ประเภทเอกสาร

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ชื่อเรื่อง **Title**	Maintaining fixed exit beam of DCM while energy changes
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คำสำคัญ **Keyword**	Double-crystal monochromator, DCM, beamline 7.2W:MX

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1. บทคัดย่อ

A double-crystal monochromator (DCM) is a key component of macromolecular crystallography (MX) beamlines, where a fixed exit beam position over a wide energy range is essential for reliable beamline alignment and automated data collection. At BL7.2W:MX, upgrading the superconducting wavelength shifter from 4 T to 6.5 T shifted the source point and introduced a significant horizontal drift of the DCM exit beam as the photon energy was varied, impairing coupled alignment of the DCM and focusing mirror. In this work, we describe a practical procedure to recover a quasi-fixed exit beam by finely adjusting the χ_1 tilt of the first Si(111) crystal in the TSR-2DCM and re-optimizing the focusing mirror. Beam centroid positions at the sample location were monitored with a xyclop camera while χ_1 was iteratively tuned using a handy controller, including backlash compensation, and the mirror was readjusted accordingly. After optimization, the horizontal beam position variation ΔX over 6–18 keV was reduced to <25 μm, with the operational 8–15 keV range for SAD/MAD experiments maintained within ~20 μm, and vertical deviations kept below 10 μm. This low-cost adjustment provides an effective interim solution to restore fixed-exit performance without re-installing the DCM, while highlighting the residual limitations when very small beam sizes (<200 μm) are required.

2. บทนำ

According to a beamline involving macromolecular crystallography, it is necessary to have a monochromator to select X-rays of single wavelength from synchrotron using Bragg's law on the angle of crystals with respect to the incoming beam. The most popular model of a monochromator for MX beamline is a double crystal monochromator which uses the first crystal surface to select a single wavelength and then the second one is used for adjusting to maintain a fixed exit beam. Both of crystals for this purpose are using silicon crystals with a reflection of (111) which gives a strong diffracted beam regarding to its large structure factor. This beamline 7.2W also employs this type of monochromator with Si (111) crystals as shown in figure 1. with main components such as two crystals system, crystal cooling system, Compton Shield, beam stopper and beam monitor, cam stages, and vacuum system.
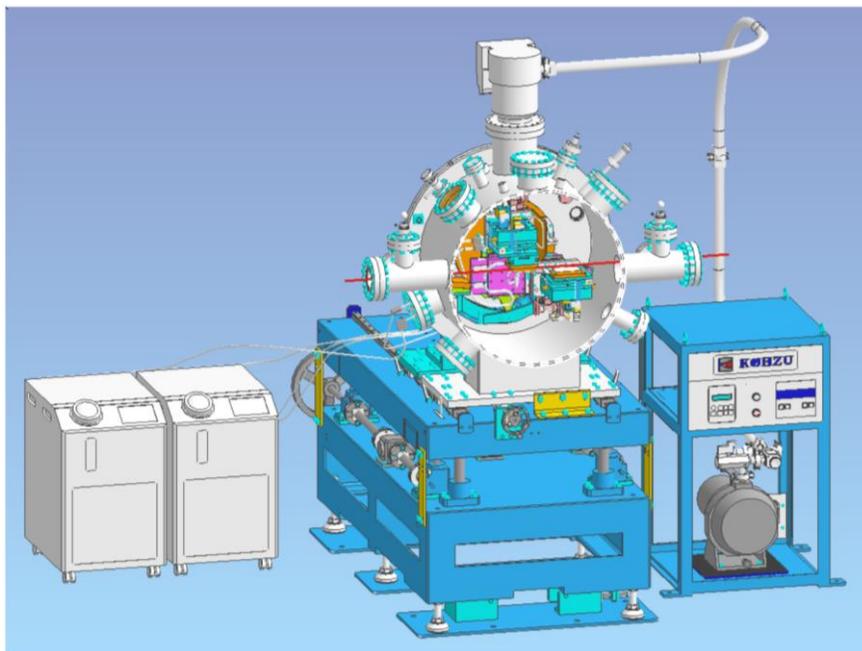

Figure 1 The TSR-2DCM design for BL7.2W:MX

For this topic, it is related to alignment stages and cam stages (figure 3) in order to maintain fixed-exit beam while Bragg angle is varying using this equation:

$$(x, z) = \left(\frac{H}{2 \times \sin \theta} , \frac{H}{2 \times \cos\theta} \right)$$

