AUTOMATION OF MICROBEAM FOCUSING FOR X-RAY MICRO-EXPERIMENTS AT THE 4B BEAMLINE OF POHANG LIGHT SOURCE-II*

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Abstract

The 4B beamline of the Pohang Light Source-II performs X-ray microdiffraction and microfluorescence experiments using X-ray microbeams. When performing X-ray micro-experiments, an X-ray microbeam should first be prepared. Up to recently, the microbeams with vertical and horizontal sizes (full width at half maximum) of less than 3 µm have been achieved, by manually adjusting the positions and pitch angles of the vertically and horizontally focusing mirrors, in a Kirkpatrick–Baez mirror system. In this research, we developed a program that automates the complex and cumbersome process of microbeam focusing. Some part of the control hardware of the K-B mirror system was replaced by corresponding components. A control routine to control the picomotors by means of proportional closed-loop control was also configured. Based on the control routine as well as the output of an ionization chamber arranged at the rear of the K-B mirror system, the whole Microbeam Focusing Automation program was completed using LabVIEW. The developed program was applied to the 4B beamline and enabled the focusing of an X-ray beam to a minimum size within one hour. This paper introduces the algorithms of the microbeam focusing automation program and also examines the performance of the program.

HARDWARE RECONFIGURATION

The main equipments for the X-ray micro-experiments of the 4B beamline at the Pohang Light Source-II consist of two slits (optics and experiment slits), two ionization chambers (ionization chamber-I and ionization chamber-II), a shutter, a monochromator, a Kirkpatrick–Baez (K-B) mirror system, a sample stage, a charge-coupled device area detector, and a fluorescence detector. The ionization chamber (IC) referred to hereafter is the ionization chamber-II, which is placed in the rear of the K-B mirror system.

The front vertically focusing mirror (VFM) and the rear horizontally focusing mirror (HFM) of the K-B mirror system are arranged to configure a K-B optic system [1]. Each 102 mm long mirror translates in a direction perpendicular to the mirror surface or pitches with respect to the beam by two picomotors. Each mirror is adjusted into the required elliptical curvature using a manual mirror bender.

An acrylic plate bolted to a sample holder attached to the sample stage is shown in Fig. 1. A 4 mm diameter hole is machined at the central part of the acrylic plate, and two vertical and horizontal 250 µm diameter tungsten wires are attached cross the hole so that the hole is divided into four quadrants.

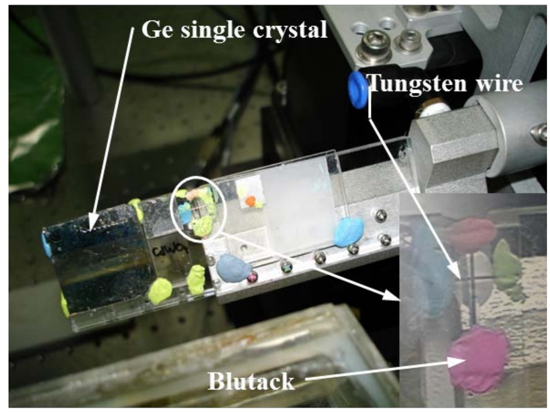

Figure 1: The sample holder and a close-up view of the tungsten wires.

In this research, the IC outputs electric current values as negative numbers, and the beam intensity is the absolute value of the IC current.

The existing picomotor drivers and control pad used to drive the picomotors, as well as the existing linear variable differential transformer (LVDT) display used to measure and display the displacements of the picomotors of the K-B mirror system, have no communication function. Thus, we replaced these components with a new picomotor controller and two new LVDT controllers with serial communication capability.

MICROBEAM FOCUSING AUTOMATION

After configuring the closed-loop control routine (i.e., Picomotor-LVDT Closed-Loop Control routine), which controls the picomotors using proportional control [2] by inputting pulses into the picomotors through the picomotor controller and reading the displacements of the picomotors from the LVDT controllers by the control computer, we developed the whole Microbeam Focusing Automation program. This program performs every step of the existing microbeam focusing process, including a half-cutting phase and a focusing phase.

In the Microbeam Focusing Automation program, algorithms that achieve a specific value of IC output while translating a mirror or a maximum of beam intensity or a minimum of beam size while rotating a mirror are required. In this research, the golden section search algorithm [3] that is very effective for this purpose was used but modified for practical reason in its application. The algorithms of coded subroutines as well as the main routine are described below.

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Picomotor-LVDT Closed-Loop Control Routine

Since the picomotors do not drive a uniform displacement for applied fixed pulses unlike a stepping motor [4], the actual displacement can be confirmed only by the output of an LVDT mounted around the adjustment screw of the picomotor. Moreover, the relation between the picomotor displacement and LVDT output varies according to the calibration of the LVDT. In this research, a LabVIEW routine using proportional closed-loop control [2] was coded to move a picomotor to a target LVDT position by directly treating the output of the LVDT as the displacement of the picomotor. In this proportional control, the gain was set to 4000 pulses/V.

