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ประเภทเอกสาร

☑ TR: รายงานเชิงเทคนิค (TECHNICAL REPORT)
☐ TN: รายงานเชิงเทคนิค (ฉบับย่อ) (TECHNICAL NOTE)
☐ MN: คู่มือการดำเนินงาน (Operation Manual) / คู่มือการใช้งาน (Instruction Manual) / แผนปฏิบัติการ (Operation Plan)

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คำสำคัญ Keyword	beamline 7.2W:MX, Rayonix SX165, sample-to-detector distance, X-ray diffraction

รายชื่อผู้จัดทำรายงานหรือผู้ดำเนินโครงการ (Name)	**ส่วนร่วมในการปฏิบัติงานในโครงการ Responsible tasks in the project**
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นายมงคล ผานาค	ติดตั้งและพัฒนาระบบติดตามตำแหน่งกึ่งกลางแสง

1. บทคัดย่อ

Determination of the sample-to-detector distance and the optimal beamstop position is essential for collecting high-quality X-ray diffraction data, particularly for non-expert users at synchrotron beamlines. In this work, we describe a practical procedure to select sample-to-detector distances such that the target resolution is reached at the edge of the detector while maintaining appropriate coverage of low-resolution reflections. We further present a systematic approach for positioning the beamstop to minimize its shadow on the detector and thereby reduce loss of low-resolution data. By explicitly linking beamline geometry, detector geometry, and beamstop position, we provide a set of easily applicable experimental setup parameters that guide users in configuring their data collection. Application of this strategy improves signal-to-noise ratios and completeness in the low-resolution range, where the beamstop shadow typically has the greatest impact, while still ensuring that the desired high-resolution limit is captured. The resulting guidelines are implemented in straightforward instructions that can be readily followed by non-expert users. Overall, this optimization of sample-to-detector distance and beamstop position is crucial for user service, enabling more reliable and meaningful X-ray datasets to be obtained across a range of experimental conditions.

2. บทนำ

For macromolecular crystallography, it is necessary to collect a dataset of protein crystal by X-ray diffraction technique. The experiment setup in the MX beamline for data collection has marDTB desktop system consisting of goniometer, beamstop, detector, cryo-cooling system as shown in figure 1. The detector is a type of CCD with sensitive sensors to detect diffracted beam. Because of sensitivity of the detector to a bright direct beam, it is necessary to have a beamstop to block the beam (figure 2).

