

# EFFICIENT MULTI-REGION FLY-SCAN ARCHITECTURE USING PLC INTEGRATION FOR SYNCHROTRON XAS

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## Abstract

A high-speed fly-scan system has been developed and implemented at the Taiwan Photon Source (TPS) 32A Tender X-ray Absorption Spectroscopy (TXAS) beamline to enhance data acquisition efficiency for X-ray Absorption Spectroscopy (XAS). Unlike conventional fly-scan systems that rely on Field Programmable Gate Array (FPGA) or CompactRIO (cRIO) platforms, this system adopts a programmable logic controller (PLC)-based architecture, offering high modularity, low development complexity, and seamless integration with existing beamline infrastructure. The system enables continuous scanning of the double-crystal monochromator (DCM) while simultaneously acquiring synchronized data from multiple detectors. Analog-to-digital converters (ADCs) digitize current signals for transmission and total electron yield (TEY) modes, while high-speed digital outputs from the PLC provide external triggers for silicon drift detectors (SDDs) used in partial fluorescence yield (PFY) measurements. This approach simplifies the coordination of asynchronous devices and eliminates the need for complex timing hardware. To further optimize performance, a multi-region scan strategy was implemented, allowing dynamic adjustment of scan speed across different energy segments. This significantly reduces total scan time by up to a factor of six compared to traditional step-scan methods, while maintaining comparable spectral quality. The PLC-based fly-scan system also supports real-time data logging, automated sample switching, and energy-axis registration, making it a robust and scalable solution for time-resolved and in-situ XAS experiments.

## INTRODUCTION

The TPS 32A is a new beamline recently established at the TPS of the National Synchrotron Radiation Research Center (NSRRC) [1]. Utilizing a bending magnet source, it covers a photon energy range of 1.7-11 keV and delivers a highly purified X-ray beam with a small focal spot and minimal higher-order harmonic contamination. Fig. 1 illustrates the beamline schematic.

A significant challenge for this beamline is its inability to employ the common quick-scanning monochromators used elsewhere for rapid data acquisition [2, 3], due to its specific energy range. Consequently, reliance on the traditional step-scan method for collecting an Extended X-ray

Absorption Fine Structure (EXAFS) spectrum is highly inefficient, with each scan requiring 25 to 50 minutes to complete. This limitation severely restricts experimental throughput and the optimal use of the synchrotron source.

To overcome this bottleneck, we have developed and commissioned a new "fly-scan" data acquisition module for the TPS 32A beamline. This system successfully reduces the time for a full EXAFS scan to under one minute while maintaining exceptionally high data quality. The module supports multiple detection modes, including transmission, TEY, and PFY. Its development hinged on the precise synchronization of the monochromator's Bragg angle ( $\theta_B$ ) movement with various detectors, while also overcoming challenges related to electronic noise and signal triggering. The resulting fly-scan system now provides data quality comparable to the conventional step-scan method, thereby significantly enhancing the research capabilities and efficiency of the beamline.

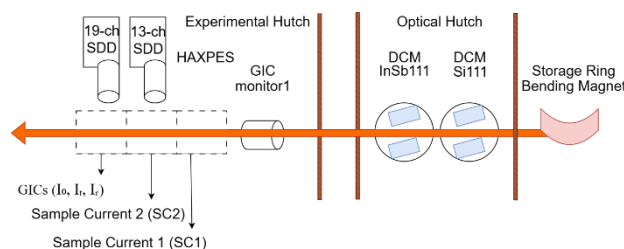


Figure 1: The schematic of the TPS 32A beamline.

During the initial phase of beamline commissioning, a conventional step-scan system was systematically established, along with several optimization tools, to verify the beamline design and support alignment and calibration procedures [4]. In traditional transmission XAS, the incident photon energy is varied by adjusting the pitch of the crystals ( $\theta_B$ ) in the DCM (Kohzu TWC-2A/B). At each energy point, the system pauses to record the current signals from gridded ionization chambers (GICs), which correspond to  $I_0$ ,  $I_i$ , and  $I_r$ . The scan then proceeds to the next energy position, repeating the measurement cycle. After numerous steps, a complete absorption spectrum is obtained. For PFY measurements, the system must dwell at each designated energy point to allow the SDD to integrate the signal over a defined exposure time, typically ranging from 0.4 to 4 seconds. Only after multiple exposures can a full fluorescence spectrum be acquired. The current signals from the GICs are amplified using NF-CA5351 amplifiers, while the sample current is measured using a Stanford Re-

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search Systems SR570. Both amplifiers convert the measured current into voltage signals, which are then processed through a voltage-to-frequency converter (Tsujiicon SVF8-01) and a counter module (Tsujiicon CT08-01C) during step-scan operation. This integration process yields averaged values to smooth the data and reduce noise. Quantum-Xpress3 SDDs configured with multiple channels are used for PFY detection. Under typical conditions, acquiring a full absorption or fluorescence spectrum spanning 1000 eV using the step-scan method requires around  $\sim 30$  minutes in high energy range ( $\sim 9500$  eV).

