INVESTIGATION OF CONTINUOUS SCAN METHODS FOR RAPID DATA ACQUISITION*

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Abstract

It is common practice to perform spatially resolved X-ray data acquisition by automatically moving components to discrete locations and then measuring beam intensity with the system at rest. While effective, scanning in this manner can be time consuming, with motors needing to accelerate, move and decelerate at each location before recording data. Information between data points may be missed unless fine grid scans are performed, which accounts for a further increase of scan time. Recent advances in commercial hardware and software enables a continuous scan capability for a wide range of applications, which saves the start and end of step motors. To compare scanning performance, both step and continuous scan modes were examined using the SPEC command language with both commercial and in-house hardware. The advantages and limitations of each are discussed.

INTRODUCTION

Step scan data collection can be achieved by a motor moving with intermittent motion and the signal collected when the system is at rest. Several studies have been made with the step scan method to acquire data [1-4]. One advantage with this method is that high position precision can be achieved. It is also a direct and simple method to collect scan data. However, there are some disadvantages with the step scan method such as induced start/stop vibrations and an increase in data collection time.

Each data point during a step scan requires the detector to accelerate, move, and decelerate, causing vibrations. A settling time can be defined to allow vibrations to dampen but this will further increase the data collection time which is already increased by the need to start and stop the motors. For example, in a typical scan application a detector moves in angle from 0° to 60° with a step size of 0.01° so the data set contains 6,000 points. As acceleration and deceleration time is required to move the motor to each point, an extra 0.5 s must be allocated for each step of the scan [5]. An extra 3,000 s is therefore required to complete the scan. The extra time can be reduced if large step sizes are used during the experiment, but significant diffraction peaks may be missed. It is therefore desirable to minimize scan time while reducing vibrations in the system.

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Continuous scanning on the other hand bypasses vibrational problems and reduces latency time. One technique that can benefit from a continuous scan is basic X-ray diffraction (XRD), often used to study the crystal structure of samples. A typical XRD experimental system is comprised of monochromatic X-rays, motion controller, a diffraction signal detector and a data processing system. The detector is moved along a path where the diffraction signal from the sample is distributed. The detector acquires an angle-dependent diffraction signal to analyse the electronic sample structure. In the past, several approaches to continuous scan measurements have been used for X-ray diffraction experiments [6-8].

This paper presents a new method for continuous scan measurements using SPEC as the command language with both commercial- and in-house motor controllers and detector read back electronics. The continuous scan mode is defined here as uninterrupted motor movement with continuous data acquisition. The motion of the detector can maintain a constant velocity or change velocity during the scan to account for changes in X-ray diffraction signal strength. As a result, vibrations in the system as well as total data acquisition time are reduced.

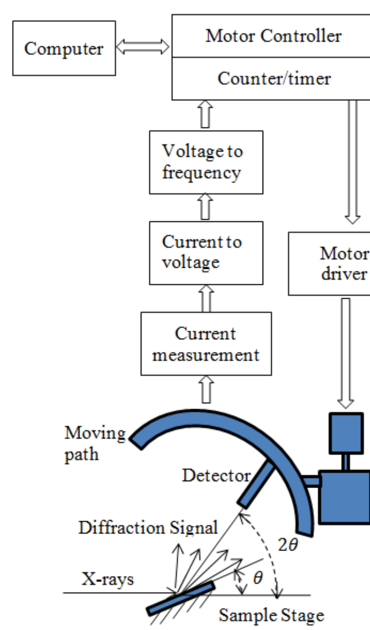

Figure 1: Schematic for the SSRL continuous scan XRD system.

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METHOD: CONTINUOUS SCAN

During a single-axis continuous scan process, the detector is constantly moved while the diffraction signal is simultaneously read by the data acquisition software. The detector can be programmed to move with different defined 'trajectories', which will cause the motors to move at a constant or changing velocity. The user can define scan variables such as data collection time and scan interval for each data point and the software will automatically create a motor trajectory for the detector scan. Counter/timers are gated in time to count pulses for each data point. Since the motors move continuously and the counters collect pulses continuously, the data point position is reported as the spatial average in that interval.

Figure 1 shows a schematic of the continuous scan system. The angle between the incident X-rays and the sample is θ, and the angle between the incident X-rays and the detector is 2θ. For these measurements 2θ is increasing while θ is fixed during the scan process.

