

SSRF MX Beamline Remote Operation Instructions

2022-12-13

This document is applicable for remote data collection operations at the Shanghai Synchrotron Radiation Facility MX Beamlines (BL02U1 and BL10U2).

Before conducting remote experiments, users must obtain prior approval from the beamline, possess practical experience in on-site data collection at the beamline, be familiar with the standard beamline operations and software usage. They are responsible for securely maintaining the account and password used for accessing the beamline control and data collection system and are not permitted to share these credentials. Remote experiments should be conducted in compliance with the network usage requirements specified by the Shanghai Synchrotron Radiation Facility.

I. Pre-Experiment Preparations

1. The box outside the liquid nitrogen tank must have wheels; boxes without wheels will not be accepted. Please do not use cardboard boxes or luggage trolleys. The box should be clearly labeled with the project leader's name, the beamline to be used, and the scheduled beamtime. Samples should be shipped to the Shanghai Synchrotron Radiation Facility at least one working day before the experiment date. In principle, no rescheduling or reallocation of beamtime will be made due to experiment delays caused by transportation.

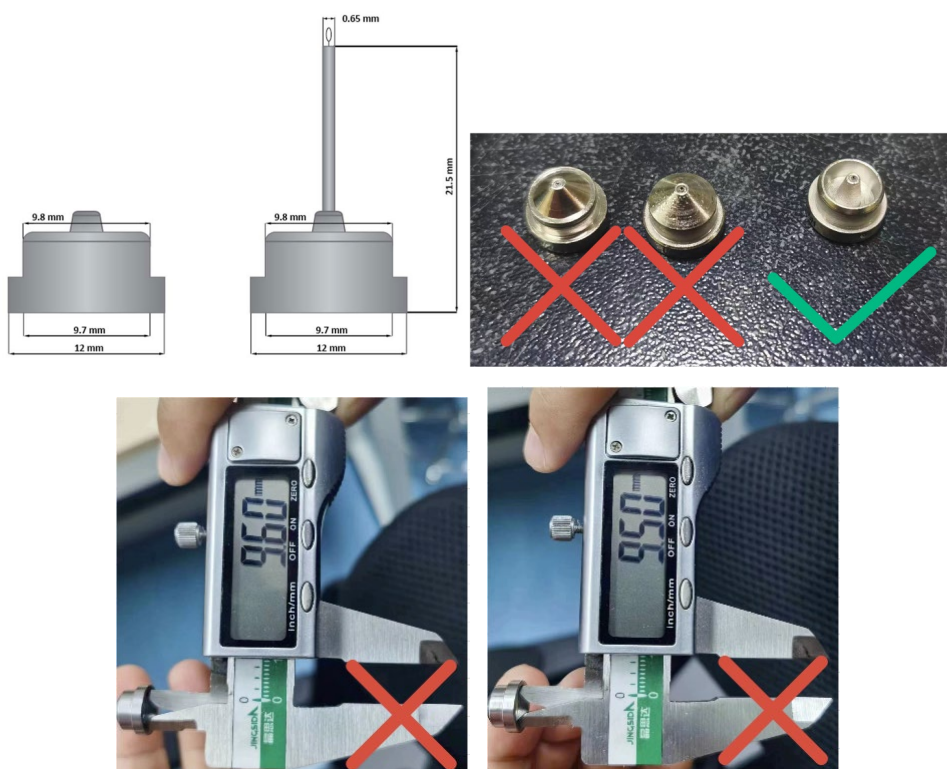
2. Do not mix samples from different research groups in the same liquid nitrogen tank. Each research group should transport their own samples in their designated liquid nitrogen tank and should not delegate the transportation of their samples to other research groups. The beamline follows the principle of 'who sends (brings) the samples, is responsible for sending them back (bringing them back).' If any issues related to mixing of samples arise (including but not limited to problems due to beamline malfunctions), the respective research groups should communicate and resolve them independently.

3. Please provide a Puck information sheet with the samples for the corresponding placement of Pucks. In the future, it is recommended to use Pucks with QR codes for sample

management, allowing for information retrieval through scanning.

4. We recommend preparing a sample information sheet. For more details, please refer to the 'Crystal Parrot' WeChat public account beamline operation guide. You can download the information sheet from the following website: <https://gitee.com/cjsy/finback-sample-sheet/raw/master/finback.xlsx>

5. Remote experiments are limited to the use of SPINE sample mounts only, and non-SPINE mounts will not be accepted. SPINE sample mounts offer the best compatibility with the sample loading robot, reducing the likelihood of malfunctions. The specifications for the SPINE sample mounts are as shown in the diagram below. Please note that the inner diameter of the lower opening is 9.7mm. Using mounts with diameters that are too large or too small can cause serious issues, so please ensure proper identification before use. It is recommended that the pin length be 18mm, approximately 22mm from the bottom of the mount to the nylon ring, for optimal centering and improved experiment efficiency.



