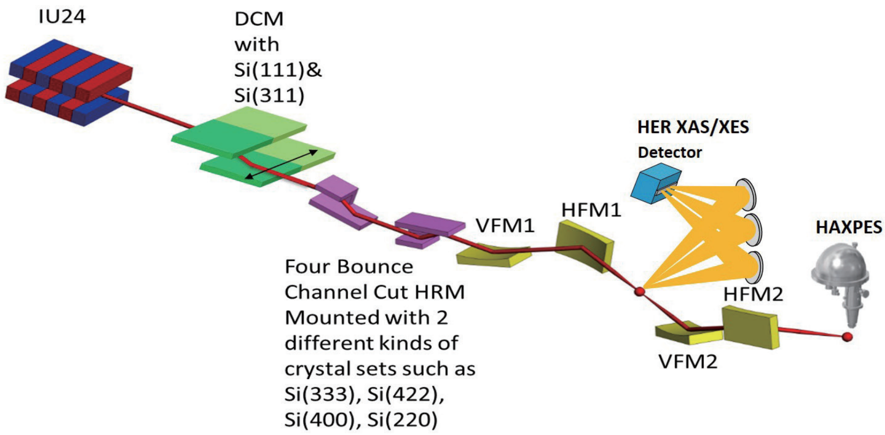

Fig. 11: Beamline **TPS 47A** concept drawing with undulator, DCM, high-resolution monochromator and focusing mirror. Two endstations—ES1: HER-XAS and ES2: HAXPES—are to be built at this beamline.

structure and spin states of materials studied for user research on a wide range of hard X-ray energy (including 3d, 4d K edge and 5d L edge). The multi-analyzer system can significantly improve the efficiency of data collection and cover a wide energy range of measurements at the HER-XAS endstation. The HAXPES endstation exhibits a high penetration depth and bulk-sensitive spectra using hard X-rays, and provides the electronic structure of the inner layer or interface of the sample. The liquid-solid interface sample under nearly ambient pressure experiment can also be performed in our HAXPES endstation. Both experimental endstations will be introduced and installed with various experimental environments *in situ/operando*, such as applied bias, electrochemistry, high pressure and temperature dependent, *etc*. We expect that these two endstations will greatly help not only for user research in energy and semiconductor study but also for industrial applications. The schematic drawing of the beamline is shown in **Fig. 11**. (Reported by Gung-Chian Yin, Chun-Hsiang Huang, Chun-Jen Su, Yen-Chung Lai, Chi-Liang Chen, Wen-Bin Wu, Shu-Chih Haw, Ting-Shan Chan, Chia-Hsin Wang, and Yen-Fa Liao)

High-Resolution Powder X-ray Diffraction

TPS 19A is a dedicated powder X-ray diffraction beamline, which was designed particularly for structure determination and structural dynamics *in situ*. It includes a high-resolution station (**TPS 19A1**) and a general-resolution station (**TPS 19A2**) for diverse scientific purposes and applications. **TPS 19A** was planned not only to investigate an average structure for periodic crystalline systems but also to analyze the local structures of nano- and amorphous materials. Rapid and high-resolution diffraction with atomic pair distribution function (PDF) was therefore both considered and proposed. As expected, powder diffraction is an essential and mature technique for material science, but we devoted effort to keep the design cover both innovative and conservative. A great breakthrough was made to use a cryogenic undulator in vacuum (CU15, length 2 m) as a radiation source. CU15 was the first to be operated near liquid-nitrogen temperature (83 K) in TPS and was made by our magnet group.[1] Based on the character of CU15, the X-ray energy of **19A** can cover from 10 to 40 keV, which will create extensive experimental possibilities for diverse research fields. The beamline specifications are shown in **Table 1**. From 2018 to 2020, after beamline construction for three years, **19A** has been ready for commissioning and invited experiments and open for user operation (10%) in 2021 Q1. The preliminary commissioning results appear in **Fig. 1**. The gap of CU15 can be decreased to a really challenging value, 4.5 mm. It can provide an extremely bright X-ray photon flux. The detailed experimental conditions and non-ambient devices provided are listed in **Table 2**; high or low temperature, high pressure, gas or solvent loading system, electrochemistry are all integrated to the data collection program, and user-friendly and easy data reduction macros are also provided.

The first endstation, the so-called high-resolution powder X-ray diffraction station, has been operated in **TPS 09A**

Table 1: Specifications of **TPS 19A** high-resolution powder X-ray diffraction beamline.

