ON-THE-FLY SCANNING: IMPROVING SCAN TIME OF XAFS AT BM08-XAFS/XRF BEAMLINE

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Abstract

In this work, we present the use of PandABox timing module to implement position-based and time-based on-the-fly scanning to continuously acquire data at the X-ray Absorption Fine Structure (XAFS) and X-ray Fluorescence (XRF) beamline of SESAME synchrotron light source. For position-based scanning, we first developed a module that automatically partitions the user-defined energy and Bragg angle ranges into sub-intervals. Within each sub-interval, the energy-angle mapping is linearly approximated to maintain accuracy within acceptable margins. The method then integrates the position encoding of the Double Crystal Monochromator (DCM) Bragg angle with the synchronous triggering of multiple detectors, including ionization chambers (ICs) and a KETEK SSD detector. For time-based scanning, PandABox is pre-configured to generate triggers at fixed time exposure time intervals. Improvements, performance and comparative results are also discussed in this work.

Keywords: on-the-fly scanning, QEXAFS, DAQ, PandABox, linear fitting, XAFS/XRF

INTRODUCTION

The BM08-XAFS/XRF beamline at SESAME Synchrotron in Jordan serves users who need to measure X-ray Absorption Fine Structure and X-ray Fluorescence spectra [1]. BM08 has traditionally operated in step-scan mode where the DCM moves to an energy point, waits for the mechanics to settle, collects data, then moves on to the next point. This stop-and-go cycle works reliably, but it wastes a lot of time. For a typical XAFS scan spanning hundreds of energy points, the settling delays add up to a significant fraction of the total beamtime time that could otherwise be spent collecting more scans or studying faster sample dynamics.

To enhance system performance, we implemented an on-the-fly scanning mode in which the DCM continuously moves across the user-defined energy range while the detectors are being triggered synchronously at specific pre-calculated energies (angle positions). This eliminates the settling overhead entirely. Similar technique has been adopted at several major facilities worldwide, including the ESRF BM29 beamline [2], the QXAS mode at Diamond B18 [3], the SuperXAS beamline at the SLS [4], and the general XAFS beamline at SSRF [5] in order to reduce acquisition times from tens of minutes to a few seconds while maintaining data quality comparable to step scanning. Continuous on-the-fly scanning can in some few cases be implemented in software (i.e. no need for hardware triggering), as demonstrated at the BEATS beamline [6], our goal is to make it available across all beamlines, on a best-effort basis and whenever applicable as it is already mentioned in our DAQ stander [7, 8]. Currently, we are implementing on-the-fly scanning on HESEB beamline [9].

In this work, we report the implementation of two complementary continuous scanning modes at the BM08 beamline: a *position-based* mode, where triggers are generated at specific encoder positions, and a *time-based* mode, where triggers are generated at fixed time intervals. Both modes rely on a PandABox timing module to synchronize all participating subsystems.

SYSTEM ARCHITECTURE

Beamline Control Infrastructure

The BM08 DAQ system is built on top of the EPICS control system and includes a modular Python-based scanning tool that supports multiple scan modalities and energy calibration. A Qt-based graphical interface, together with epicsQt for live experimental data visualization, allows users to configure and execute scans without interacting directly with low-level control system commands [10]. The detectors connected to the system include ICs for transmission measurements and a KETEK detector for fluorescence measurements.

PandABox Synchronization Module

Continuous scanning is achieved using PandABox, an FPGA-based timing and position-capture module [11]. The module reads the Bragg-angle encoder in real time and continuously tracking of the position during motion. Depending on the selected scan mode, it generates hardware gate signals to trigger all detectors simultaneously, either when the encoder reaches predefined angular positions or at fixed time intervals. As synchronization is handled at the hardware level, the timing remains precise and consistent for every acquired data point.

Architecture and pipeline is described in Figure 1. Also, the internal PandABox block configuration used for this work is shown in Fig. 2.