6. Network bandwidth

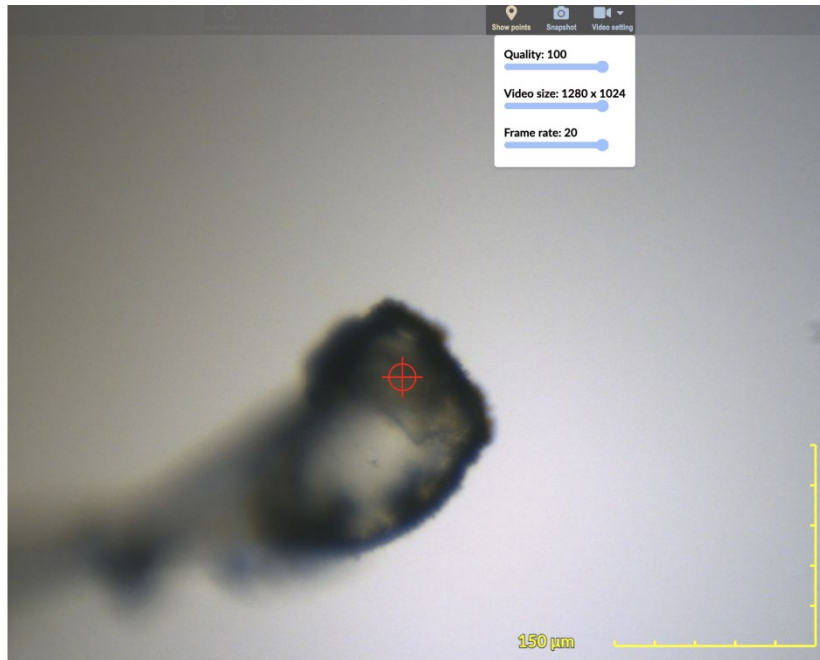
6.1 Before formal usage, please test the connection speed using the network speed testing tool provided by the beamline.

URL for the network speed testing (BL02U1): <http://10.30.74.219:5100>

URL for the network speed testing (BL10U2): <http://10.30.84.179:5100>

6.2 Sample videos that closely resemble the on-site beamline experience typically require a bandwidth of approximately 10 Mbit/s. In cases of unstable network conditions, adjustments can be made by selecting different video settings parameters. Real-time monitoring videos from the beamline typically require a bandwidth of around 10 - 15 Mbit/s.

6.3 You can adjust the video settings using the "Video setting" dropdown menu on the toolbar above the sample video. You can configure the video's Quality, Video size, and Frame rate. It's recommended to set the Frame rate to no lower than 15 Hz.

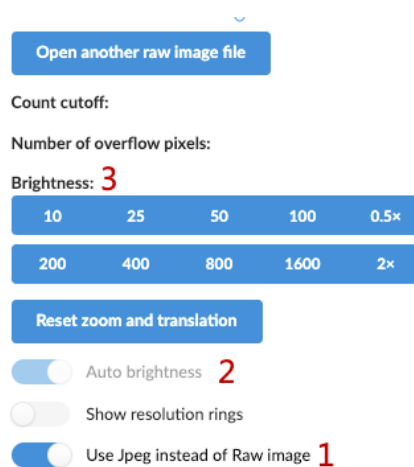


6.4 The table below shows the required bandwidth for different sample video test parameters for your reference:

Quality	Video size	Frame rate	Required Bandwidth
100	1280 × 1024	20	~ 80 Mbits/s
75	1280 × 1024	20	~ 10 Mbits/s
75	960 × 768	18	~ 7.2 Mbits/s
75	640 × 512	15	~ 4.0 Mbits/s

6.5 At SSRF BL10U2, using the Eiger X 16M detector, the original uncompressed diffraction images are approximately 70 MBytes each, and when compressed, they are approximately 15 MBytes each. At SSRF BL02U1, using the Eiger2 X 9M detector, the original uncompressed diffraction images are approximately 35 MBytes each, and when

compressed, they are approximately 9 MBytes each. When the available bandwidth is greater than 50 Mbit/s, you can attempt to view the original diffraction images. However, the viewing experience may have a delay of 7-10 seconds, depending on your internet speed. In cases where the bandwidth is lower than 50 Mbit/s, two options for viewing diffraction images in JPEG format are provided, with each JPEG diffraction image size being approximately 1 MByte. If the delay in viewing the original diffraction images is too long, it is recommended to switch to JPEG format for faster display. Additionally, the performance of the client's computer can also affect the speed of image viewing. This information is helpful for users to optimize their data viewing experience during remote experiments.