Photon energy range	10–40 keV
Photon flux @ 10 keV	> 10^{13} photons/s
Energy resolution $\Delta E/E$	< 10^{-4}
Beam size	500 x 500 μm^2 20 x 20 μm^2 (focused beam)
Detectors	• Multi-crystal analyzer • MYTHEN 18K • XRD1611

for four years (2017–2020), and has already produced over 40 scientific publications. It includes a large three-circle diffractometer with detectors of two types, a one-dimensional position-sensitive detector MYTHEN 18K and multi-crystal analyzers (**Fig. 2**). The detailed design and preliminary results have been reported in references 2 and 3. The second endstation of **TPS 19A** is specially designed for complicated setups such as a non-ambient environment or a sample that could not be loaded into a capillary tube, a diamond anvil cell for large pressure, gas loading, battery charge or discharge, reaction chambers with custom devices *etc*. The size of the incident beam can be focused from 600 to 20 μm with Kirkpatrick-Baez (KB) mirrors and hexapods (Physik Instrumente) for motion control (**Fig. 2**). The benefit of a smaller beam spot could be applied to those experiments requiring a small

Table 2: Experimental parameters and available non-ambient devices at **TPS 19A1** and **TPS 19A2**.

19A1	X-ray energy range: 12–20 keV Beam size: 500 x 500 μm^2 High-resolution PXRD measurement: MYTHEN 18K (Δ2θ: ~ 0.02°) Ultra-high-resolution PXRD measurement: Multi-crystal analyzer (Δ2θ: ~ 0.005°) Available non-ambient sample environments: 1. LN_2 cryostream (90 K–RT) 2. Hot-air gas blower (RT–1000 °C) 3. LHe Dynaflow cryostat (10 K–150 K)
19A2	X-ray energy range: 12–40 keV Beam size: 500 x 500 μm^2 (without KB focusing mirrors) Beam size: 20 x 20 μm^2 (with KB focusing mirrors) General resolution XRD measurement: XRD 1611 (Δ2θ: ~ 0.06°) Available non-ambient sample environments: 1. LN_2 cryostream (90 K–RT) 2. Hot air gas blower (RT–1000 °C) 3. Potentiostat (single cell: Autolab PGSTAT204; multi-cell Biologic VSP3e) 4. Gas loading system (N_2, CO_2, Ar, CO, H_2) 5. High-temperature oven (Anton Paar HTK1200N, RT–1,200 °C) 6. High-pressure (diamond anvil cell)

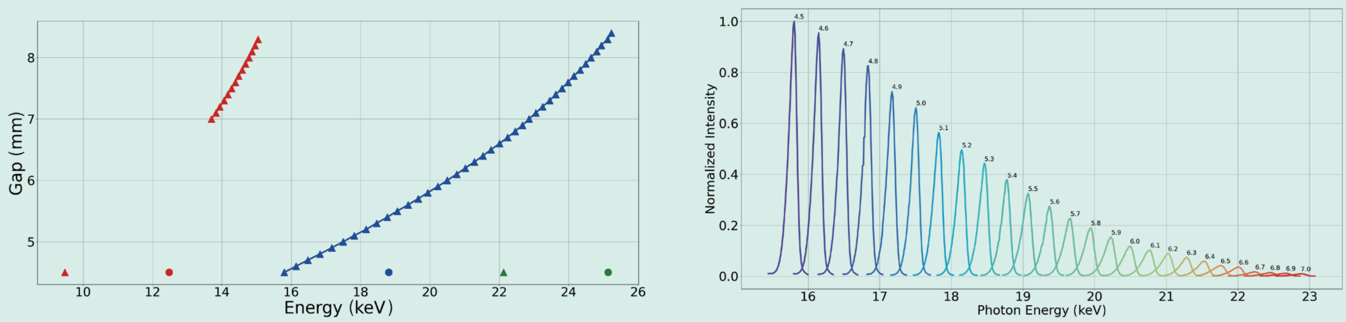

Fig. 1: Experimental gap size as a function of photon energy between the third and fifth harmonics.

