CURRENT STATUS OF HES (HARD X-RAY ENDSTATION)-2 BEAMLINE AT PAL-XFEL*

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Abstract

The HES (Hard X-ray EndStation)-2 Beamline is located at the hard X-ray experimental hall at PAL-XFEL. The main objective of HES-2 is to deliver a hard X-ray FEL beam to target materials in such as a manner that a coherent diffraction study is possible. In particular, the instruments are designed for coherent diffraction imaging (CDI) and serial femtosecond crystallography (SFX). Here we report the current status of the HES-2 beamline construction and key component (X-ray focusing system, diagnostics and sample environments) for the scientific application.

INTRODUCTION

Pohang Accelerator Laboratory X-ray Free Electron Laser (PAL-XFEL) is a research facility. It will generate extremely intense (assuming 1 X 10^{12} photon/pulse at 12.4 keV) and ultra-short (10-60 femtosecond) pulsed X-rays. This machine will allow us to travel into the ultra-fast and ultra-small world [1, 2].

The HES-2 endstaion is located at the hard X-ray experimental hall. This endstation is built to deliver the FEL beam in the energy range from 2 to 20.4 keV [1]. The initial complement of this beamline has been chosen to serve the needs of the diverse community of Korean scientists. The HES-2 endstation is most often used for coherent diffraction imaging (CDI) and serial femtosecond X-ray crystallography (SFX). Therefore, the first phase of the design of the HES-2 instruments focused on science program of the CDI and SFX based on user demand. To allow these science programs, endstation instruments are applied in the forward-scattering geometry. This instrument can be applied together with time-resolved study with optical laser system. Major specification for the HES-2 are summarized in Table 1.

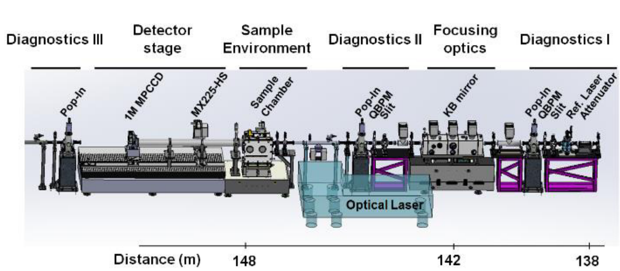

Figure 1. Overview of the HES2 experimental hutch. HES-2 instruments consist of the diagnostics, focusing optics, sample environment and detectors.

Table 1: Major Specification of HES-2

	HES2
Scientific application	Coherent X-ray Imaging Serial Femtosecond Crystallography Timer-resolved CXI/SFX Other technique with forward scattering geometry
Energy range	2-20.4 keV 5-12.4 keV (optimized)
Beam size	1500 µm (unfocused beam)@ 12.4keV 2 µm (KB mirror) @ 12.4keV
Sample Environment	High Vacuum (~10-7 Torr) He ambience
Detector	1M MPCCD MX225-HS

CONSTRUCTION

The dimension of the HES-2 experimental hutch is 22 m (optical axis) x 8.2 m (width) x 3.5 m (height). The HES-2 instruments will be placed <17 m downstream of the hutch. This design saves 5 m of space (optical axis) for future scientific application. At first phage, we installed the FEL diagnostic, focusing optics, sample environment and detectors (Fig. 1). The purpose of details instruments is summarized in Table 2.

Table 2: Summary of the Instruments of HES2

Instruments	Purpose
Reference Laser	Instrument alignment
Attenuator	Reduction of the incident XFEL flux
Slit	Remove the halo Beam definition
Profile monitor (Pop-in)	Measurement of the spatial distribution
Intensity monitor (QBPM)	Measurement of the incident XFEL flux
KB mirror	X-ray focusing optics
Mirror manipulator	KB mirror positioning
Optical laser	Laser pump for time-resolved studies
Sample environment	Sample positioning
Detector	Measurement of the diffraction pattern
Detector stage	Detector positioning

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X-ray Focusing Optics

A Kirkpatrick-Baez (K-B) mirror have been designed for the HES-2 endstation at PAL-XFEL. The focal beam size of the K-B mirror was designed to be 2 μm at the interaction point; the half of mirror surface is coated with carbon material to obtain high reflectivity while avoiding damage by the XFEL. The sample-interaction position of the HES-2 endstation is located ~148 m from the source. The estimated source size at 12.4 keV is 50 μm FWHM vertical and horizontally. The mirror optics have demagnifications of about 1:25 horizontal and vertically. The focal length is 5.86 m. This mirror will cover the energy range of 5-12.4 keV. The carbon coated mirror substrates are shown in Fig. 2.