6.5.1) Use Jpeg instead of Raw image: Based on the available bandwidth, choose whether to display JPEG diffraction images or original diffraction images. For remote users, the default setting upon opening the page is to display JPEG diffraction images.

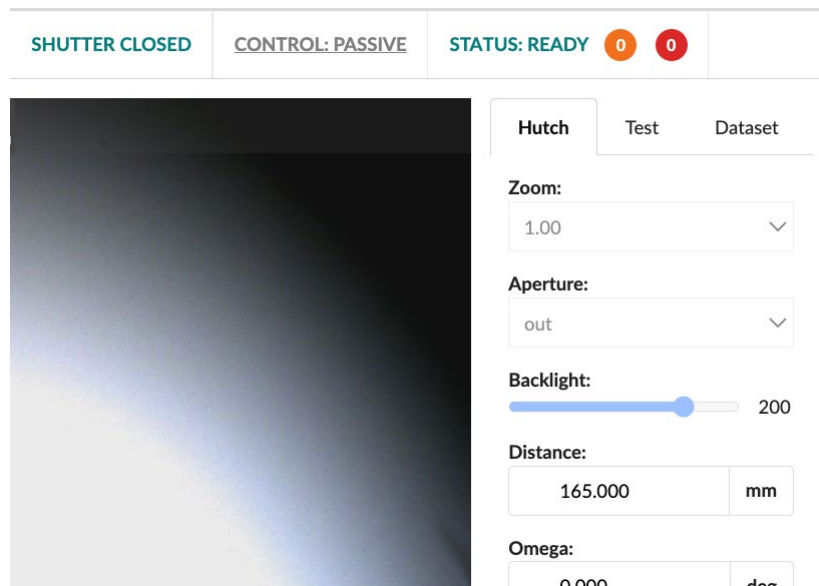
6.5.2) Auto brightness: If you choose to display original diffraction images, the 'Auto brightness' feature will be enabled by default to automatically adjust the brightness (contrast) of the diffraction image.

6.5.3) Brightness: If you select the original diffraction image display and do not wish to use 'Auto brightness,' you can deactivate 'Auto brightness' and manually adjust the brightness (contrast) settings.

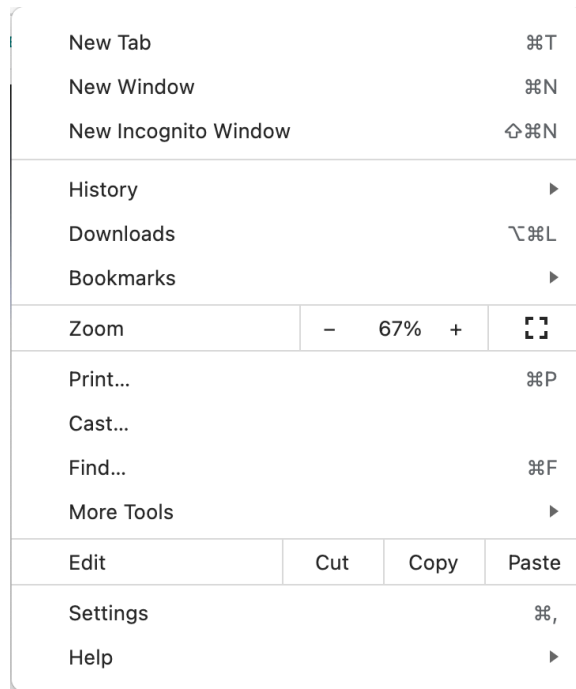
7. Prepare a high-performance and stable computer. It is recommended to have four screens, each with a resolution of 2K (2560×1440) or higher, dedicated for data collection, displaying automated data processing results, viewing diffraction images, and real-time beamline monitoring videos. If you have fewer than four screens, content that cannot be displayed on a

separate monitor can be accessed through browser tabs on the same screen. Real-time monitoring videos from the beamline provide live updates on the status of the robotic arm and goniometer, making it easy to understand simple issues that may arise during use. In case of malfunctions, communication with on-duty staff is facilitated.

8. The Finback page is optimized for 2K screens, and if you are using a monitor with a resolution lower than 2K, you may need to utilize your browser's zoom function to fully display the entire Finback page, including data collection and diffraction image viewing. For example, if you are using a 1920×1080 resolution monitor, you may need to reduce data collection and diffraction images to 90% for complete display. On a 1440×900 resolution monitor, you may need to reduce them to 67% (or 70%) for full visibility. The lowest resolution we have tested is 1440×900. We do not recommend using monitors with resolutions lower than 1920×1080.



After opening the Finback page, carefully inspect the top information bar and make sure that the rightmost sections, including CONTROL, STATUS, warning count, and error count, are fully displayed. Incomplete display of the information bar may prevent the activation of Finback.