We define three functional requirements (FR) for the continuous scan method:

FR-1: define the motor/detector trajectory,

FR-2: data collection while the motor is moving, and

FR-3: synchronization of data to detector position.

The device solution to satisfy FR-1 is as follows. First, the relation between the detector position and velocity is calculated from Eq. 1, where $v(N)$ is the motor velocity at each data point N, v_{start} and v_{end} are the start end velocities, s and f are the start and finish positions, and d is the distance between two data points. The Eq.1 provides a general means to calculate motor velocities. The exponent p determines how the motor velocity will be changed during the scan. This can be used for constant velocity ($p = 1$), or variable velocity ($p \neq 1$) scans. To make a motor move at a defined velocity at the start position, an acceleration segment must be added before the start position. Similarly a deceleration segment must be added after the end position.

$$v(N) = v_{start} + (v_{end} - v_{start)}\left(\frac{N \times d}{|s - f|}\right)^p \qquad (1)$$

For a constant velocity scan, the start velocity is equal to the end velocity, so Eq. 1 shows the motor must accelerate to the start velocity, move at that velocity during the whole scan, and finally decelerate to zero velocity. For a variable velocity scan, the motor must be accelerated to the start velocity and is then adjusted during the scan process as defined by Eq. 1. The motor then decelerates to zero at the end position. Variable velocity scans are especially important when the precise spatial information about weak diffraction peaks is required.

To fulfil requirement FR-2, internal counter/timers in the motion controller are gated to count pulses during the scan. Controlling motors and measuring counter/timer inputs on the same hardware device helps to minimize latency and allows the computer to communicate with a single device for both motion control and detector readbacks.

Before proposing a device solution to fulfil requirement FR-3, a note is given; the signal intensity is not recorded at a fixed detector position but at an 'average' detector position for each data collection interval. To fulfil FR-3, the data collection begins half of the step distance before the center and terminates half the step distance after the center. For example, the diffraction intensity recorded at the detector position $2\theta = 20^\circ$ with sample interval $\Delta 2\theta = 0.02^\circ$ is the result of integrating photon counts between 19.99° and 20.01°.

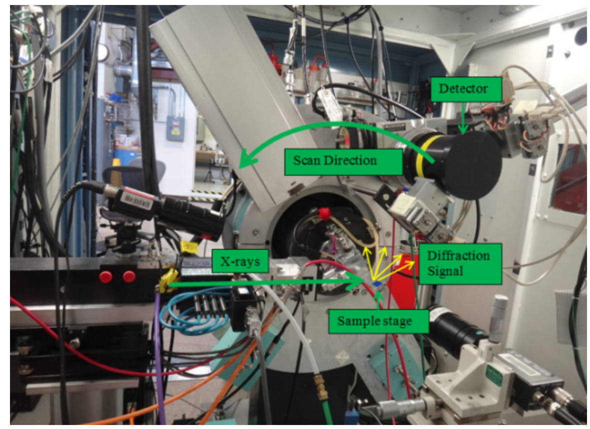

Figure 2: Test system for continuous and step scan.

EXPERIMENTAL SETUP

Figures 1 and 2 show how the continuous scan system tested at SPEAR3 beam line 2-1 contains two main parts: the motor control system and the data acquisition system. The common software package used for both step scan and continuous scan measurements was SPEC version 6.02.08 (Certified Scientific Software, Cambridge, MA, USA).

For step scans, a Galil DMC-4183-NRE motor controller and a National Instruments 6602 counter/timer were used to control the motor and count–pulses. The diffraction signal is measured with a low-current photomultiplier tube, then amplified and converted to voltage using an SRS low noise current preamplifier (SR570). This signal is then converted to frequency through a Nova R&D Inc. N101 voltage-to-frequency converter. A motor control chassis developed at SSRL both amplifies pulses from the motor controller for the stepper motor (Oriental Motor Co., LTD., Torrance, USA) and counts the frequency pulses.

For the continuous scan experiment, a zinc oxide, ZnO, crystal was used because it has many narrow diffraction peaks which span a wide range of angles at 12.5 keV X-ray beam energy. For the scan tests only one ZnO peak at about 20.4° was considered, a count time of 200 ms was found to provide sufficient signal, and 200 data points were sufficient to clearly resolve the peak.

In order to establish the peak position and compare the two scan methods, a preliminary calibration test was conducted as follows. First, the ZnO sample was installed on the sample stage, and motor position recorded. A diffraction peak was identified between 20.3° and 20.7°

using the traditional step scan method. Then, the peak was scanned multiple times using both the step scan and continuous scans technique.