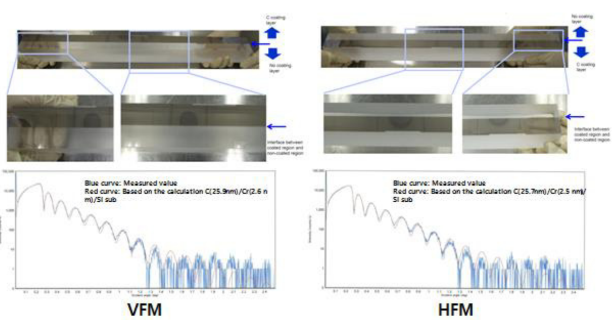

Figure 2: Carbon coated mirror substrate. VFM (vertical focusing mirror) and HFM (horizontal focusing mirror).

Mirror Manipulator

To realize X-ray beams with an ideal focal size and high efficiency, correct alignment of the two K-B focusing mirrors important, particularly the adjustments for perpendicularity and for glancing angles. The final fine adjustment proceeds by repeating measurement of beam size with a wire scanning method and adjusting the glancing angles and focal lengths. The required specification of the manipulator resolution is determined by the focal beam size and focal length between mirror center and sample position. The desired specification of the mirror stability was decided by scientific programs. The K-B mirror manipulator must meet stringent requirements in five motions, and must have a stable alignment. The mirror manipulator has the performance of the high resolution motion of < 0.2 arcsec and high stability of 1 arcsec/8 hours. The inside of a mirror mirror manipulator is shown in Fig. 3.

Figure 3: KB mirror manipulator.

Diagnostics

The diagnostics play a critically important role in accurate monitoring of XFEL beam position and intensity. It provides the beam stability and position with real-time and widely used in the endstation area. In HES-2, two-types of diagnostics will be used such as beam position monitor (Pop-in) and beam intensity monitor (QBPM).

Sample Environment

CXI Sample Environment

The goal of CXI system at PAL-XFEL is to conduct single-shot CXI experiments with optical pumping-laser and focused probing-XFEL. To achieve this goal, CXI instrumentation will be established as a common experimental platform which can be summarized as follows:

-high vacuum (~10-6 Torr) for metallurgical
-He ambience (~1 atm) for hydrated samples
-various pump-probe laser ports (10°,15° and 40°)
-large exit angle (45°) from focus spot

Considering high repetition rate of PAL-XFEL (60 Hz), an efficient sample-providing system (Fig. 4A) is another key factor to determine the capability of HES-2endstation. The quantity of measured data is determined by the efficiency of the sample-providing system, which consists of a sample chamber, a viewer, and a scanning system. To provide samples efficiently, the sample-providing system should be operated systematically. The design concept for this instrument focus on quick sample loading, vibration-free conditions, and maintenance of the desired sample environment. The focused XFEL can cause ablation patterns on the sample surface, thus these patterns should be observed through a high-resolution microscope. A long-focal-length microscope (Union UWZ100 model) is installed to observe it. The CXI sample chamber shown in the Fig. 4B.

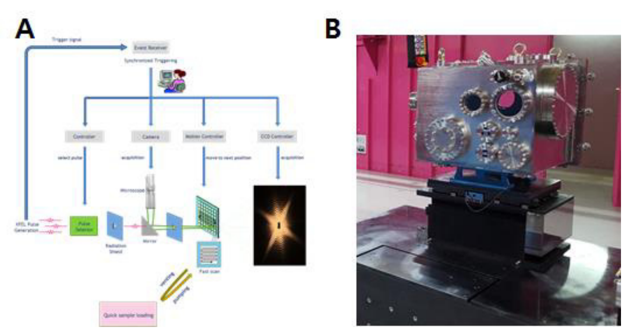

Figure 4: CXI sample chamber. (A) Schematic of sample-providing method. (B) CXI sample chamber.