When x and z reflect horizontal and vertical distance between two crystals' surface point, respectively whereas H represents beam position. From that equation, the plot of beam position in horizontal or vertical direction as a function of main theta is shown in figure 2. The dramatical change in horizontal position occurs in a theta range of 5 – 30 degrees which should be resolved by adjusting χ_1 position of the first crystal whereas the most change in vertical position appears from main theta of 50 degrees onwards that must be fixed by Z1 of the first crystal. For the parameters of the second crystal, it is unnecessary to adjust them; χ_2, Δtheta2, and Z2.
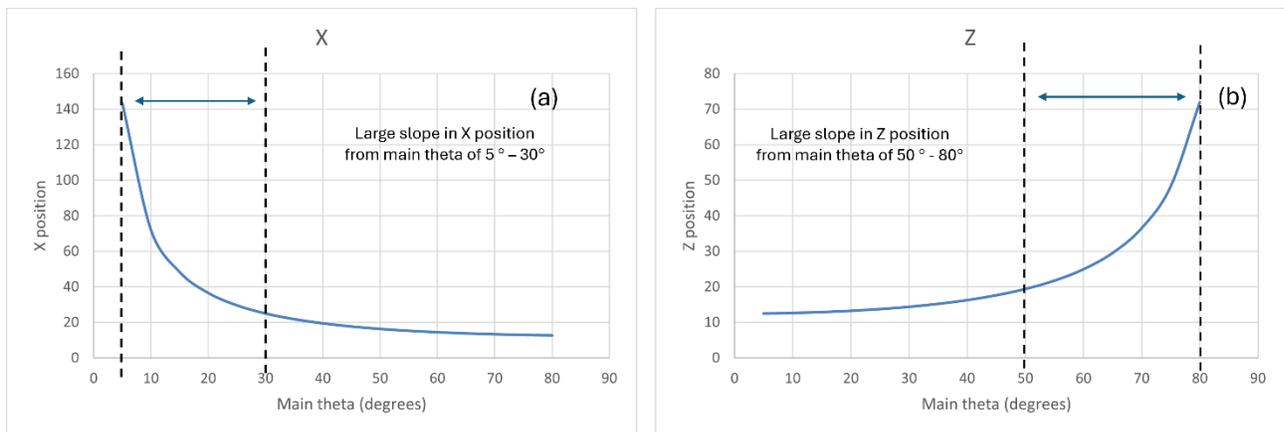

Figure 2 Beam position of horizontal (a) or vertical (b) as a function of main theta (degrees)
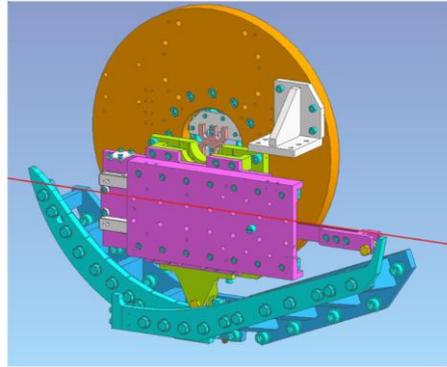
Figure 3 Two cam stage in the DCM