EXPERIMENTAL RESULTS

Using the approach outlined above, ZnO sample scans were conducted using both the step and continuous scan methods. Each scan covered the same angular range and collected 200 data points with each data point integrating for 200 ms. Table 1 shows that the average time for a step scan is 61 seconds while the average time for a continuous scan is 40 seconds. This shows a 34.4% reduction in data collection time. In cases where counting times are short compared to moving times, step scans take a much longer time to complete than a continuous scan. The required beam time can easily be doubled compared with an identical quality continuous scan.

Table 1: Comparison of Data Collection Scan Times for Continuous and Step Scans

Scan number	Continuous scan time (s)	Step scan time (s)
1	40	61
2	40	61
3	40	61

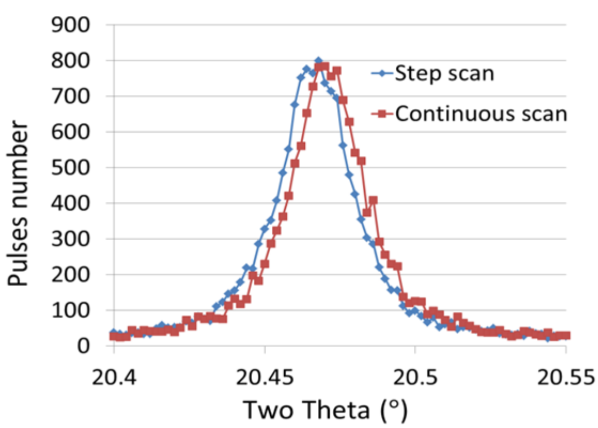

Figure 3: The collected diffraction data for the peak between the two scan methods.

ZnO diffraction peak data for a step scan and continuous scan are shown in Figure 3. For the step scan the peak position is 20.471° and for the continuous scan is 20.467° or a 0.004° difference. The error is mainly caused by the different motor controllers for the step and continuous scans, respectively. All other components of the system were the same.

For this case the data point intervals for the step and continuous scans are 0.0025° with a motor resolution of 10,000 pulses/°. The peak position was also measured three times using continuous scan method. The result shows that the maximum difference among the results is 0.0004°, which means that the continuous scan result is repeatable.

The continuous scan approach can also be extended to other techniques and experiments. In a separate, 2-axis experiment, the continuous scan system was used to rotate a beam polarizer and vertically scan a stepper motor to characterize the polarization state of visible light emitted from SPEAR3. Details for this experiment can be found in reference [9].

CONCLUSION

A continuous motor scan system has been developed at SSRL to acquire X-ray diffraction peak data at the SPEAR3 beam line 2-1. Tests with a ZnO sample show that the required detector scan time can be significantly reduced using the continuous scan method when the count time is short compared with the stepper motor motion time. The results also show the diffraction peak data is nearly identical for both the step scan and continuous scan methods. Ongoing tests will be carried out to determine optimal continuous scan rates as a function of X-ray diffraction signal intensity in the future.

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REFERENCES

[1] R.H. Blessing, "Computer analysis of step scanned X-ray data," Applied crystallography, 1972, p.488.
[2] J.C. Hanson et al., "A limited-range step-scan method for collecting X-ray diffraction data," Acta. Cryst, 1976, p. 616.
[3] H.J. Wang, "Step size, scanning and shape of X-ray diffraction peak," App. Crystallography, 1994, p.716.
[4] J.H. Reibenspies, "Peak width determination of step scan profiles: the floating baseline method," Applied crystallography, 1993, p.426.
[5] V.K. Pecharsky et al., "Fundamentals of powder diffraction and structural characterization of materials", (New York: Springer, 2005), p. 319.
[6] B.C. Chakoumakos et al., "Four circle single crystal neutron diffractometer at the high flux isotope reactor," Applied crystallography, 2011, p.655.
[7] B.E.H. Claus et al., "Continuous scan Tomosynthesis system and method," US 6940943B2, 2002.
[8] J.Fu et al., "Methods determining the angular increment of a continuous scan cone beam CT system," IEEE transactions on nuclear science, June 2010, p. 1071.
[9] J. Corbett, A. Kiss, C.L. Li, et al., "Characterization of Visible Synchrotron Radiation Polarization at SPEAR3", IPAC'15, Richmond, VA, USA, May 2015, paper MOPWI035, these proceedings.

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