SFX Sample Environment

The liquid jet sample injector is installed in the SFX sample chambers to provide fully-hydrated protein crystal samples for diffraction experiments. This injector capillary consists of liquid-channel to deliver the protein crystal solution and gas-channel for liquid focusing. This injector is designed for easy assembly and disassembly. This will reduce the sample exchange time during the experimental operation. The flexible tubing connections enable simple manipulation of the injector position to submicron resolution in the sample chamber. To minimize the sample consumption and background noise from sample solution, the liquid beam is focused to a few microns in diameter by a coaxial aerodynamic lens (Fig. 5A). Other sample delivery method is lipidic cubic phase (LCP) injector, which can be applied for the membrane protein crystal (Fig. 5B). The LCP with crystal sample will inject in continuous and stable states by hydrodynamic forces in a helium environment. The speed of the both SFX injectors is finely-controlled considering the XFEL repetition rate and the endsation optics. These injectors will be operated in the SFX dedicated chamber. This instrument contains the multi-function including multi-nozzle, temperature control and time-resolved study using optical laser.

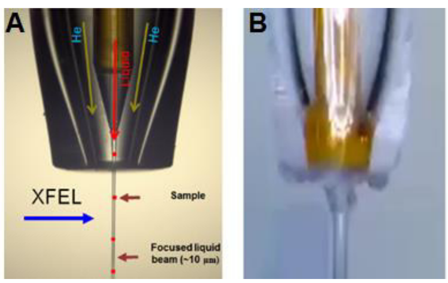

Figure 5: SFX sample delivery system. (A) liquid jet sample injector (B) LCP injector.

Detectors

The FEL provides coherent X-rays in femtosecond pulses of unprecedented intensity. Many experiments at the HES-2 require a detector that can image scattered X-rays on a per-shot basis with high efficiency and excellent spatial resolution over a large solid angle and both good signal-to-noise ratio (for single-photon counting) and large dynamic range (for coherent X-ray diffractive imaging). At first phase, 1M MPCCD (Multiple coupled charge detector) and MX225-HS (Rayonix) will be applied into the CXI and SFX science program (Fig. 6).

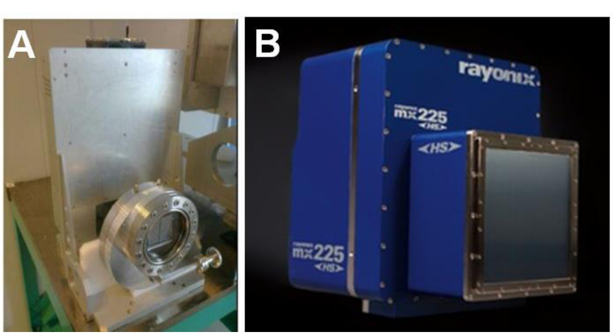

Figure 6: HES-2 detector systems. (A) 1M MPCCD (B) MX225-HS.

Detector Stage

Detector stage serves the purpose of positioning the detector relative to the sample and the incoming beam. The dimension of the HES-2 detector stage is 4 m (optical axis) x 1.5 m (width). This distance allows the CXI and SFX experiment without distance limitations (Fig. 7). The 1M MPCCD detector will be mounted in vacuum inside the detector stage, whereas MX225-HS detector will be installed in atmospheric ambient. Both detectors will be mounted in a detector stage and operated individually without physical interference. Both detector is not including the beam-pass hole in the centre of the detector area. To prevent X-ray damage to the detector, beam stopper will be installed into the front of both detectors.

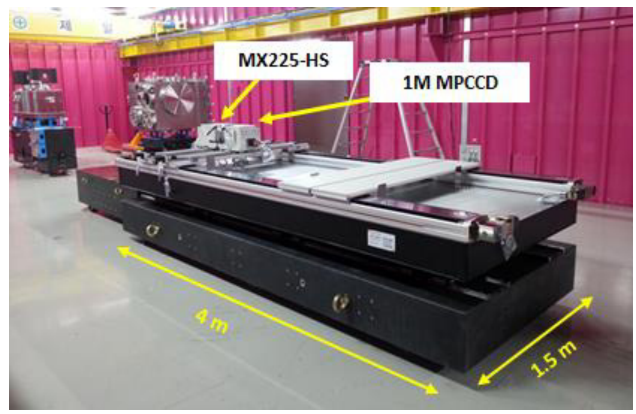

Figure 7: HES-2 detector stage. 1M MPCCD (for CXI) and MX225-HS (for SFX) will be installed in the arrow indicator.

SUMMARY

Here we report the scientific application and instruments of the HES-2 at PAL-XFEL. It will provide a better understanding of the HES-2 instruments at PAL-XFEL. HES-2 will open up new opportunities for high-resolution X-ray imaging of nano-materials and biomolecules. Time-resolved experiments at this endstation will combine high spatial resolution to delineate dynamic processes of molecules in chemical and biological reactions.

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