Thus, in this issue, when changing photon energy in the monochromator in order to proper wavelength for anomalous scattering and dispersion absorption edge in SAD technique, it is noticeable that DCM's exit beam had not been in same position over a range of energy. It had moved dramatically in relatively horizontal direction as shown in figure 4, which would be an obstacle on performing auto-alignment that involves both DCM and focusing mirror. The beam position was observed by the maximum intensity from a xyclop camera at the end of beamline.
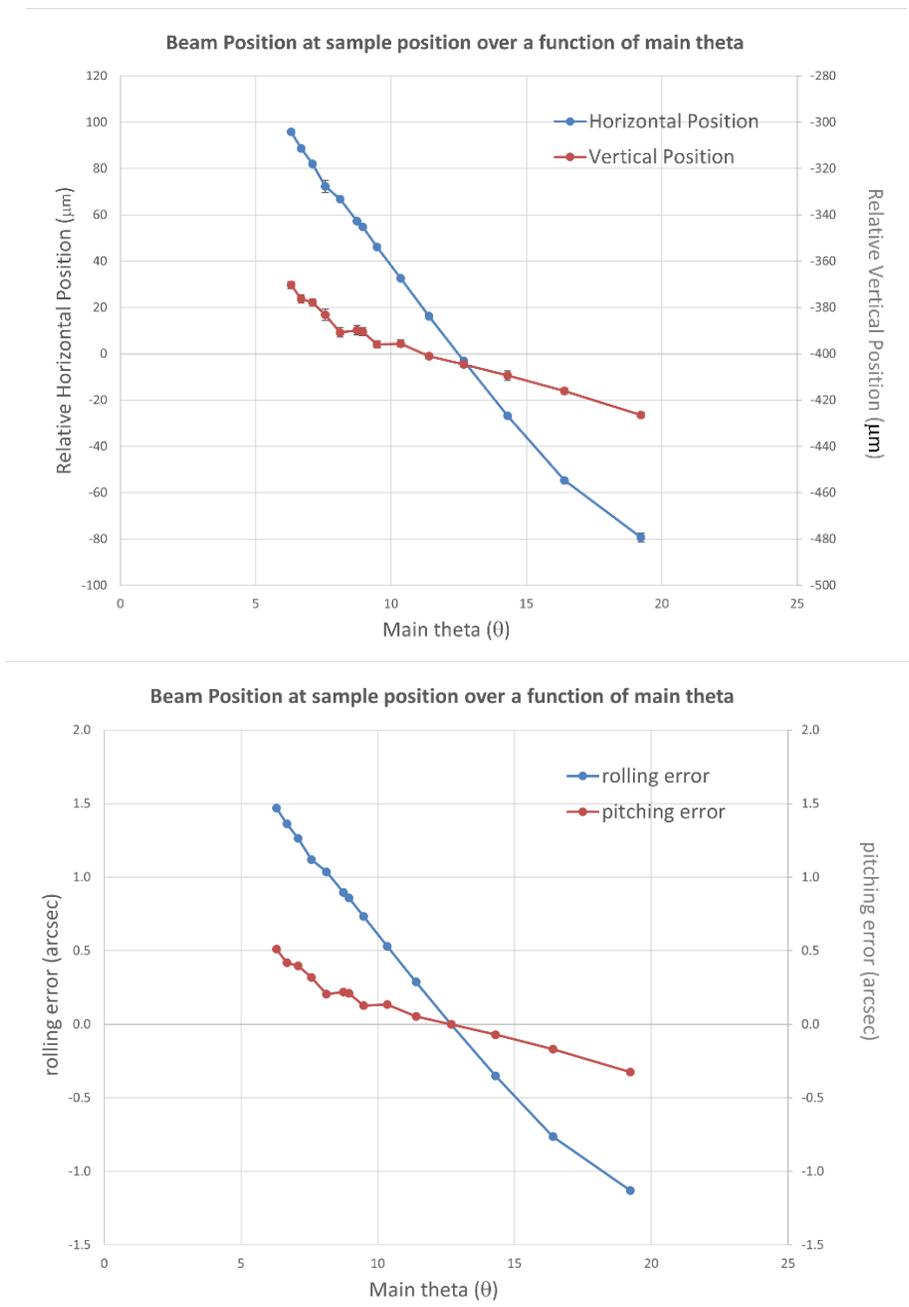
Figure 4 The relative beam position/relative rotation error at sample position as a function of main theta before adjusting a position of fixed exit beam

3. วัตถุประสงค์

To resolve the issue on instability of an X-ray beam position after energy change due to inaccurate χ_1 position in a double-crystal monochromator.

