variable focusing capability would permit simple optimization of the focus of the two endstation branches. In addition, the focusing capabilities of this design could easily adapt to multiple endstation positions on each branch, although separate exit slits and refocusing optics would be needed for each endstation.

We endorse the planned use of a combination of KB and Wolter-type refocusing mirrors to provide a variable focal spot size at the sample which will be, if successful, an innovative solution to providing a desired "zoom" capability for the endstation techniques. We offer a warning about potential sample heating: focusing high-flux soft X-ray photon beams to ~50 nm spot size can result in undesirable heating of the sample, certainly under vacuum conditions.

If the method of splitting the beam for the branch line away from the main beamline is, as described in the branch beamlines section (section 3.3 of the Coalition BL Report), by a planar diverting mirror located between the M0 mirror and the two M1 mirrors, various problems are envisaged: (i) optimized alignment of the branch line optics must depend to some extent on the amount of beam that is intercepted by the diverting mirror; if this amount is not fixed, realignment would be desirable any time the fraction changes; (ii) even tiny lateral instabilities in the position of the diverting mirror will change the amount of flux going to each beamline (branch and main); techniques such as MCD are quite sensitive to changes in flux as the photon energy is scanned, for example. If such issues were to lead, eventually, to a reversion to the traditional mode of operating (one beamline branch at a time), it would have been more efficient (in both photons and cost) to simply insert the M1 mirror for the branch line when it is used and retract it for main branch use.

Simultaneous usage of two branches: The stated goal of using both branches of this beamline simultaneously (via usage of different gaps for the two helical undulators), while risky technically, will (if successful) be highly demanded because it will double the output of this beamline per unit time. This success would necessarily interfere, schedule-wise, with the MCD program, which depends inherently on usage of both helical undulators, set to the same gap value, at the same time. In addition, any changes in the gap setting of one helical undulator would almost surely lead to noticeable changes in the flux measured at the sample of the other branch (the one with its monochromator set to a different photon energy), owing to tails in the angular distribution of undulator radiation. This risk is noted in the Coalition Beamline Report. We suggest to optimize the design of each branch of this beamline independently, which will most likely lead to separate (in time) operation of the two branches. This strategy will support state-of-the-art performance of the beamline and endstations, which in turn will extend the useful long-term lifetime of this beamline and both of its branches compared to compromised performance of a simultaneous-usage design.

Endstation techniques:

The coherence-hungry ptychographic and scanning microscope techniques will be well-matched to the beamline properties and represent state-of-the-art SR techniques.

Comments:

- Fast switching is conceptually very nice but in practice not that often used or needed.
- Care has to be taken that x-ray flux and illumination don't change and that there is no cross talk when beam is split between the branches, e.g., when changing the energy/gapin one branch

IV. Branch lines - especially wiggler lines, possible soft x-ray beamlines

To provide the coalition with the experimental capabilities needed the use of branch lines is an important option. The specific choice of branch lines can only be made after the initial operation of the NGSR and the 7 coalition beamlines have been commissioned. Based on the demand from the coalition members the specific branch lines can be defined. It is recommended however to install the initial hardware to accommodate the splitting optics so as not to adversely impact the operations of the main lines as the branch lines are developed.

Wiggler beamlines at many existing SR sources have a main branch using the central milliradians of the 'wiggler' fan and side or branch lines using the outer portions of the fan. There are wiggler lines at the NGSR source and of course branch lines should be considered. These are developed using crystal optics in either Bragg or Laue geometry depending on the wavelength range. The coalition beamlines should consider this approach carefully, noting that the use of the sides of the fan introduces a larger effective source size. It may also be useful to consider a Laue geometry crystal in the 'central' portion of the fan if source size is an important consideration. Of course, 'splitting' undulator lines in the x-ray regime, by necessity, uses Laue case reflections from 'transparent' crystals, most often diamond. As photon energy is set by the main branch and thus the side branch needs to be flexible in the photon energy to make maximal use of the radiation or the choice of 'technique' to be developed with the side branches that would depend on the source, wiggler versus undulator. The thinking behind this is simple, the undulator beamline will have the photon energy chosen by the main branch.

Developing side branches in the soft x-ray spectral range is much more challenging and since in this energy range the majority of the techniques are 'spectroscopic' the main branch-side branch photon energy issue is much more crucial. For soft x-rays the proposed 'division of wavefront' using a sharp edge of a splitting mirror must be very carefully evaluated in particular with regard to vibrations of the splitting mirror to avoid the introduction of unwanted fluctuations in intensity of the main branch.

V. Possible other areas for development

1. Bio/medical research

Synchrotron x-rays are heavily used in medical and biological research and by the pharmaceutical industry. Bio-SAXS, XRD, micro and nano-CT, full-field and scanning x-ray imaging, synchrotron IR nanoimaging could be of interest to the bio/medical research community and the high brightness of the ring would likely enable strong academic and industrial research programs. Beamlines could have impact in the areas of solving protein structures, cell imaging, 3D and surface chemical imaging of tissues, plants, bio-minerals, etc.

2. Environmental sciences

X-rays are an important tool to identify contaminants in soils, to image and chemically identify organic, inorganic and biological components across length scales in minerals, soils, sediments, water. High-brightness x-rays from a state-of-the-art ring would enable high-throughput, high-resolution imaging techniques, such as soft x-ray STXM and ptychography under operando conditions (e.g., flow cells) or at cryogenic temperatures (especially of biologicalsystems), and micro and nanoprobes using tender and hard x-rays.

3. Energy sciences

The program in energy sciences, e.g., related to industrially important materials and systems such as membranes for water purification, electrochemical systems, batteries, fuel cells, carbon capture technology, structural materials, could benefit from a broadened suite of tools including SAXS/WAXS, soft x-ray scattering, chemical crystallography, tomography and operando imaging and spectroscopy techniques.