Half-Cutting Algorithm

The K-B mirror is in a half-cut state when each of the VFM and HFM blocks exactly half of the beam in a posture parallel to the beam. The half-cut states of the K-B mirrors are imposed to minimize the beam size while adjusting only the picomotor for the pitch angle of each mirror in the focusing phase using the fact that mirror rotation in the K-B mirror system is realized on the pivot axis, which is the transverse axis passing through the center of a mirror surface. The steps of the half-cutting phase used in the program are shown in Fig. 2.

1) The mirror is translated from a position away from the beam to a position where the front end of the mirror barely breaks through the beam center line, in a state in which the front end is higher than the rear end [Refer to Fig. 2(a).].

2) The mirror is rotated in a direction in which it can accept more of the beam, and whether or not the current pitch angle maximizes the beam intensity is checked using the IC output [Refer to Figs. 2(b) and 2(d).]. If the beam intensity is the maximum, we proceed to step 5); otherwise, we proceed to step 3).

3) Whether or not further rotation causes the front end of the mirror to move out of the beam is checked [Refer to Fig. 2(b).]. If yes, we proceed to step 4); otherwise, we proceed to step 2).

4) The mirror is again translated so that the front end of the mirror, which descended below the beam center line by the prior mirror rotations, breaks through the beam center line [Refer to Fig. 2(c).].

5) The mirror is again translated so that a straight line connecting the front and rear ends of the mirror coincides with the beam center line [Refer to Fig. 2(e).].

If the front end of the mirror is higher than the rear end as in Fig. 2 when a mirror advances toward the beam or rotates, analyzing the IC output becomes much easier without considering the effect of reflection on the IC output.

In steps (b) or (d) in Fig. 2, much more beam transmits to the rear of the mirror as the mirror rotates, and the beam intensity of the IC increases. However, if the mirror exceeds the pitch angle parallel to the beam, the beam intensity of the IC decreases. Thus, the parallelized pitch of the mirror is achieved by searching the position at which the beam intensity is at a maximum, as in steps (b) and (d) in Fig. 2.

Steps 1), 4), and 5) are executed by the Mirror for I routine, whereas steps 2) and 3) are executed by the Mirror for Max I routine.

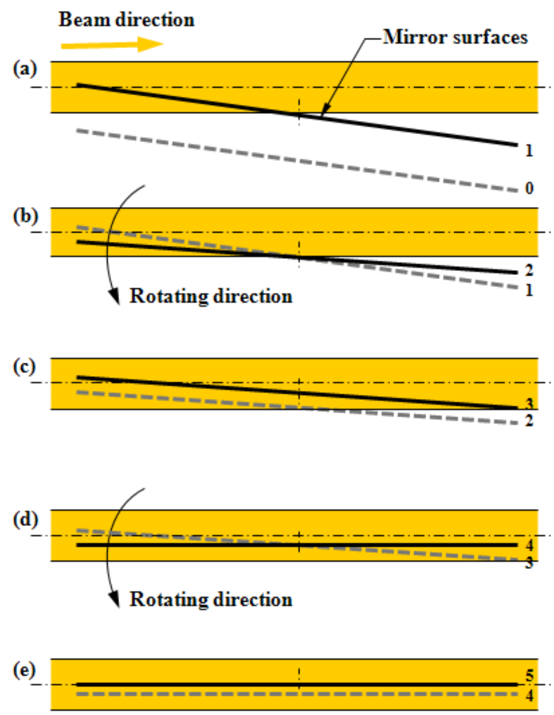

Figure 2: Process of achieving the half-cut state of a mirror.

As, to complete the half-cutting, repetitive operations of the combined Mirror for I and Mirror for Max I routines are required, a while loop was configured. Inside the while loop, a segment that calls the Mirror for I routine, a segment that calls the Mirror for Max I routine, and an escape criterion segment exist.

Microbeam Focusing Routine

The Microbeam Focusing routine rotates a mirror to the pitch angle of the mirror that yields the minimum beam size by repeating the measurement of beam size while changing the pitch angle of the mirror. Among the steps of the Microbeam Focusing routine, the steps that measure beam size is performed by calling the Beam Size Scan routine.