4. วิธีการดำเนินงาน

Since it was relating to DCM thus Dr.Yuji suggested it was linked to Chi tilt (χ) on the 1st crystal within DCM due to the change occurring in a range of 5 – 20 degrees. According to TSR-2DCM technical proposal Rev 1.1 by Kohzu, the χ_1 tilt is parallel to the 1st crystal surface and it adjusts the error between crystal surface and crystal lattice plane. Therefore, this problem is from inaccurate χ_1 position of the first crystal which needed to be adjusted in favour of horizontal beam direction as shown in figure 5.
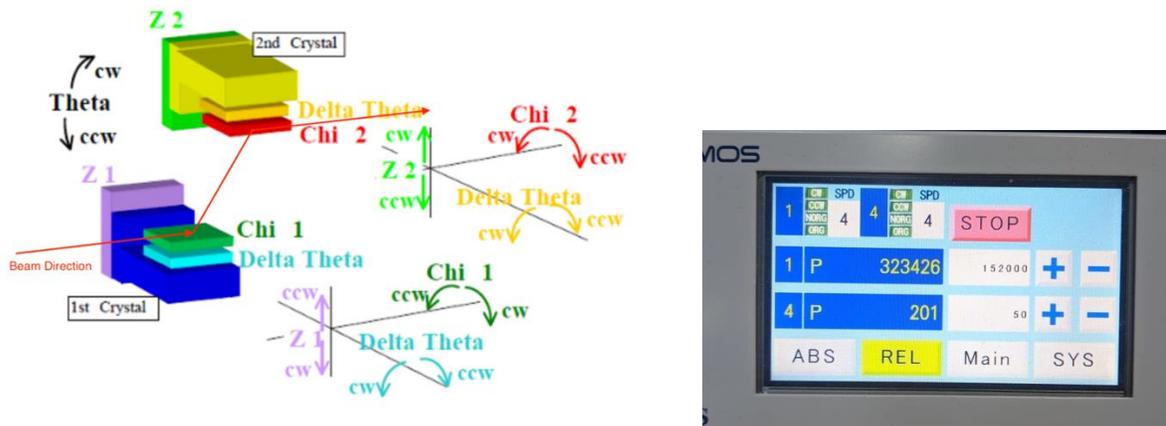

Figure 5 Diagram of coordinate system within BL7.2W's DCM (left, adapted from Double Crystal Monochromator for BL7-2 MX by Kohzu, 2015) and a handy controller to control motion of each coordinate parameter manually (right)
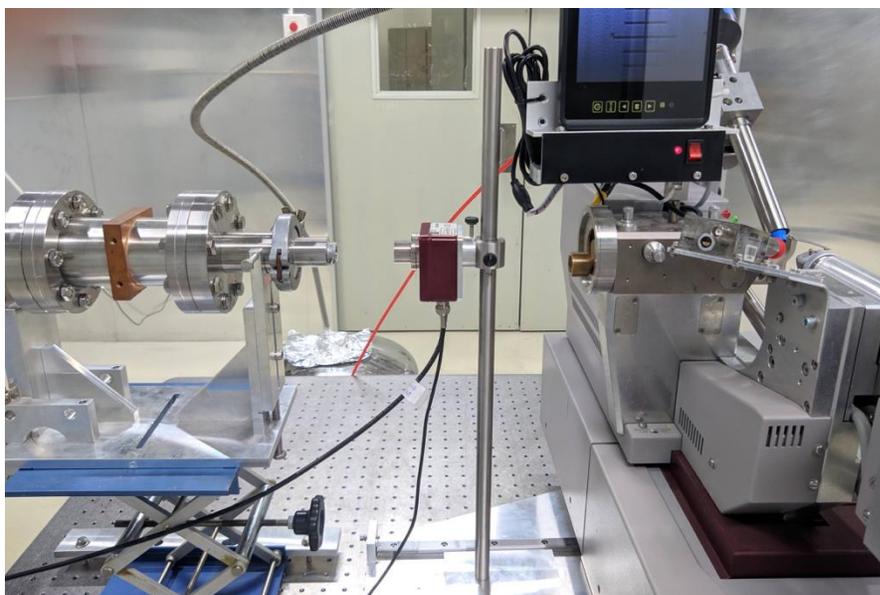
Figure 6 The position of a xyclop to attach the end of beamline in order to observe beam position which is installed at the focus position in a distance of 13906 mm from the DCM

To adjust proper angle can be done by observing relative beam position at sample position whilst adjust χ_1 which is P3 (Channel 3 blue tab) on the handy controller. Initially, χ_1 angle of "-1000" had given large number on difference of each beam position (ΔX >> 0) since energies of 12.7, 9.0 and 7.5 keV thus the χ_1 should be moved in either CCW or CW direction on trials (more negative or positive pulses, respectively). In between of adjustment, the beam position at sample position would be observed. If the difference on each beam position in a range of energy is less than 30-40 μm, it would be acceptable. Besides that, there should be adjustment on positions of the focusing mirror in corresponding to the DCM as well. The example is as shown in Table below.

χ_1 (pulse)	Relative beam centroid (horizontal) position (micron)			
	12.7 keV (8.982°)	9.0 keV (12.684°)	7.5 keV (15.288°)	Δx
-1000	55.0	-3.6	-70.3	125.3
-1800	388.0	362.0	350.0	38.0
-1900	405.4	384.7	380.8	24.6

Note: After changing χ_1, the backlash movement should be performed as well by plus 1000 and then minus 1000 on P3 blue tab because it would reduce error in profile in gears within motors of DCM.