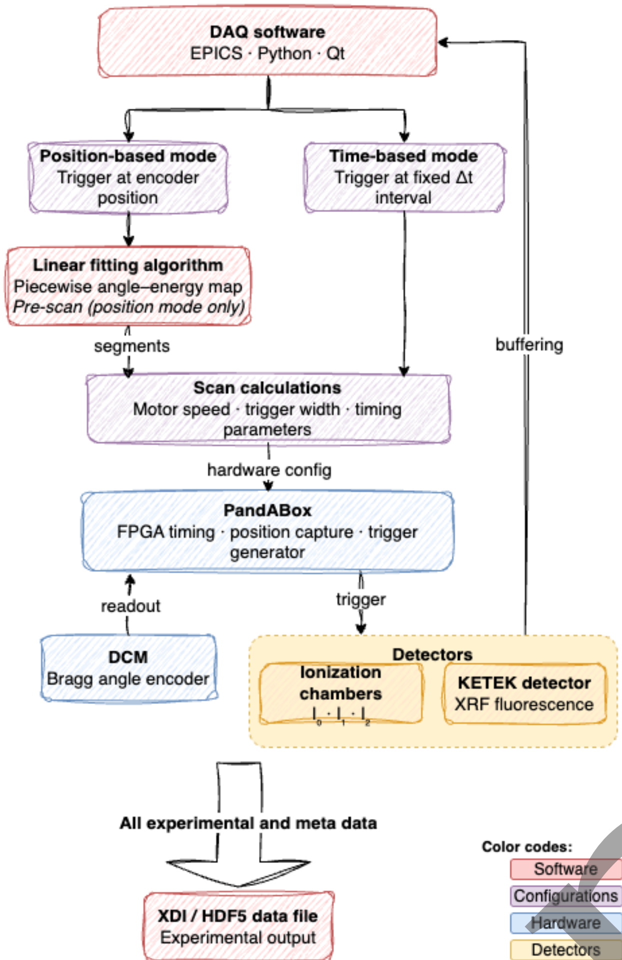

Figure 1: On-the-fly scanning system at BM08 (architecture and pipeline).

CONTINUOUS SCAN IMPLEMENTATIONS

Position-Based Continuous Scan

In this mode, PandABox generates a trigger every time the Bragg angle encoder reaches a pre-calculated position. The main challenge is the nonlinearity between Bragg angle and photon energy, that means uniformly spaced energy points do not map to uniformly spaced angles. To avoid solving this relation in a restricted operation that would limit users to predefined intervals, a piecewise-linear approximation is used.

A head of each scan, DAQ divides the full angle range into sub-intervals and fits a straight line to the angle–energy relationship within each sub-interval (linear segments). The fitting is validated to stay within a confirmable tolerance. Trigger positions are then calculated from the user-defined settings such as exposure time and step size, together with the linear-segment approximation, and loaded into the lookup table of PandABox segment by segment to avoid table overloading. The implementation is available in `linearIntervals.py` and `engScanContPos.py` in the open-source scan tool [10].

The main advantage of this mode is that each data point is tied directly to an encoder position, so the energy assignment is independent of how fast or slow the DCM was moving at that moment. This makes it the preferred mode when energy accuracy matters most.

Time-Based Continuous Scan

In this mode, the PandABox triggers the detectors at fixed time intervals while the energy changes continuously. The energy of each data point is determined after acquisition by matching timestamps with the recorded encoder positions. This mode is simpler to configure and is suitable when uniform time sampling is preferred over uniform energy sampling. However, any variation in DCM speed during the scan results in non-uniform energy spacing between data points [11].

PERFORMANCE RESULTS

We performed the same scan using the three acquisition modes and compared the total scan time for each. Table 1 summarises the results of some samples where the continuous scan modes achieved a reduction of approximately 70% in total scan time relative to the step scan.

Table 1: Comparison of Scan Time for a Representative XAFS Scan Using Three Acquisition Modes

Scan Mode	Energy Points	Scan Time [s]
Step scan	1468	5109
Continuous (pos.)	1527	1532
Continuous (time)	1566	1580

For data quality, spectra collected in continuous mode were compared with the step-scan reference. Figure 3 shows the Cu K-edge spectrum of a Cu foil measured in step-scan and position-based continuous modes. The two spectra overlap closely across the XANES region, the EXAFS oscillations, and the Fourier transform, indicating that the continuous mode introduces no measurable artifacts. Figure 4 presents the same comparison for the Ni K-edge using the time-based mode.

CHALLENGES AND LIMITATIONS

The speed of continuous scans is limited by the maximum angular velocity of the DCM motors, which imposes a lower bound on the achievable scan time. This is usually not restrictive for wide energy ranges, but it becomes a practical constraint for narrow scans where maximum speed is desired.

In contrast, the ICs at BM08 are connected to an Analog to digital Converter (ADC) that generates internal data pulling triggers independently of the PandABox. This causes a timing mismatch that introduces latency between the two subsystems. Moreover, the minimum integration time supported by the ADC is 0.7 s, limiting the achievable energy resolution during fast continuous scans.