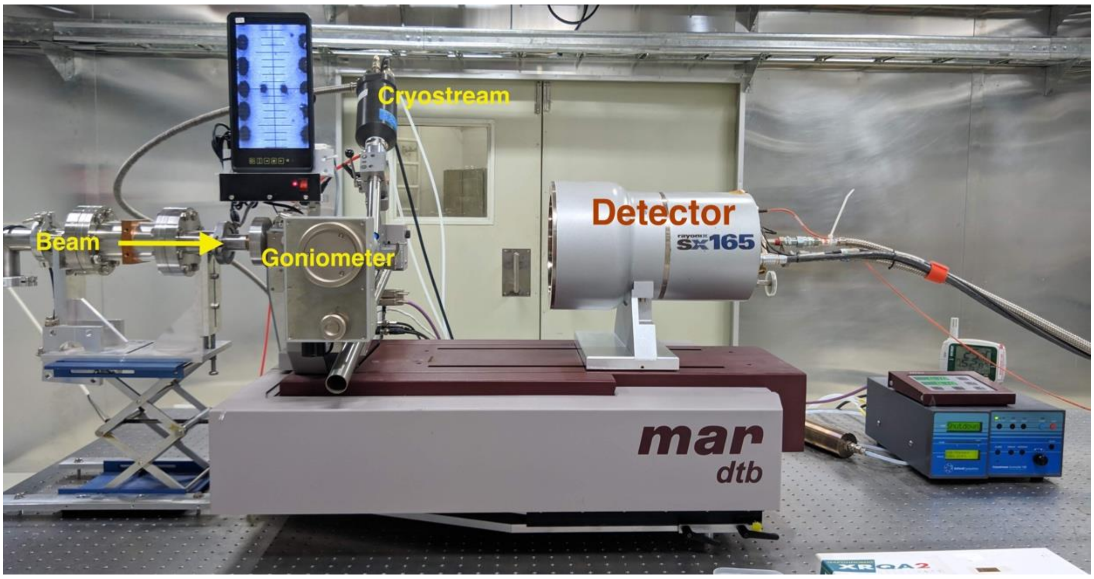


Figure 1 Main components in the Experimental endstation at BL7.2W:MX

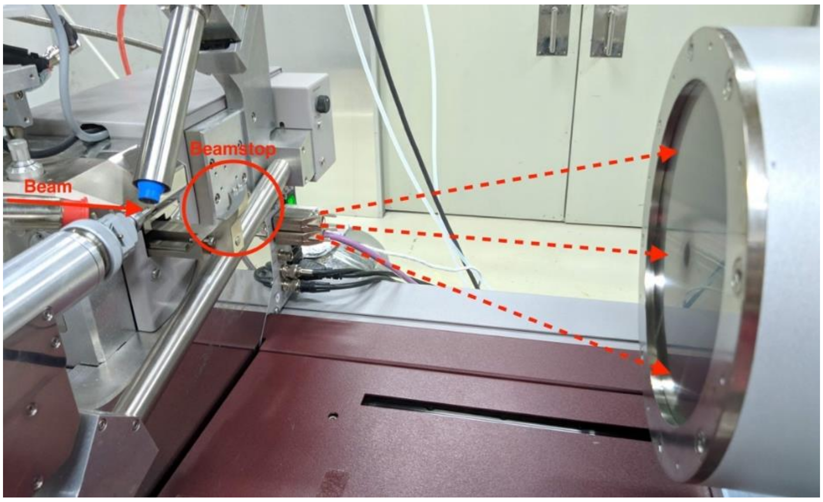


Figure 2 The direction of beam through beamstop towards the detector

In MX technique, diffraction pattern at low resolution somehow is important to data processing in order to solving structure at level of C-backbone. The low-resolution data is necessary to be used in Patterson calculation for molecular replacement. Recently, it is noticeable that scattering spots at low resolution disappeared whilst collecting diffracted data at distances of detector and beamstop of 180 and 20 mm, respectively as shown in figure 3.

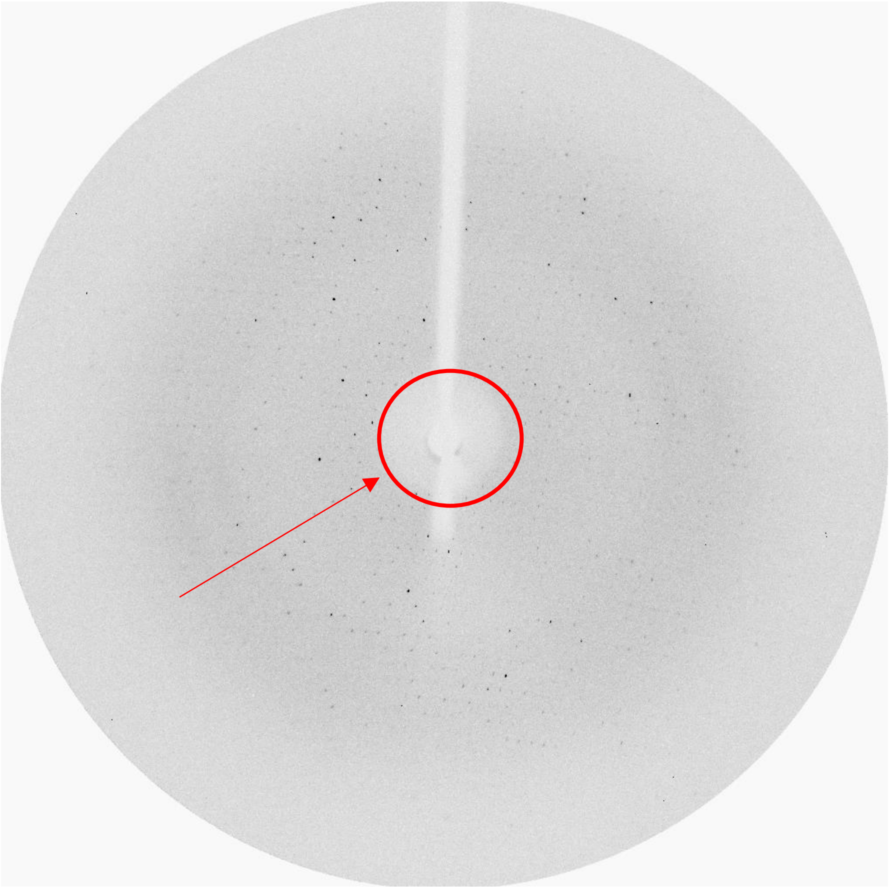


Figure 3 Low resolution data loss due to non-optimized beamstop set up

(courtesy of Dr.Buabarn's experiment)