5. ผลลัพธ์

After adjustment on χ_1 together with the focusing mirror, the beam centroid position was monitored at the end of the beamline about the sample position as shown in figure 7. It is noticed that the difference of horizontal position (rolling error: ΔX) at different energy falls less than 25 microns or 0.4 arcsec whilst the one of vertical position (pitching error) is less than 100 microns or 1.25 arcsec over the energy range of 6 – 18 keV (main theta of 5 – 20 degrees). According to the report of delivery specification Rev 1.1 (TSR2_deliver_spec_v11) given by Kohzu, the maximum rolling and pitching errors are 1.68 and 5.49 arcsec, respectively, which our results are fit into the acceptance test as shown in figure 8.
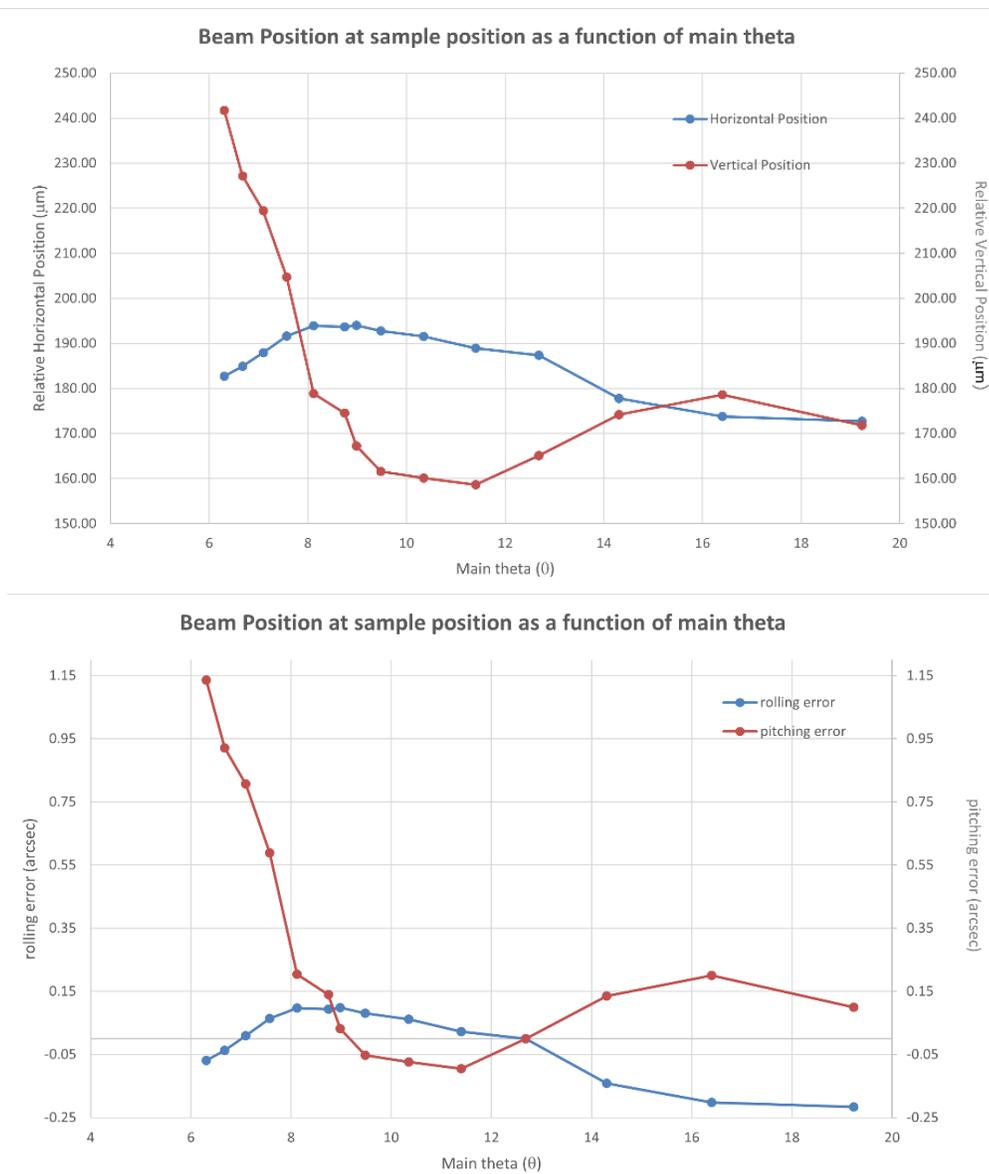
Figure 7 The relative beam position/relative rotation error at sample position as a function of main theta after adjustment on the 1st crystal in DCM and focusing mirror.