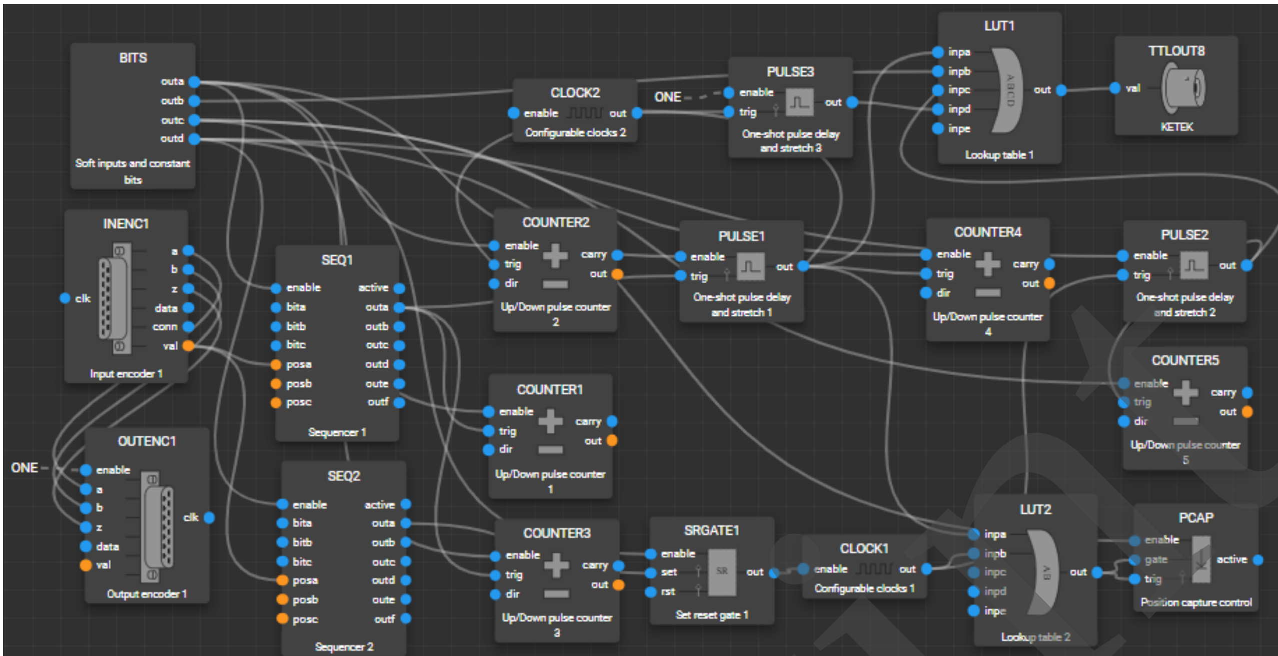

Figure 2: PandABox internal block configuration for the continuous scan system at BM08. The input encoder block (INENC1) reads the DCM Bragg angle in real time. Two sequencer blocks (SEQ1, SEQ2) generate the trigger sequences for the position-based and time-based scan modes respectively. Pulse, counter, clock, and lookup table (LUT) blocks handle timing logic and route gate signals to the ICs and the SSD KETEK detector (TTLOUT8). The position capture block (PCAP) records encoder positions at each trigger for post-processing.

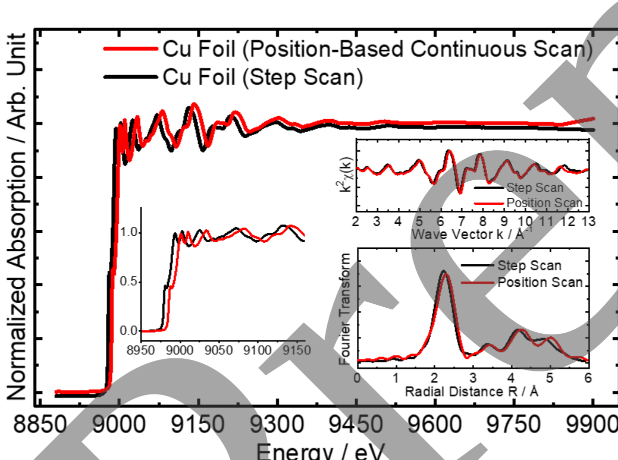

Figure 3: Cu K-edge (8979 eV) XAFS of Cu foil: step scan (grey) vs. position-based continuous scan (red). Insets show the XANES region, $k^2\chi(k)$, and Fourier transform of $\chi(k)$.