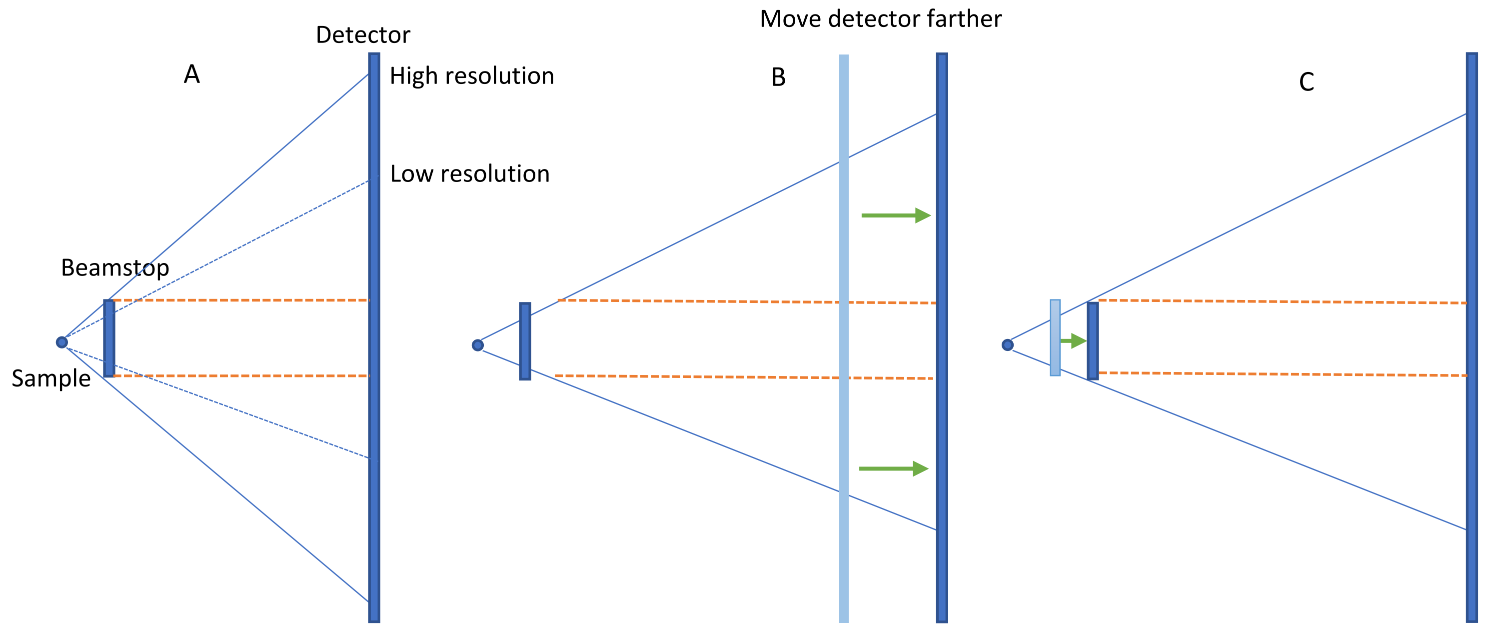
3. วัตถุประสงค์

To determine the proper correlation of detector distance and the resolution at the edge of detector, Rayonix SX165 for experimenting X-ray diffraction.

4. วิธีการดำเนินงาน

To determine the correlation of detector distance and the resolution at the edge of detector, different crystal to detector distances w adjusted and the resolution at the edge of detector was observed using marDTB software. For optimizing the beamstop position at different resolution range, a test diffraction image was observed and the beamstop position was re-adjusted to obtain no low-resolution loss in diffraction image.

According to a paper, “X-Ray Data Collection From Macromolecular Crystals” by Garman et. al. (2007), it pointed the correlative geometry on distance of detector and beamstop to sample position. Usually, it necessary to make the beamstop shadow as small at low resolution by putting the beamstop as far as possible. The diagram is shown in figure 4.



At 100 mm Distance-to-detector (1.5 Å resolution) and 20 mm beamstop distance, it makes beamstop shadow as small as possible.

At 180 mm Distance-to-detector (2.3 Å resolution) and 20 mm beamstop distance, it causes beamstop shadow appear larger at low resolution

At 180 mm Distance-to-detector (2.3 Å resolution) and 35 mm beamstop distance, it makes sufficient size of beamstop shadow for the low resolution

Figure 4 Correlation between beamstop shadow and distance-to-detector

5. ผลลัพธ์ และอภิปรายผล

The detector distance was determined to correspond to the resolution at the edge of detector as shown in Table 1. After that the beamstop position at different resolution was optimized to provide the smallest beamstop shadow. The optimized beamstop distance was listed in the table below and therefore users could be used those parameters for their X-ray data collection. Test experiment shows that adjusting the beamstop position can improve the low-resolution data as shown in figure 5.