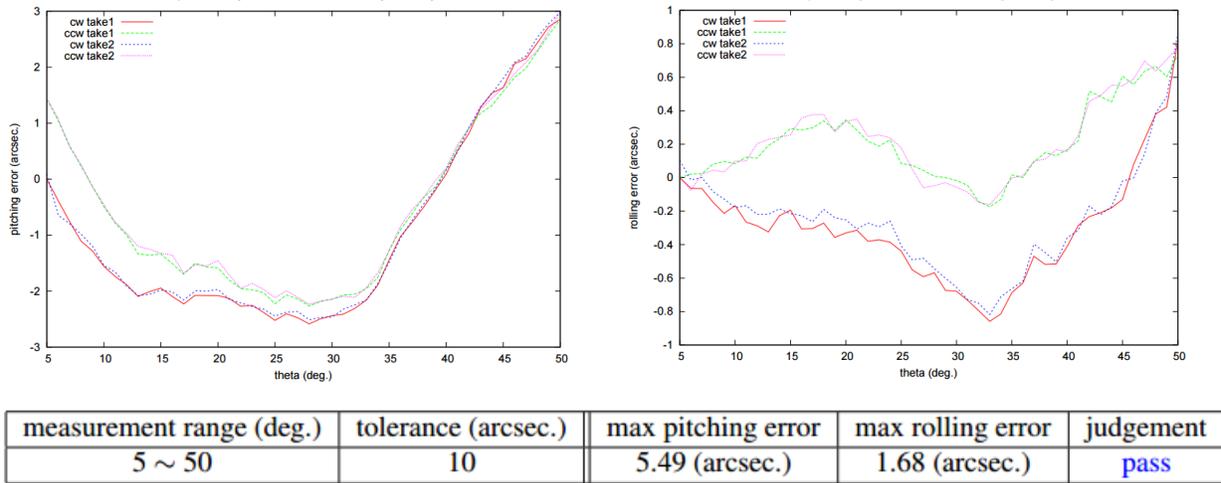| measurement range (deg.)	tolerance (arcsec.)	max pitching error	max rolling error	judgement
$5 \sim 50$	10	5.49 (arcsec.)	1.68 (arcsec.)	pass

Figure 8 Pitching error (left) and rolling error (right) on site acceptance test including Table for result of acceptance test according to the report of delivery specification Rev 1.1 (TSR2_deliver_spec_v11) by Kohzu

6. สรุปผล

The DCM was designed, installed and commissioned previously in 2016 according to the beamline parameters with the SWLS operation at 4 Tesla. Currently, BL7.2W: MX operates on the 6.5T SWLS, resulting in the relative beamline parameters change with the beam position at 1 mm above compared to the previous operation. This would affect the exit beam position due to mismatched height of DCM however, according to Kohzu, to perform reinstallation could have high cost. Therefore, Dr. Yuji offered simple solution but yet to effective by fixing on χ_1.

After success on adjustment on χ_1, the exit beam after DCM was able to be fixed at the same position with an error acceptance of 20 microns for energy range of 8-15 keV that is most operational energy for SAD/MAD techniques. However, this solution can be done temporarily because it cannot be fulfilled for whole energy range of 5-20 keV and sometimes the position error of 20 microns can still cause a problem on performing experiment with a small beamsize of less than 200 microns with 10% error. Therefore, if it is necessary to perform a small beamsize of less than 200 microns, it needs better competence such as re-installation of DCM.

7. กิตติกรรมประกาศ (Acknowledgements)

We would like to thank Dr.Yuji Fukumoto of Kohzu for his supervision. Also, Dr. David Hall, a group leader of MX village at Diamond Light Source for his comments and suggestions.