## FLY-SCAN SYSTEM ARCHITECTURE

Compared to the conventional step-scan method, which requires significant time for mechanical settling at each energy point, the fly-scan approach enables continuous motion and synchronized data acquisition, significantly improving measurement efficiency. To implement this, the team evaluated core architectures commonly used in various facilities, including PandABox [5] and the NI cRIO platform [6].

In our system, the  $\theta_B$  of the DCM is driven continuously while synchronized gating signals are sent to the SDD controller. These signals are generated by a high-speed digital output module, enabling time-resolved integration without interrupting motion. The fly-scan system is built on the Keyence PLC platform, with the following modules integrated:

- KV-8000 – Main controller for motion coordination and signal routing.
- KV-SAD04 – 16-bit ADC for real-time current signal acquisition.
- KV-SSC02 – BiSS-C encoder reader for precise position feedback from the DCM motor.
- KV-SIR32XT – High-speed digital output module for generating synchronized trigger pulses to the SDD controller.

Motion commands are issued via EPICS, while energy positions and timestamps are recorded directly by the PLC. This dual-layer architecture ensures precise synchronization between mechanical motion and data acquisition.

To accommodate varying resolution requirements across the energy range, the system supports multi-region scanning. Finer energy steps are applied near the absorption edge, while coarser steps are used in pre-edge and post-edge regions. This segmented scanning strategy balances spectral resolution and total acquisition time.

### The Schematic of the Fly-Scan System

The overall architecture of the fly-scan system is illustrated in Fig. 2. At its core is a PLC-based control framework, which integrates multiple modules to coordinate motion, signal acquisition, and timing synchronization. The encoder module continuously reads the  $\theta_B$  value, while current signals from the GICs are amplified by preamplifiers and converted into voltage signals. These analog signals are digitized by a 16-bit ADC module and subsequently read into the PLC for processing.

To ensure precise timing across all modules, the system utilizes the KV-8000's "unit interrupt / inter-unit synchronization" function [7], which guarantees that data acquisition and recording are completed within a  $4 \mu\text{s}$  window. This mechanism effectively minimizes timing jitter between modules and ensures that all signals are captured in a tightly synchronized manner.

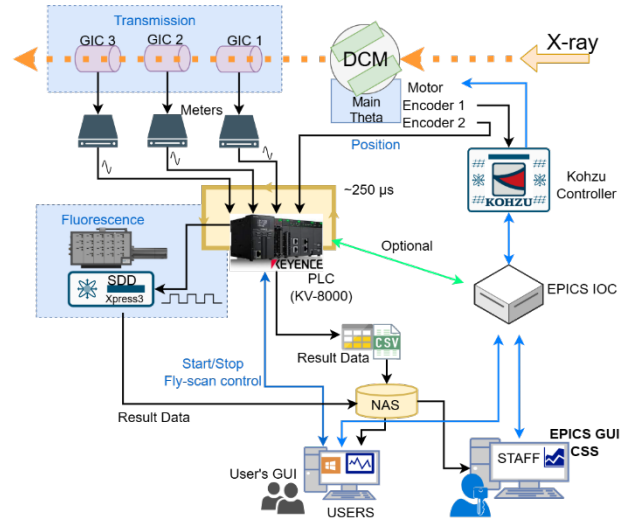


Figure 2: Architecture of the fly-scan system at TPS 32A beamline.

### Timing System Overview

To ensure that the SDD receives a gating signal precisely during each acquisition cycle, the KV-SIR32XT high-speed digital output module is used to generate square wave pulses. The timing relationship of these pulses is illustrated in Fig. 3.