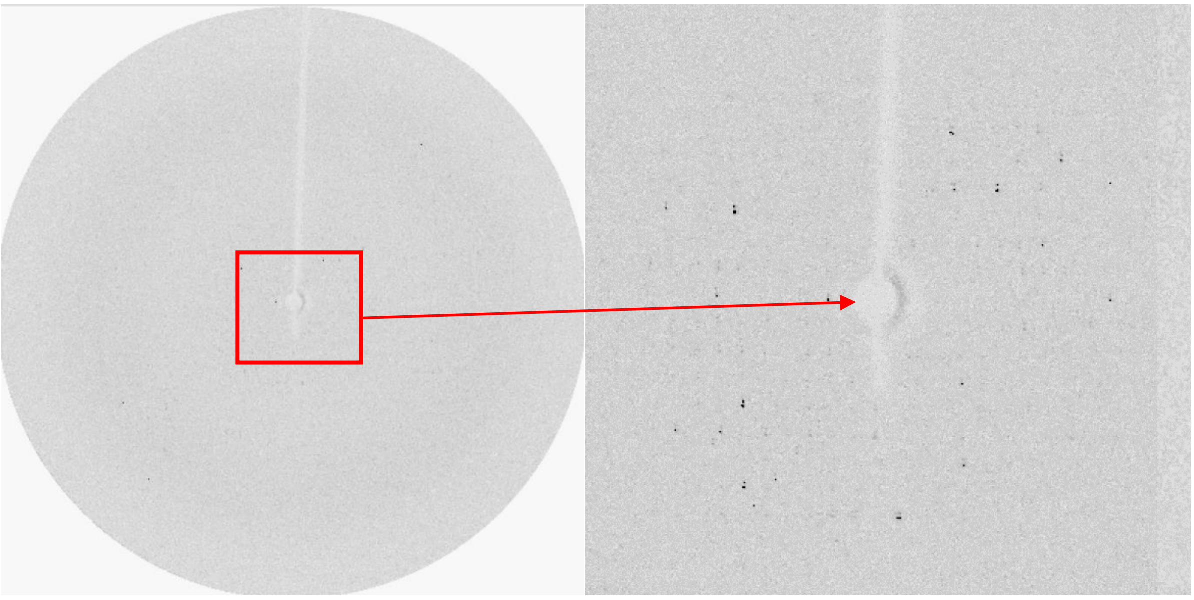


Figure 5 Appearance of scattering spots at low resolution after beamstop optimization

Table 1 Experimental set up parameters for data collection at BL7.2W: MX at an energy of 12.658 keV (0.979 Å)

Detector distance (mm)	Beamstop distance (mm)	Resolution (Å)
45	10	0.96
50	10	1.00
60	10	1.08
70	10	1.17
80	20	1.26
90	20	1.36
100	20	1.46
110	20	1.56
120	25	1.66
130	25	1.77
140	25	1.87
150	30	1.98
160	30	2.09
170	30-35	2.20
180	35	2.31
190	35	2.43
200	40	2.54
210	40	2.65

220	40	2.77
230	40	2.88
240	40	2.99
250	45	3.11
260	45	3.23
270	45	3.34
280	45	3.46
290	45	3.57
300	45	3.69
320	45	3.92
350	45	4.28
390	45	4.75

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6. สรุปผล

To facilitate non-expert users, we have provided experimental set up parameters which are necessary for data collection. Since the acknowledge on a position of beamstop has linked to its shadow on some area at low resolution, the problem on data loss at low resolution has been sorted out as well as improving signal to noise of the X-ray data. Therefore, to optimize experimental setup parameters appropriately is crucial for user service in order to obtaining a meaningful dataset.

7. ผู้ใช้ประโยชน์

Staff and beamline’s users who have encountered data loss due to low-resolution while doing data acquisition with marDTB coupled with Rayonix SX165.

8. เอกสารอ้างอิง

- Garman E., Sweet R.M. (2007) X-Ray Data Collection From Macromolecular Crystals. In: Doublié S. (eds) Macromolecular Crystallography Protocols. Methods in Molecular Biology™, vol 364. Humana Press. https://doi.org/10.1385/1-59745-266-1:63
- Ed Lowe (2010) Sources, Detectors and Data Collection. Handout from lecture on instrumentation for protein crystallography in BCA/CCP4 Protein Crystallography Summer School 2010