Exploring the Dynamic Structural Evolution of Materials: TPS 20A Two-Dimensional X-ray Diffraction Beamline

Contemporary technology has evolved rapidly on the back of a solid understanding of material properties at the atomic level. Whether developing next-generation batteries, high-performance catalysts, or novel quantum materials, their properties such as conductivity, magnetism, thermal stability, and reactivity are governed by their internal crystal structures. However, in real-world applications, materials operate in complex environments involving heat, pressure, electricity, or gas adsorption. Consequently, modern materials science has shifted from merely identifying "static structures" to exploring the "dynamic evolution" of materials, such as how they undergo phase transitions, lattice distortions, or reconstruction under external stimuli.

To capture these dynamic processes under real-world operating conditions, the selection of appropriate experimental techniques is critical. Powder X-ray Diffraction has emerged as the preferred method for observing structural evolution under working conditions owing to its flexible sample preparation and compatibility with various environmental chambers. In this regard, the **TPS 20A** beamline was specifically designed to serve as a high-throughput platform with excellent temporal resolution. It allows researchers to continuously monitor structural evolution and capture transient phase transitions, thereby revealing the underlying kinetics and reaction mechanisms of functional materials.

The **TPS 20A** beamline uses a bending magnet source, delivering tunable X-ray energy of 8–30 keV. When using an Si (111) crystal monochromator, the energy resolution ($\Delta E/E$) reaches 2×10^{-4}, ensuring superior spectral quality. The photon flux at 10 keV is approximately 6×10^{11} photons/s, significantly exceeding that of the **TLS 01C2** beamline. This high flux is crucial for improving diffraction signal quality and dramatically reducing data acquisition time. The optical system has been optimized to provide a focused spot size of approximately 300 μm × 300 μm at the sample position, ensuring sufficient flux density and sampling volume.

The configuration of the endstation is illustrated in **Fig. 1**. This design balances the needs for "high-throughput screening" and "high-precision control". For large-scale powder analysis, the station features an automatic capillary alignment system paired with a robotic arm, allowing for fully automated sample exchange and maximizing data

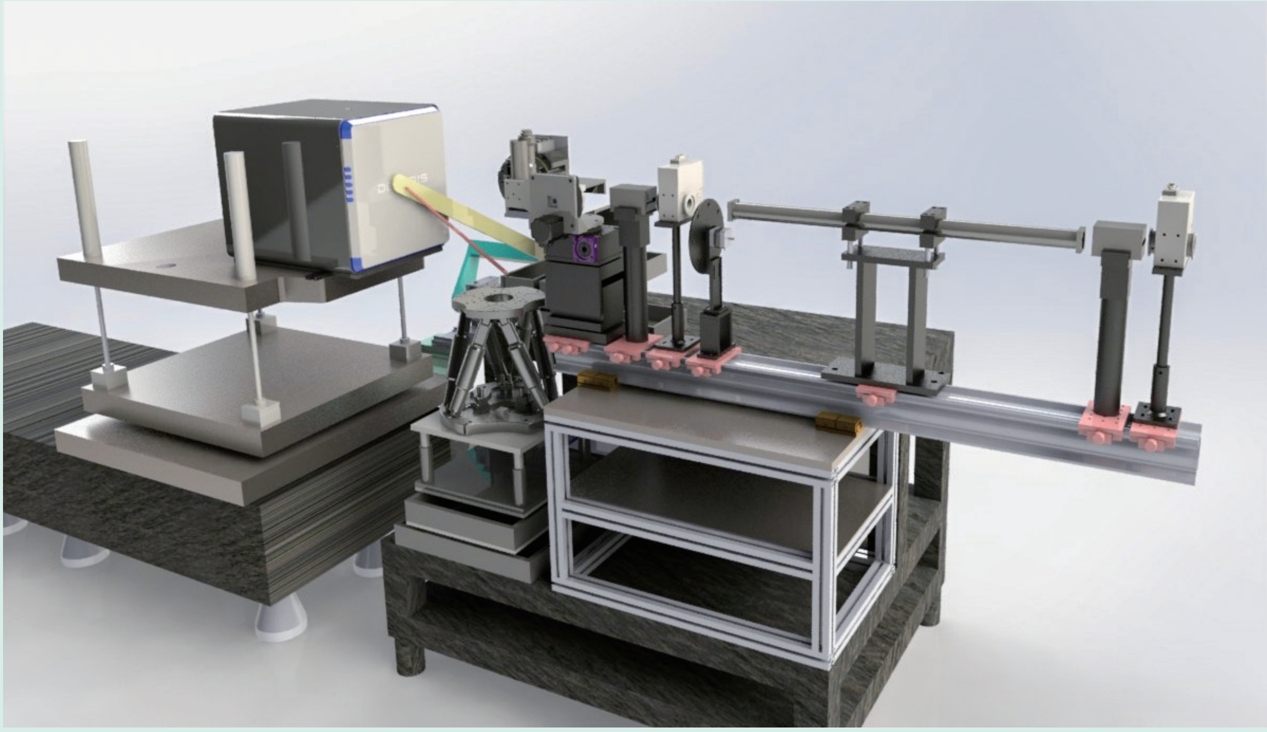

Fig. 1: Schematic diagram of **TPS 20A** endstation. The layout illustrates the arrangement of the Eiger2 S 16M detector, six-axis hexapod sample stage, and optical path configuration.