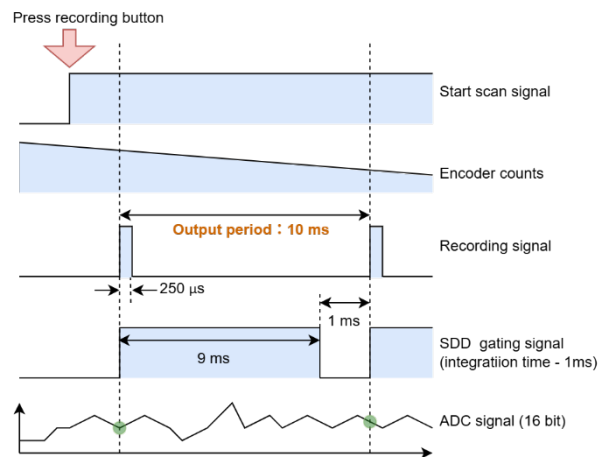


Figure 3: Signal timing structure of the fly-scan system, including encoder, ADC, and SDD gating.

For example, with a data output period of 10 ms, the actual integration time provided to the SDD is 9 ms. A 1 ms gap is intentionally inserted between pulses to allow the multichannel analyzer (MCA) to clearly distinguish each gating event. The timing control is governed by the PLC's built-in  $10 \mu\text{s}$  clock, which ensures consistent pulse generation and precise synchronization throughout the scan.

In fly-scan measurements, the digital pulse processor (DPP) paired with the SDD exhibits a variable delay of 0.9–1.2 s between receiving the trigger from the PLC and initiating integration. This delay desynchronizes the acquisition of the incident intensity  $I_0$  and the fluorescence intensity  $I_f$ , leading to energy-axis misalignment and producing anomalous features (glitches) in the EXAFS region, as indicated by the red trace in Fig. 4. To correct the misalignment, an energy-axis registration algorithm was developed that minimizes the root-mean-square error (RMSE), thereby suppressing spectral distortions arising from acquisition asynchrony. The RMSE of a spectrum is defined as

$$RMSE = \sqrt{\frac{1}{N} * \sum_{E_i \in N} (u(E_i) - u_b(E_i))^2} \quad (1)$$

Where  $u(E_i)$  denotes the absorption coefficient at the  $i$ -th energy point,  $u_b(E_i)$  is the corresponding reference background absorption coefficient, and  $N$  is the total number of spectral points. In implementation, a three-point moving average is first applied to smooth the spectrum and estimate the background  $u_b(E)$  used for RMSE evaluation. Subsequently, the spectrum is shifted stepwise along the energy axis within a window of  $\pm 5$  data points, and—after subtracting the background from the raw spectrum—the corresponding RMSE is computed for each trial shift. The energy position associated with the minimum RMSE is taken as the corrected registration. As shown in Fig. 4, the corrected spectrum agrees with the step-scan data, and the glitch originally present in the EXAFS region disappears, demonstrating that the energy-axis alignment algorithm effectively compensates spectral distortions induced by the DPP integration-onset delay.

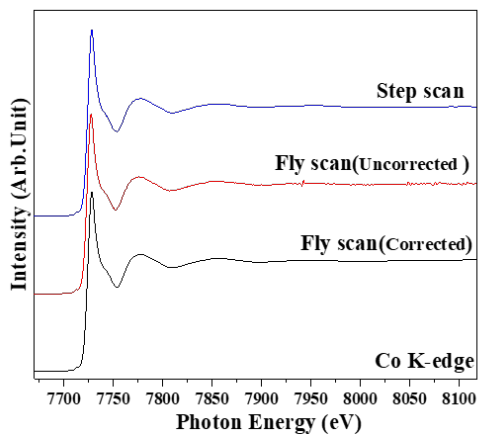


Figure 4: Co K-edge spectra acquired by step-scan, fly-scan (uncorrected), and fly-scan (corrected).

### Motion Control and Data Logging

In the fly-scan system interface, motion control—specifically the variation of the DCM's crystals ( $\theta_B$ )—is executed via EPICS, which communicates with the Kohzu motor controller and driver. Once the scan is initiated, the system simultaneously activates the PLC's built-in operation logging function. This feature enables real-time and synchronized recording of position and voltage data into a .csv

file, which is automatically stored on the internal FTP server, eliminating the need for custom programming.

Regarding data from the SDD, since it operates under external triggering, its output is stored internally in HDF5 format by the Quantum system [8]. The number of trigger events corresponds directly to the number of entries recorded by the PLC, allowing for straightforward data alignment. By matching these entries, the HDF5 fluorescence data can be integrated into the .csv file for consolidated analysis. For data verification, the PLC model used also supports built-in playback functionality. This allows frame-by-frame review of each register based on the scan time resolution ( $\sim 250 \mu\text{s}$ ), providing a reliable method for validating the integrity and timing of recorded data.