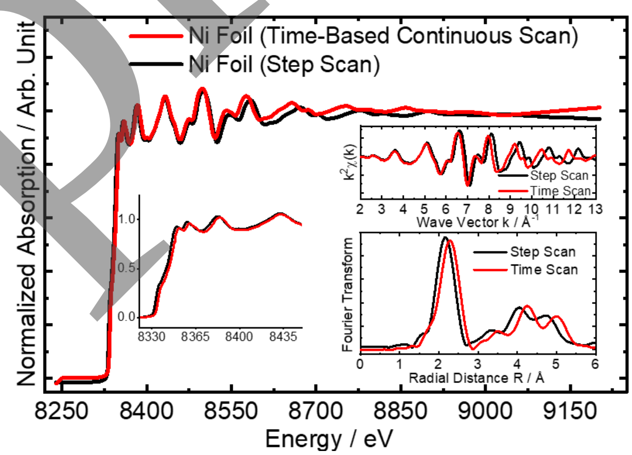

Figure 4: Ni K-edge (8333 eV) XAFS of Ni foil: step scan (grey) vs. time-based continuous scan (red). Insets show the XANES region, $k^2\chi(k)$, and Fourier transform of $\chi(k)$.

Because the current detector drivers do not support streaming, the DAQ software writes each data point to storage as soon as the corresponding trigger is received. This point-by-point I/O introduces latency that partially reduces the time savings gained from continuous motion.

CONCLUSION

We have successfully implemented on-the-fly scanning at the BM08-XAFS/XRF beamline of SESAME Synchrotron. In addition to step scanning and mapping scan, this offers two continuous scan modes, position-based and time-based. Such enhancements have dramatically improved scan time and user satisfaction. By changing energy without stopping at DCM and using a PandABox module to trigger detectors at the right moments, we eliminate the settling overhead that makes step scans slow. Experimental data comparisons confirm that data quality is preserved in both modes. The position-based mode goes a step further by using a piecewise-linear fitting algorithm to ensure accurate energy assignment even across wide scan ranges. Known limitations, the 0.7 s ADC integration floor and per-point data writing are being addressed in future work. The scan tool, PandABox settings and other related modules are open source and available on SESAME's GitHub repository [10].

REFERENCES

[1] M. Harfouche *et al.*, "Emergence of the first XAFS/XRF beamline in the Middle East", *J. Synchrotron Rad.*, vol. 29, pp. 1107–1113, 2022. doi:10.1107/S1600577522005215

[2] C. Prestipino *et al.*, "Quick-EXAFS implementation on the general purpose EXAFS beamline at ESRF", *J. Synchrotron Rad.*, vol. 18, pp. 176–182, 2011. doi:10.1107/S0909049510046546

[3] A. J. Dent *et al.*, "B18: A core XAS spectroscopy beamline for Diamond", in *J. Phys.: Conf. Ser.*, vol. 190, p. 012039, 2009. doi:10.1088/1742-6596/190/1/012039

[4] O. Müller *et al.*, "Quick-EXAFS setup at the SuperXAS beamline for in situ X-ray absorption spectroscopy with 10 ms time resolution", *J. Synchrotron Rad.*, vol. 23, pp. 260–266, 2016. doi:10.1107/S1600577515018007

[5] Y. Zhou *et al.*, "A new QEXAFS system on the general XAFS beamline at the Shanghai Synchrotron Radiation Facility", *J. Synchrotron Rad.*, vol. 29, pp. 1461–1468, 2022. doi:10.1107/S1600577522008177

[6] G. Iori *et al.*, "BEATS: BEAmline for synchrotron X-ray microTomography at SESAME", *J. Synchrotron Rad.*, vol. 31, pp. 1358–1372, 2024. doi:10.1107/S1600577524005277

[7] M. Alzubi *et al.*, "Experimental Data Collection Standards at SESAME Synchrotron", in *Proc. PCaPAC'22*, Dolní Břežany, Czech Republic, 2023, pp. 116–119. doi:10.18429/JACoW-PCaPAC2022-FRO23

[8] M. Alzubi, A. Mohammad, S. Matalgah, and M. Harfouche, "Data Acquisition in SESAME Synchrotron", *Synchrotron Radiat. News*, vol. 37, no. 6, pp. 23–28, 2024. doi:10.1080/08940886.2024.2432346

[9] A. Abbadi *et al.*, "HESEB Soft X-ray Beamline ID11-L at SESAME: Performance and First User Experiments", *J. Phys.: Conf. Ser.*, vol. 3010, no. 1, p. 012043, 2025. doi:10.1088/1742-6596/3010/1/012043

[10] M. Al-Zubi *et al.*, "XAFSScanTool: BM08 XAFS/XRF Beamline DAQ System", SESAME Synchrotron, open-source software, 2024. https://github.com/SESAME-Synchrotron/XAFSScanTool

[11] T. Cobb *et al.*, "PandABox: A Modular Detector Trigger and Position Capture System", in *Proc. ICALEPCS'19*, New York, USA, Oct. 2019, pp. 871–875. doi:10.18429/JACoW-ICALEPCS2019-WEPHA083