For Google Chrome or open-source Chromium, you can find the Zoom option in its menu bar. You can click the plus (+) and minus (-) buttons to adjust the zoom level. Alternatively, you can directly use the keyboard shortcuts Ctrl+ and Ctrl- (on macOS, it's Cmd+ and Cmd-) to adjust the zoom level.

9. For hard drive preparations, please refer to the relevant content in the 'Crystal Parrot' WeChat public account.



10. It is recommended to use Google Chrome or its open-source counterpart Chromium as your web browser.

11. Prior to your experiment, it is essential to test your network bandwidth and adjust appropriate video settings. Network bandwidth, computer performance, and display

resolution are critical factors for a smooth user experience. We recommend a minimum network bandwidth of at least 30 Mbit/s and, ideally, no less than 100 Mbit/s (as networks with over 100 Mbit/s have become quite common). Please control the number of simultaneous users logging into the beamline (since beamline bandwidth is shared, reducing unnecessary bandwidth consumption is important). Robust computer performance and compliant displays are also highly beneficial for improving experiment efficiency.

12. Prior to remote experiments, it is crucial to have your own beamline account and password. In principle, we will create accounts and passwords for the Principal Investigator (PI). If you are unsure whether you have your own account and password, please do not hesitate. Make sure to contact the beamline user coordinator at least one week before the experiment. Account issues cannot be resolved on-site during the experiment. If you still do not have an account and password at the start of the experiment, we can provide a temporary user account (tempuser), but please note that temporary accounts do not have access to automated data processing functions.

II. Remote Data Collection

1. VPN Login: <https://159.226.222.242:6443>, Enter the username and password to log in.

BL02U1 VPN Username for login: bl02u1user

BL10U2 VPN Username for login: bl10u2user

Passwords are periodically changed. Please contact the beamline staff before your experiment to obtain the most up-to-date password.

2. First-time login may require downloading the Atrust client.
3. Open the beamline's web page in your web browser.

BL02U1

Data Collection (Finback) : <http://10.30.74.219>

Diffraction Image (Finback) : <http://10.30.74.219/rawimages> (Original Diffraction Image and JPEG Diffraction Image)

Data Processing (SealWeb) : <http://10.30.74.219:4500> (For academic users only)

Real-time Beamline Monitoring: <http://10.30.74.219:5000>

BL10U2

Data Collection (Finback) : <http://10.30.84.179>

Diffraction Image (Finback) : <http://10.30.84.179/rawimages> (Original Diffraction Image and JPEG Diffraction Image)

Data Processing (SealWeb) : <http://10.30.84.179:4500/> (For academic users only)

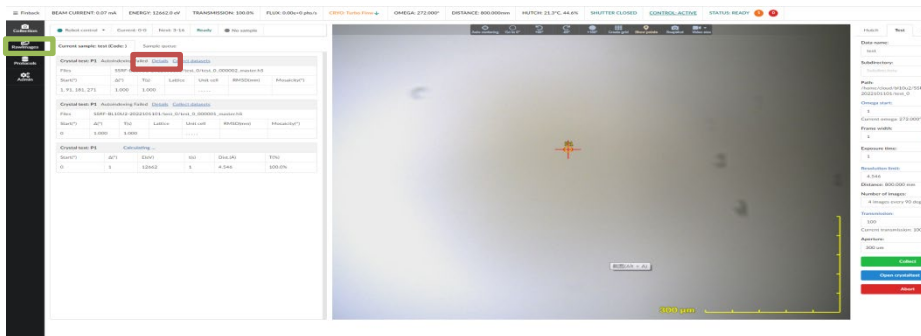
Real-time Beamline Monitoring: <http://10.30.84.179:5000>

4. To ensure proper data collection, remote users need authorization from the beamline staff before logging into the Finback system. Please do not log in during unallocated beamline time. SealWeb system login does not require prior authorization and provides the capability to download data processing result files, including mtz, sca, pdb, and log files. After data collection is completed, you can still access and download processing results and files through the SealWeb system.

5. Follow the beamline's operational instructions for data collection.



6. In addition to the dedicated 'Raw Image' page for diffraction image viewing, you can also view JPEG diffraction images under 'Details' in the data collection interface.



III. Post-Experiment Operations

1. Close the software and log out of the VPN.
2. Please contact the company to provide the return address and recipient information for the liquid nitrogen tank. Arrange for the return shipping with 'collect on delivery' payment.

Shanghai Synchrotron Radiation Facility will provide necessary experimental support for remote experiments. However, the facility will not be held responsible for damages, losses, or other unexpected incidents, including but not limited to damage or loss of containers or materials during transportation and the experimental process.

The Shanghai Synchrotron Radiation Facility reserves the final right to interpret remote experiments.