On-the-fly Scan: Improving the Performance of Absorption Spectrum Measurement

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Abstract. The efficiency of conventional point-to-point scan is limited by overheads from mechanical system and data acquisition system. With network-friendly development interface provided by commercial software and hardware, the DAQ system, the position encoding system, the undulator, and the monochromator system can be easily controlled by synchronizing various instruments for on-the-fly scanning operation. In this work, an on-the-fly scanning method is developed for absorption spectrum measurement under the Labview’s programming environment. We have tested its performance on Dragon type beamlines at NSRRC. For a given energy resolution and a S/N level our preliminary results show that the time required to obtain a spectrum of Near Edge X-ray Absorption Fine Structure (NEXAFS) and X-ray Absorption Spectroscopy (XAS) using the on-the-fly scanning system is about 10 times and 20 times shorter than those using the point-to-point scanning with bending magnet and undulator sources, respectively. The higher efficiency gained from the on-the-fly scanning system results from minimizing system communication time and mechanical system overheads. The new improved technique should significantly contribute to the study and measurement of photon dose sensitive samples.

Keywords: On-the-fly scan, point-to-point scan, monochromator
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INTRODUCTION

The traditional point-to-point scan method has been used for photo-absorption measurements, e.g., Near Edge X-ray Absorption Fine Structure (NEXAFS) and X-ray Absorption Spectroscopy (XAS). However, there are photon dose sensitive samples that will face serious radiation damage during sample illumination time. For example, octadecyltrichlorosilan (OTS) exhibits self-assembled monolayer in the presence of X-ray photons. Thus, the NEXAFS spectrum of OTS depends on illumination time. For a conventional point-to-point scan method, the undulator, the grating and slit positions are sequentially driven to the required positions for a given photon energy. Much of the times are wasted in the system communication and mechanical overhead. Developing a high efficient on-the-fly scanning measurement scheme is one of the ways to solve this problem.

The on-the-fly scanning technique has previously been demonstrated and successfully operated for PGM type beamlines at SLS [1]. In this work, we are currently developing an on-the-fly scanning method for Dragon type beamlines [2,3] at NSRRC. The on-the-fly energy scan requires synchronizing various motions including undulator gap, grating and exit slit positions during energy scanning to obtain the optimum flux throughput, energy accuracy and resolving power to meet the spectral quality as that obtained by the point-to-point scan. Because the monochromator of Dragon type consists of grating and entrance/exit slits only, the synchronization of monochromator and undulator motions are thus simpler than that of PGM. In this preliminary work, we have introduced a software-based on-the-fly scheme for Dragon beamline without even upgrading any hardware, and have found that the data acquisition time is about 10 and 20 times shorter than that of point-to-point scan on the bending magnet and undulator sources, respectively. In the following we shall describe the detailed working scheme and show the obtained NEXAFS and XAS spectra to evaluate the performance of the on-the-fly scanning method.
THE DATA ACQUISITION AND ENERGY SCANNING SYSTEM SCHEME

Data acquisition (DAQ) system is one of the bottle necks for on-the-fly-scanning performance. In this work, a high speed NI USB-6259 M-series DAQ module is used for acquisition of the detecting system signal. A LabVIEW program working with NI-DAQmx driver software can easily control this DAQ module with automatic timing, triggering, and synchronization. Base on this hardware and software environment, the signals steams can be easily downloaded to the computer with high speed. We only need to define the DAQ system sampling rate. The data signal array can be automatic synchronization with equal time interval.

The on-the-fly scan control flow and data acquisition scheme are shown in Fig. 1. The Dragon type beamline energy setting is defined by the grating rotation angle and the exit slit, i.e., moving to the image point of grating in order to optimize the monochromator resolving power. During energy scanning the computer can read the scanning drive system position by linear encoder through RS232 interface with an 8 Hz reading rate. The relation between the grating rotation angle and the linear encoder reading was calibrated by interferometer. The optimization slit scanning rate was set to match the moving of exit slit to a preset position during energy scan.

The DAQ and monochromator scanning is synchronized by software trigger for which the time jitter is smaller than 10 ms. After the trigger, the DAQ module downloads the signal data steam with the preset sampling rate and the monochromator does the energy scan under linear slider with constant scanning velocity. Because the data steam time internal and linear slider position are well defined, the data steam can be directly converted from time scalar to energy scalar.

Because bending magnet beamlines provide light sources with continuum radiation we only need to vary the monochromator energy setting during the absorption measurements. However, the outputs of undulator consist of regularly separated, narrow bands of radiation. During the energy scan, the monochromator energy and the undulator energy settings are required to synchronize to obtain the maximum throughput. Similar to the exit slit controlling concept, the undulator energy setting was calibrated by the beamline monochromator. And then, we select an optimization velocity to synchronize the undulator and monochromator energy setting during the absorption measurements.