The Microbeam Focusing routine also adopts the modified golden section search algorithm when searching for the pitch angle that corresponds to the minimum beam size. The routine rotates the mirror by the rotation interval, which increases by a factor of 1.618, to reduce the search duration from the initial rotation interval. For every rotation, the routine translates the tungsten wires to predetermined offsets away from the beam by executing the Cross-Wire Reposition routine and measures the beam size by executing the Beam Size Scan routine. When searching for the interval corresponding to the minimum beam size, the search criterion employed is $\psi_u > \psi_m$, where ψ_u represents the beam size measured at the current picomotor position (p_u), and ψ_m represents the beam size measured at the prior picomotor position (p_m). The routine repeats the step which moves to the next picomotor position and measures the next beam size as long as the search criterion is not satisfied.

Once the interval containing the pitch angle corresponding to the minimum beam size is captured, the routine subsequently measures the beam size at each equally partitioned position after dividing the length of the interval by ten. The routine then finds the final minimum beam size by fitting the 11 measured beam sizes to a third order polynomial function.

The golden section search algorithm is modified in the step of searching for the minimum value within the interval, because the algorithm is rather prone to fall into error due to the low actual stability of beam size measurements within a quite narrow pitch angle interval. A graph of beam sizes measured at the equally partitioned positions within the captured interval is shown in Fig. 3.

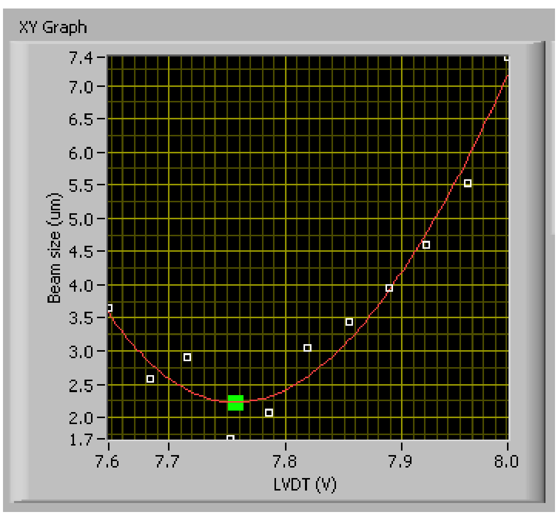

Figure 3: Graph of the beam sizes measured at equally partitioned positions within the interval containing the pitch angle corresponding to the minimum beam size.

Microbeam Focusing Automation Routine

The Microbeam Focusing Automation routine, namely the main routine, fulfils the whole microbeam focusing process by achieving the half-cut states and performing the focusing phase of both the mirrors using the subroutines.

First, by adjusting the picomotors, the main routine not only translates the mirrors in a direction opposite to the beam to avoid interference with the raw beam but also rotates the mirrors so that the front ends of the two mirrors are higher than the rear ends.

The main routine finds the coordinates of the beam center on the x-axis and y-axis by calling the Beam Centering routine. In this state, the main routine translates the sample stage to the lowest position away from the beam.

The next step involves the configuration of the half-cut states. The main routine performs the while loop for half-cutting to configure the half-cut state of the VFM. Subsequently, the main routine performs the while loop for half-cutting of the HFM. Subsequently, the main routine makes the tungsten wires unblock the beam as well as approach the beam in the half-cut state by executing the Cross-Wire Reposition routine.

As the first step of the focusing phase, the main routine rotates the pitch angles of the VFM and HFM by 2.2 and 1.9 V, respectively, from their present positions so as to rotate the pitch angles immediately to the vicinity of prior optimum pitch angles. By calling the Cross-Wire Reposition routine, the main routine positions the tungsten wires in predetermined offsets away from the beam, of which the path is altered because of the large rotations of both the VFM and HFM.

By calling the Microbeam Focusing routine, the main routine consecutively focuses the beam on the y- and x-axes. The main routine subsequently finds the center of the focused beam by executing the Beam Centering routine and stores it.

Finally, the main routine positions the tungsten wires in predetermined offsets away from the beam center to prepare for an X-ray micro-experiment and terminates the whole Microbeam Focusing Automation program.

EXECUTION RESULTS

Beam Intensity with Respect to the Pitch Angles

Since the preliminary Mirror for Max I routine often could not capture the maximum beam intensity, we inquired into the variations in beam intensity according to the pitch angles of the VFM and HFM. Figure 4 shows the beam intensity measured from the IC while adjusting only the pitch angle of the VFM from the half-cut states of both mirrors.

The IC output decreases from the left up to point A and then increases up to point B. The output presents the second minimum value at point C and increases continuously after point C in Fig. 4 for the VFM. This phenomenon also appears with almost the same tendency for the HFM. We found that point A corresponds to the pitch angle of the half-cut state by comparing with another half-cut state, which was manually achieved. Since the beam which starts to reflect cannot enter the IC because of the concave curvature of the mirror from point A up to point B, even if the rotation continues, the beam intensity decreases. Hereafter, as the reflected beam on the mirror surface enters the IC, the IC output decreases. Point C can be deduced as the state in which the entire beam that passes the experiment slit reflects on the mirror surface. As only the increase of the reflection angle affect the output from point C onwards, the beam intensity starts to decrease.