### Graphical User Interface (GUI) Interface and Multi-Region Scan Configuration

The scan software developed for TPS 32A is built on the LabVIEW platform, featuring a GUI that integrates a wide range of functionalities [4]. These include real-time trend plots for individual electrometers, sample thickness inspection, standard sample and filter switching, parameter import/export, energy calibration, and more.

The fly-scan functionality was successfully integrated into the software, which includes a unified operational interface and a dedicated configuration panel for multi-region fly-scan setup, as shown in Fig. 5.

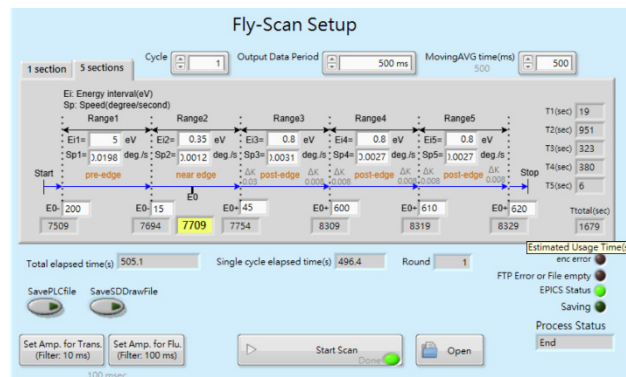


Figure 5: Fly-scan configuration panel with multi-region energy range setup.

The fly-scan interface allows users to specify the number of scan cycles, enabling repeated scans over the same energy range. The output data period defines the time interval between each recorded data point and can be selected from predefined values: 0.01, 0.1, 0.5, 1, 1.5, 2, 3, or 4 seconds.

Once the user inputs a desired energy interval ( $E_i$ ), the interface automatically calculates the corresponding scan speed ( $Sp$ ). This design reflects user habits, as energy is typically specified in electron volts (eV), while the monochromator operates in angular units. Because the relationship between energy and  $\theta_B$  is nonlinear, the system must dynamically adjust scan speed to maintain consistent energy spacing.

For the TPS 32A beamline using the DCM model S111, the conversion between energy and  $\theta_B$  is defined by the following equation:

$$\theta_B = \sin^{-1} \frac{1977.293022}{E} \times \frac{180}{\pi} \quad (2)$$

Due to this nonlinear relationship, different energy regions require different angular velocities to achieve uniform energy intervals. By varying the scan speed within the same energy range, users can fine-tune the energy resolution as needed.

The maximum allowable scan speed is limited to 0.11 degrees per second, based on the mechanical constraints of the DCM and the manufacturer's recommended operating limits.

In previous studies, fly-scan techniques were typically executed using a single scan speed across the entire energy range. However, in XAS, only the near-edge region requires finer energy intervals ( $E_i$ ), while the pre-edge and post-edge regions do not demand such high resolution.

As illustrated in Fig. 6, applying uniformly fine steps throughout the spectrum would significantly slow down the overall scan. To reduce total acquisition time without compromising spectral quality, we divided the energy range into three or more segments and assigned different scan speeds to each region. This approach allows for efficient data collection by applying slower speeds where high resolution is needed and faster speeds where coarse sampling is sufficient.

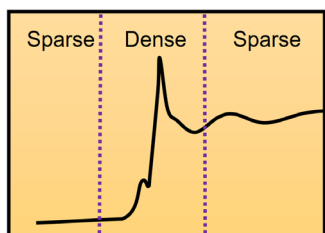


Figure 6: Energy segmentation strategy for multi-speed fly-scan.

However, the current Kohzu motor controller does not support dynamic speed changes during motion. As a result, the system must pause between scan segments to switch speeds, which introduces unnecessary delays and reduces overall efficiency. A comparison between the ideal speed transition and the current implementation provided by Kohzu is illustrated in Fig. 7.

To address this limitation, we have initiated plans to replace the motor controller with a model capable of real-time speed modulation. Details of the motion control upgrade strategy will be discussed in a later section.

In the post-edge region of EXAFS, data is often analyzed in terms of momentum space using the  $k$ -value, which relates to photon energy ( $E$ ) through the following equation:

$$k = \sqrt{0.2625 \times (E - E_0)} \quad (3)$$

This nonlinear relationship implies that a single scan segment across the post-edge region would result in uneven sampling—dense at the beginning and sparse toward the end. To address this, the energy range was divided into five distinct segments, each configured with appropriate scan speeds to match the required energy resolution.