In the next section, the results of gas and solid samples absorption measurements obtained using on-the-fly scan are presented. As can be seen the absorption measurement qualities, such as the noise level, the resolving power and energy position accuracy, are as good as those obtained by the point-to-point scan.

![FIGURE 1](image)

(a) Control flow of the on-the-fly for the undulator beamline. (b) On-the-fly data acquisition scheme for undulator beamline. For the bending magnet, the control flow and the data acquisition are the same as in the case of undulator beamline with the exception that the undulator control part is omitted.

RESULTS AND DISCUSSION

Fig. 2 shows on-the-fly and point-to-point XAS scans for Ar and SrTiO$_3$ with a bending magnet source. For the SrTiO$_3$ case the scanning time is around 1 min. and 18 min. for the on-the-fly and point-to-point scan, respectively. On-the-fly scanning time can be shorter than 30 s, but the measured peak profile will be distorted. It may imply that the sample or pre-amplifier noise filter responding time is too long to the rapidly photon energy scanning under the on-the-fly scan. The DAQ sampling rate is 200 Hz. All on-the-fly spectra were smoothed by 11-points average
because the data point energy spacing in the on-the-fly scan is 10 times smaller than that of point-to-point scan. This data smoothing process does not change the resolution in the on-the-fly spectra. The smoothed on-the-fly scan spectra exhibit a same noise level as that of point-to-point scan. Note that the signal level is around 2 – 20 pA. The results of Ar measurements show that the spectral resolution is the same for both scanning methods. The results of spectra exhibit a same noise level as that of point-to-point scan. Note that the signal level is around 2^{3.0}. Because the OTS is sensitive to the exposure of soft x-ray, its NEXAFS spectra exhibit strong dependence of data smoothing process does not change the resolution in the on-the-fly spectra. The smoothed on-the-fly scan because the data point energy spacing in the on-the-fly scan is 10 times smaller than that of point-to-point scan. This

The results of C k-edge NEXAFS for OTS measured by the point-to-point and on-the-fly scan are shown in Fig. 3. Because the OTS is sensitive to the exposure of soft x-ray, its NEXAFS spectra exhibit strong dependence of scanning times, as can be seen in the point-to-point scan. These changes in spectral features are due to the radiation damage since each spectrum took around 18 min. to complete. However, using the on-the-fly scanning method each OTS NEXAFS spectrum will only need a scanning time less than 1 min. The OTS NEXAFS spectral profiles do not change even after five repeated scans. This result demonstrates that the on-the-fly scan method can provide an effective way to measure NEXAFS for photon sensitive materials.

FIGURE 2. (a) Comparison between results obtained by the point-to-point scan and on-the-fly scan for Ar XAS. (b) Comparison between results obtained by the point-to-point scan and on-the-fly scan for SrTiO\textsubscript{3} XAS. The accuracy of energy position is within 0.05 eV between point-to-point scan and on-the-fly scan.

FIGURE 3. The C k-edge NEXAFS spectra for OTS SAM on SiO\textsubscript{2} are obtained by (a) point-to-point scan and (b) on-the-fly scan at a photon incident angle of 20°.
Finally, in Fig. 4 we show the results of F4-TCNQ/Co/Si XAS measured by point-to-point and on-the-fly scans employing an undulator light source. The undulator energy and gap setting was established and calibrated by the beamline monochromator. For the on-the-fly scan, we firstly set up the undulator gap scanning rate and the scanning range. After starting the XAS measurement the program will check undulator motion status via network. When it detects that the undulator is moving, the program will trigger the monochromator to do on-the-fly scan to acquire the spectrum data with a constant sampling rate. The results show that the measured spectra energy positions are quite consistent for both methods. However, slight difference in signal intensity between them has been noted. This may possibly be due to flux variation and could be improved by improving the accuracy of incoming light flux measurement. However, further study is warranted.

Summary

We have setup a software control system to synchronize the on-the-fly scan for absorption measurements with undulator or bending magnetic light sources. This system has signal collection efficiency 10 - 20 times faster than the conventional point-to-point scan while maintaining a same resolving power and accuracy of photon energy. Under this scheme, the beamline and undulator do not need to upgrade any system control hardware and software. This system is currently under minor modification and commission, and will be opened for user in the spring of 2013.

It is important to point out that since the grating, slit and undulator gap motions are non-linear trajectories, this software type on-the-fly scheme is hard to optimize flux and energy resolution for a long range energy scanning. In the future, we shall propose a hardware type on-the-fly system to improve system motions control. It can let system multi-motions be “quasi-synchronous” during long range energy scan to solve this problem.

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