Consequently, the conventional golden section search algorithm of which the interval increases by a factor of

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1.618 cannot be applied for finding point A, since the valley of the curve, including point A, is too narrow.

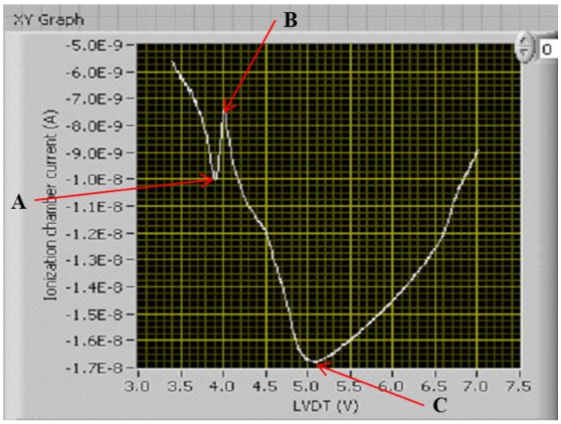

Figure 4: Variations in the IC outputs with respect to the pitch angles of the VFM.

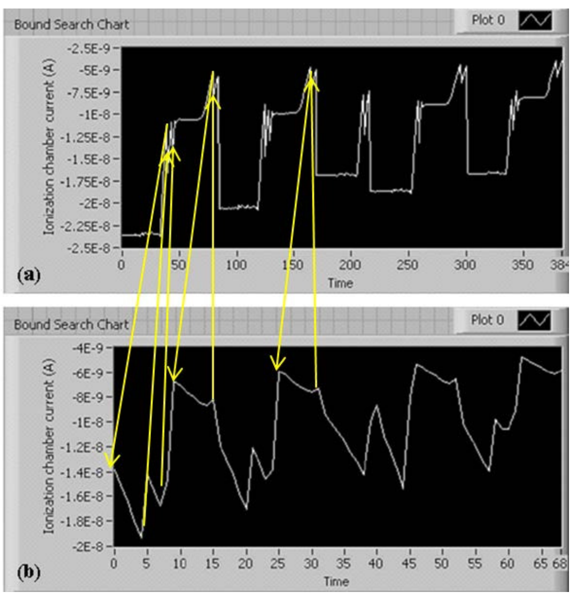

Figure 5: Interval search charts of the Mirror for I (a) and Mirror for Max I (b) routines.

Examination of the Execution Results

After defining a beam of 100 μm (H) × 100 μm (V) using the experiment slit, we performed microbeam focusing using the developed program. The execution results of the Mirror for I and Mirror for Max I routines among several routines are examined. The interval search charts of the Mirror for I and Mirror for Max I routines are shown in Figs. 5(a) and 5(b). These interval search charts show processes from initial stages until the routines find the intervals containing the minimums of the respective object functions. The horizontal axes represent the number of measurements, whereas the vertical axes represent the currents measured from the IC. The two figures resulted from a case that after first two cycles of the half-cuttings of both the VFM and HFM had been achieved, one cycle of the half-cutting of the VFM was performed, followed by two cycles of the half-cuttings of both the VFM and HFM.

The leftmost flat region in Fig. 5(a) represents a process where the VFM is advancing toward the beam starting from a position where both the VFM and HFM do not interfere with the beam. Minute fluctuations of IC output are observed even in this flat region. The IC output increases rapidly at the rear end of the flat region as the VFM begins to make contact with the beam. Subsequently, two sawtooth waveforms with gradually diminishing amplitude appear, where the half-cutting of the VFM is being accomplished in tandem with the Mirror for Max I routine. The leftmost region of Fig. 5(b) shows that the IC output decreases twice. It is this region that is increasing beam intensity while lowering the front end of the VFM. The half-cutting of the HFM can also be analyzed in the same manner.

CONCLUSIONS

In this research, in order to automate the focusing of X-ray microbeams, we replaced some of the hardware of existing experimental equipments and developed Microbeam Focusing Automation program to perform the microbeam focusing process using LabVIEW.

A vertical beam size of approximately 2.2 μm and a horizontal beam size of approximately 2.0 μm resulted from the experimental operation of the developed program. These beam sizes are either equal to or smaller than those obtained from the existing manual microbeam focusing process. In addition, the total duration of microbeam focusing using the program was about 50 minutes. Thus, the developed program is both labor- and time-saving. The developed Microbeam Focusing Automation program was immediately applied to the 4B beamline of the Pohang Light Source-II. The program enhances beamline users' convenience and shortens experiment periods.

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