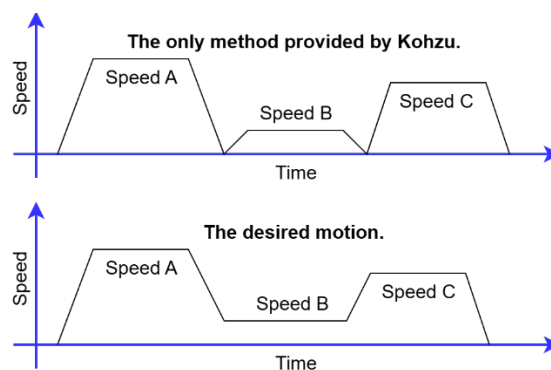


Figure 7: Comparison between ideal speed transition and current Kohzu implementation.

Despite the need for brief pauses between segments due to hardware limitations, this segmented approach offers substantial time savings. Compared to a single-speed scan designed to satisfy the fine energy interval ( $E_i$ ) requirements of the near-edge region, the five-speed configuration reduces total scan time by a factor of six or more.

For example, the conventional step-scan method typically requires approximately 25 minutes to complete a typical EXAFS Fe K-edge spectrum of the Fe foil obtained in transmission mode. In contrast, a single-speed fly-scan reduces the acquisition time to around 15 minutes. By employing a five-region fly-scan configuration, the total scan time can be further reduced to approximately 5 minutes, while maintaining comparable data quality. This demonstrates the significant efficiency gains achievable through segmented scanning strategies.

### Data Optimization

In the fly-scan system, two primary methods are available for data optimization: moving average smoothing and filter adjustment on the preamplifier. Each plays a distinct role in improving signal quality.

The moving average function is located in the upper-right corner of the GUI and is automatically configured based on the selected output data period. Manual adjustment is also supported. Given that the PLC's scan time is 250  $\mu$ s, selecting a 1-second output data period results in each data point being averaged over 4000 samples. This function is built into the Keyence ADC module (KV-SAD04), which supports averaging times up to 1500 ms. As a native feature, it requires no additional programming, making it highly convenient for users.

Another effective method for signal enhancement is low-pass filter adjustment on the preamplifier. This filter is commonly available on most preamplifier models and is particularly useful for suppressing high-frequency noise that cannot be fully eliminated by moving average alone. However, the filter parameters must be tuned according to the scan speed. In the near-edge region, where signal variation is rapid, a filter frequency that is too low may cause edge features to drift or smear.

Based on our experience, PFY scans involving SDD detection typically use a 10 Hz (100 ms) low-pass filter setting. For transmission scans, which do not involve the SDD

and generally operate at higher scan speeds, a 100 Hz (10 ms) filter is preferred. These settings strike a balance between noise suppression and spectral fidelity, ensuring that edge features remain sharp and data remains stable.

### *Multi-Sample Scanning and Automation*

At the TPS 32A beamline, two methods are employed for automated sample switching. For samples measured under ambient conditions, a robotic arm is used to pick and place specimens. For vacuum-based experiments, multiple samples are mounted on a single platform at predefined positions, and switching is achieved by adjusting the stepper motor to align each sample with the beam.

Both configurations support fly-scan and step-scan modes, enabling one-click execution of multi-sample scans—up to 99 samples per session. This automation significantly improves experimental throughput and minimizes manual intervention during extended measurement campaigns.

## CONCLUSION

The fly-scan system developed at TPS 32A is now officially available for external users. Compared to the traditional step-scan method, it achieves equivalent data quality while reducing acquisition time by up to two orders of magnitude. The PLC-based architecture offers several advantages, including high scalability, broad compatibility, low implementation cost, ease of replication, and straightforward development. Moreover, the design of DCMs at TPS 32A allows single-axis motion during scanning. This simplifies system control and contributes to the efficiency of the fly-scan implementation. The fly-scan approach described in this work will be extended to the upcoming beamlines, which will require coordinated multi-axis motion to maintain beam height during scanning. To meet these demands, a PLC-based controller with EtherCAT communication will be adopted to support synchronized

multi-axis control and data acquisition. This upgrade represents a major advancement in extending fly-scan capabilities across additional beamlines in the TPS facility.

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