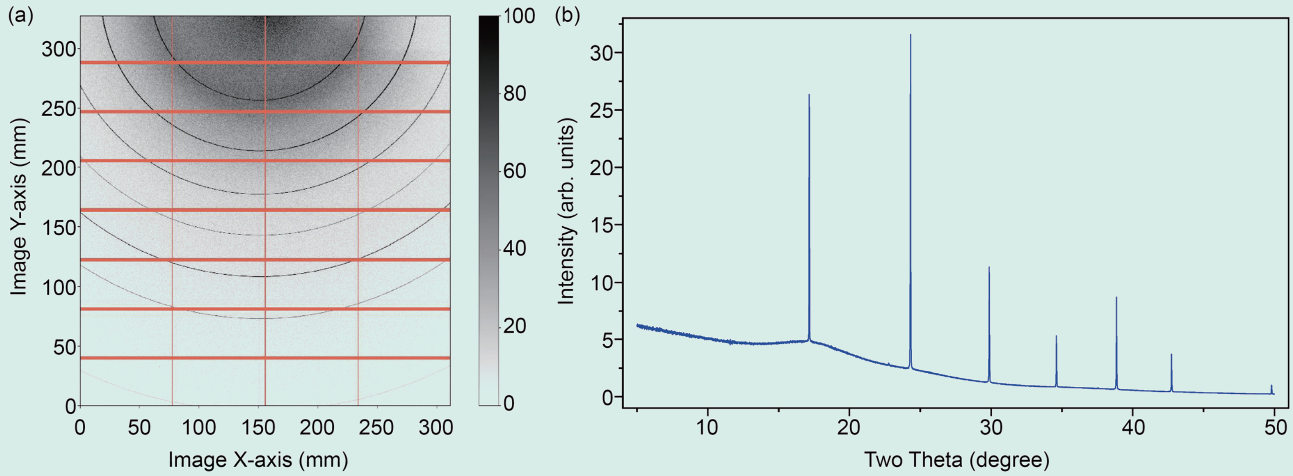

Fig. 2: Preliminary commissioning results at **TPS 20A**. (a) Two-dimensional powder diffraction pattern of a LaB6 standard, showing very low background noise. (b) Corresponding integrated intensity versus 2θ profile. Experimental conditions: Sample-to-detector distance of approximately 300 mm, covering a 2θ range of approximately 50°.

collection efficiency. For non-standard samples such as thin films, planar devices, or *in-situ* reaction chambers, a high-precision six-axis hexapod positioning stage is used. Unlike traditional stacked linear motors, the hexapod uses a parallel kinematic structure to provide exceptional stiffness and positioning accuracy across six degrees of freedom (X, Y, Z, pitch, roll, yaw). This capability is crucial for grazing incidence X-ray diffraction, where precise angular alignment is critical. Furthermore, the high load capacity of the hexapod allows it to stably support heavy *in-situ* equipment while maintaining micron-level stability.

To cater to diverse research needs, **TPS 20A** is equipped with comprehensive *in-situ* environmental equipment, including a high-temperature heat gun, low-temperature liquid nitrogen cryostream, potentiostat for electrochemical studies, and gas loading system. This versatility allows users from various fields to select environmental conditions appropriate for their specific experimental requirements. The detection system utilizes an Eiger2 S 16M photon-counting detector, which features a large active area (327.8 × 311.2 mm^2) and high pixel resolution (75 × 75 μm^2). These features help overcome the limitations of traditional image plates, such as slow readout and high noise, thereby significantly improving efficiency and dynamic range.

The hardware construction of **TPS 20A** is complete, and the beamline is undergoing commissioning with excellent preliminary results. Recent validation tests were performed using a LaB6 standard. With a sample-to-detector distance of approximately 300 mm, the system successfully collected diffraction signals covering a 2θ angle of approximately 50°. **Figure 2** shows the collected two-dimensional (2D) diffraction pattern and the corresponding integrated one-dimensional profile. The 2D pattern exhibits extremely low background and an exceptional signal-to-noise ratio. Compared to the image plate system at **TLS 01C2**, **TPS 20A** provides superior data quality and significantly shorter acquisition times, highlighting the advantages of photon-counting technology. Moreover, commissioning confirmed the flexibility of the detector stage, which allows users to adjust the detector position (centered or off-centered) and distance (closer to or farther from the sample) to optimize angular resolution and coverage according to experimental needs.

Looking forward, NSRRC's powder diffraction facilities will follow a strategic division of labor: **TPS 19A** will focus on high-resolution structural analysis, while **TPS 20A** will support experiments requiring longer reaction times and complex setups. Users of the existing **TLS 01C2** beamline will gradually be transitioned to **TPS 20A**, where they will benefit from more convenient and superior experimental facilities. During this transitional phase, the team will continue commissioning tasks, such as system integration, optimization, and testing various experiment types to ensure optimal beamline performance. **TPS 20A** is scheduled to open for general user proposals in the first quarter of 2026. In this initial phase, 20% of the beamtime will be allocated to general users. This facility is expected to be a powerful tool for the materials research community, facilitating deep exploration of functional materials, energy storage systems, and frontier physical properties. (Reported by Yen-Chung Lai)