8. เอกสารอ้างอิง

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- Technical proposal Rev 1.1 regarding Double Crystal Monochromator for BL7-2 MX Model: TSR-2DCM
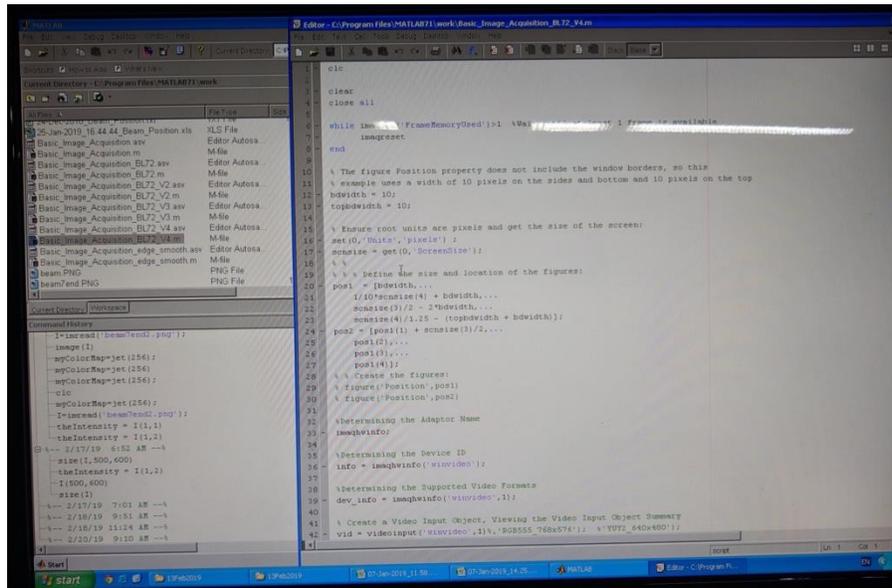
ภาคผนวก

Figure 7 Source code for monitoring beam centroid in Matlab program developed by our mechatronic engineer.
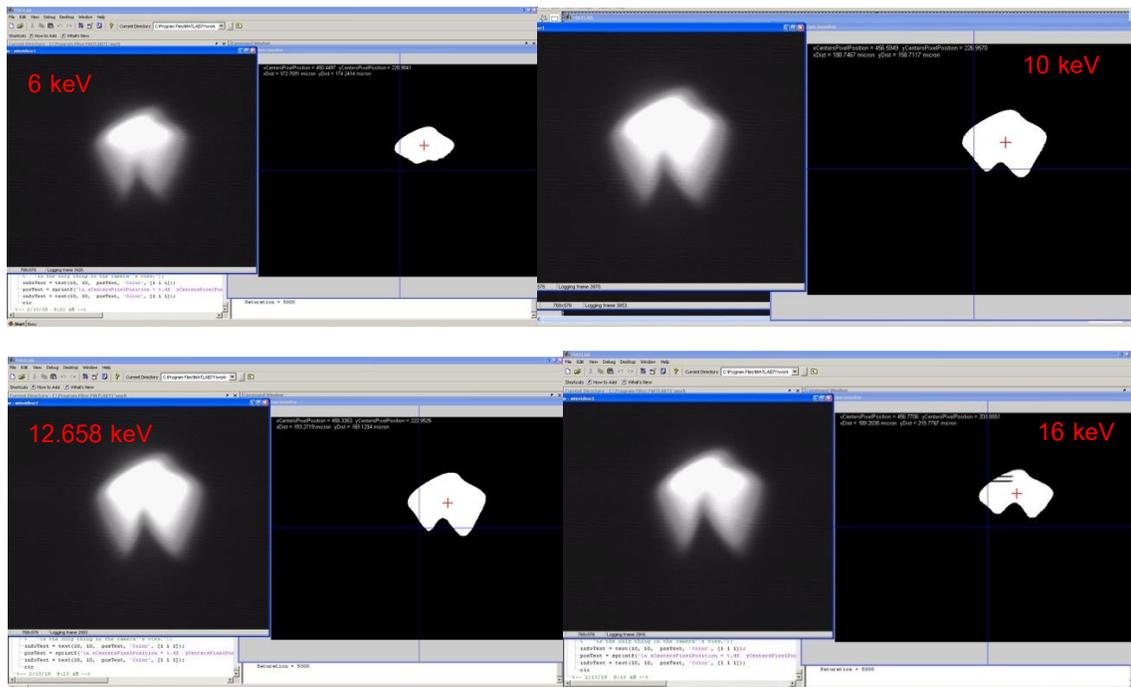

Figure 8 Beam centroid monitoring by a software encoding from the xyclop