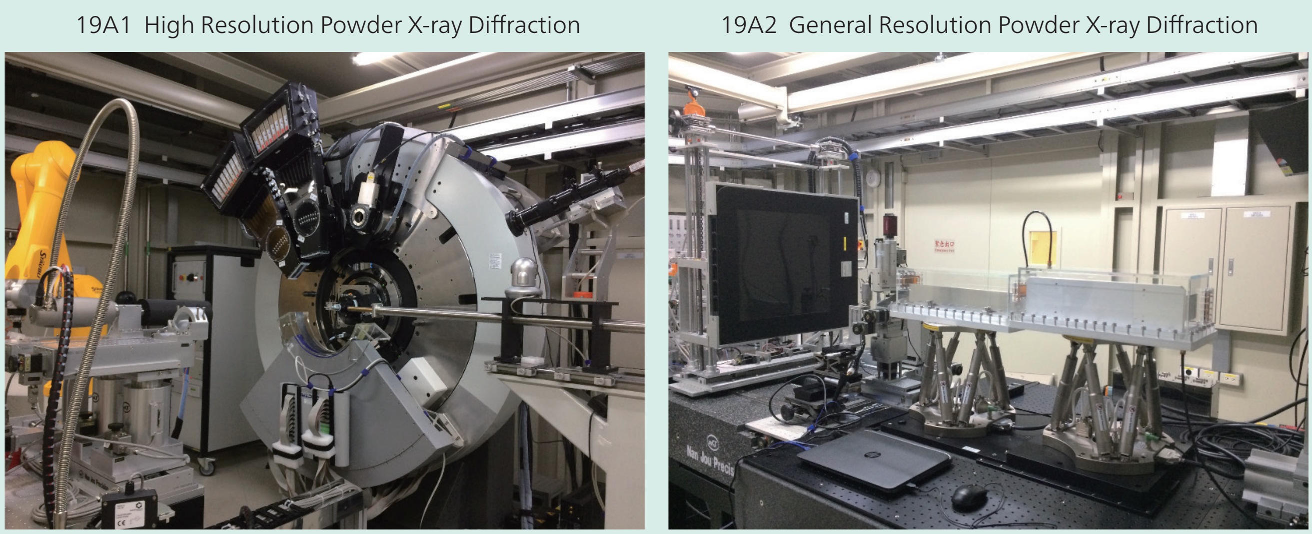

Fig. 2: Two endstations of **TPS 19A**: **TPS 19A1**, high-resolution XRD; **TPS 19A2** general-resolution XRD.

sampling area, such as a diamond anvil cell, deposition-coating films, or mapping study of bulk specimens. For a high acquisition rate and micro-structure analysis such as crystalline orientation, graininess and texture, an area detector (Perkin Elmer, Varex Imaging, XRD 1611) was selected as the scanning detector on **TPS 19A2**. This area detector provides a frame rate up to 15 frames per second and a Q coverage by 4096 x 4096 with pixel size 100 µm. In summary, **TPS 19A2** offers the option of X-ray diffraction (XRD) measurements focusing on structure or phase evolution with complicated setups *in situ*; it could otherwise be used as rapid scanning before the high-resolution experiment at **TPS 19A1**.

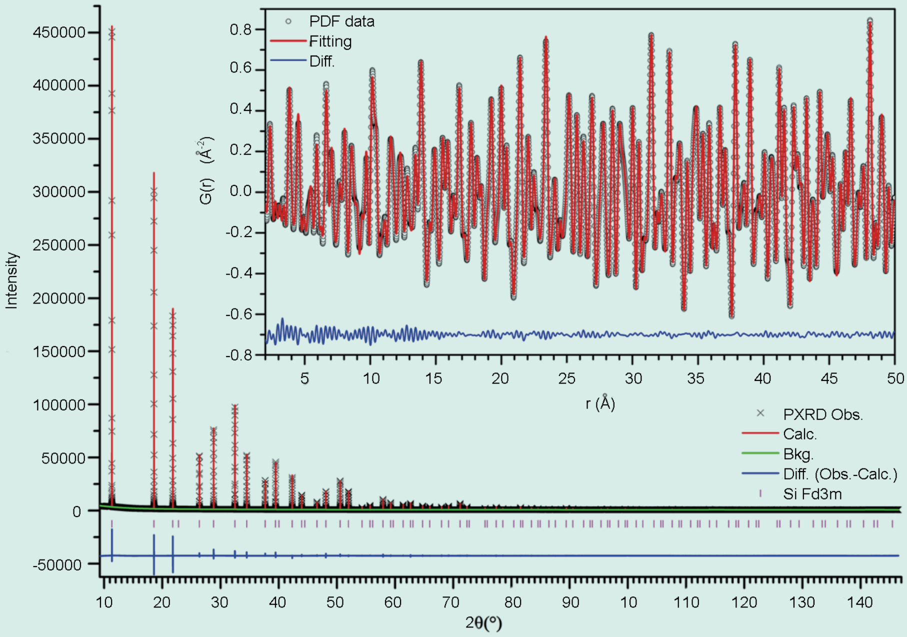

Fig. 3: Preliminary result for the pair distribution function of Si powder collected by MYTHEN 24K.

Apart from a material system with long-range ordering, many materials show their practical and interesting physical properties because of the short range of their local structure; developing PDF and rapid PDF (rPDF) is hence our long-term project. The expected X-ray energy for PDF is 30 to 40 keV, for which the maximum Q range can attain 20–30 $Å^{-1}$. A preliminary PDF study for a NIST standard material, Si (640d), is shown in **Fig. 3**, which was measured with a MYTHEN detector with X-rays of energy 20 keV. The rPDF is expected to be measured using a detector (2D XRD1611) with an integrated non-ambient system. Combining both high-resolution powder XRD and PDF techniques, **TPS 19A** provides a total solution for structure determination. It is believed that the users will appreciate the beamline performance and create many scientific results in the near future. (Reported by Yu-Chun Chuang, Chung-Kai Chang and Bo-Hao Chen)

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