Short Manual to Operate CLS-SM Ambient-STXM and Ptychography

1. Using the SM beamline **STXM BRANCH** control software to click a grating button:

LEG: 150 eV to 900 eV, Mirror Pt (outboard), LEG 200 (outboard), Cff mode

MEG: 350 eV to 2100 eV, Mirror Pt (outboard), MEG 500 (outboard), Cff mode

HEMG-Omega: 700 eV to 3000 eV, Mirror CrB4C (outboard), HEMG 1370 (outboard), Ω = 0.68 (optimized)

HEMG-Cff: 700 eV to 2100 eV, Mirror CrB4C (outboard), HEMG 1370 (outboard)

2. EPU Harmonics and Polarization settings:
1st EPU Harmonics: 150 eV to 900 eV; Polarization: Circular Left, or other polarizations as needed
3rd EPU Harmonics: 900 eV to 1700 eV; Polarization: Linear Horizontal
5th EPU Harmonics: 1700 eV to 2300 eV; Polarization: Linear Horizontal
7th EPU Harmonics: 2300 eV to 2700 eV; Polarization: Linear Horizontal
9th EPU Harmonics: 2700 eV to 3000 eV; Polarization: Linear Horizontal

3. On computer **OPI1610-003**, first run the **NX Server** application, then launch the **pySTXM GUI** application, and finally start the **pyMono** application to monitor and fix the monochromator issues.

4. **(Optional)** The pySTXM software can also run on Linux. On computer **OPI1610-003**, use Windows **Remote Desktop Connection** to connect to the computer **VOPI1610-005** by the account name: **sm-user**, and the password given to you. On **VOPI1610-005**, open a console/terminal and type **cd bin** to enter the **bin** directory (/home/sm-user/bin), then execute the command: **./runpyStxm.sh**

5. On **pySTXM 3.0** software, set **Ao** to **80-90%** of the **maximum Ao** on the **Preference** tab.

6. Enable "**FL change with Energy**" if it was disabled.

7. Enter the energy you will be working with to update the STXM **Zone Plate-Z** motor position.

8. Move **Coarse Z = Ao + 400 µm for Si3N4 window samples**; **For TEM grids**, **Coarse Z = Ao + 200 µm.**

9. At an empty hole or a known empty area of a sample, run the **Detector Scan** and center it, and then run the **OSA Scan** and center it. If the OSA edge is not sharp, run the **OSA Focus Scan**. Then, optimize **M3STXM Pitch** and **EPU Offset** at an empty hole or region on the sample, and then adjust the beamline **Exit Silts** size if necessary to achieve a beam flux of around **5 MHz**.

10. Start **Sample Image Scan** from sample #1 (coordinates (-5000,5000)), using (1000x1000 µm), (500 x 20 points), **Polarization: CircLeft, Offset: optimized value**, **Single energy** checked, dwell time **1 - 5 ms**, **Line by Line** image mode. If the image is way out of focus, you should move **Coarse Z** to an estimated position or do a focus scan, and then click **"Set Focus to Cursor" (Button #1)**.

11. Scan a smaller-sized image in focus and in good resolution, i.e., (600x600 µm) (300-600x100 points). Zoom in until the coarse scan size is at (200x200 µm) (100x100 points).

12. Scan a fine image with (70x70 µm) or (50x50 µm), (100x100 points) for a selected sample region. If a piezo stage voltage reaches **-20 or +120 V** with a **red highlighted background**, click **"AutoZero and Reset Interferometers"**.

13. Do a focus scan at a selected energy and click **"Set Focus to Cursor" (Button #1)**. If the focal point is close to the center of the image, less than about 20 µm in the Y-axis, you should click **"Set Ao to Cursor" (Button #2)**.

14. Set up a stack map using two energies, one below the edge and the other on the edge/peak, (50x50 µm) (200x200 pixels). Analyze the data and choose an interesting sample region.

15. Set up a stack scan with a size typically **from 5 to 50 µm**. **Load energy scan definition** for the scan from Jian/C1s/.... The beamline slits' size could be changed to avoid saturation at any elemental edge; other parameters will not be changed if they are optimized.

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Procedure to open the STXM Branch Control Interface & FMB Monochromator Control Interface

1. Open the **MobaXterm** or **NoMachine** software on any SM Windows computer, if the software is on the computer desktop.

2. For **MobaXterm**, click "**Start local terminal**", and type the command "**ssh -Y sm@OPI1610-002**"; or use the up-arrow key to scroll to the command. As the password has been remembered by MobaXterm, you should log in to the OPI computer directly. Type the command "**runSTXM**"; or use the up-arrow key to scroll to the command.

3. For **NoMachine**, open the software and connect to the computer **OPI0000-004**, and then you will find the **STXM BRANCH** control interface, Ambient-STXM Motor Control and Interferometer Status GUIs on the computer desktop.

4. Click **runSM_MonoFMB2022** on the **STXM BRANCH** beamline control GUI. To fix the monochromator motor frozen problems if the pyMono application doesn't work, do the following:

   4.1 Click the Status "**Enable**", or each button of "**Single Axis Panel**" for "**Mirror Pitch**", "**Grating Pitch**", "**Mirror Trans**", and "**Grating Trans**".

   4.2 Click "**Enable**" and do it for all four panels.

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Ptychography Scan Procedure

1. Manually or use the "**TPLink Kasa Control**" software to switch on the power for the CMOS liquid cooler and the Tucsen Dhyana-95V2 sCMOS camera after the STXM tank is **filled with 1/6 atm helium or in vacuum**. (Note: running under vacuum is optional, and it may introduce OSA drift and stronger vibrational noise.)
2. Open the **MOSAIC** software on the STXM-ptychography data acquisition computer (**WKS-W004516**).
3. **Temperature Control** tab → **Cooling: -10°C** → **Fan Speed: Off(Water Cooling)** (Note: cooling to -20 °C is optional as the background noise is not reduced below -10°C.)
4. **Main Control** tab → **Resolution 2048 x 2048** → **HDR** → **Exp Time: 300 ms** (Or other time user can define based on image intensity.) The live video mode is automatically on. If you want to turn off the video mode, click **Main Control** → **Stop**.
5. **Image Capture** tab → **Path:** C:\CMOS-data\Dhyana95V2\2026\2026_06\A260606072 (create a folder for each scan) → **Image Name:** A260606072 (for example) → **Total Frame:** the same as the STXM scanning points for each image → Ignore "Total Time" and "Interval Time" as you will be using the Trigger Mode for image acquisition. → File Format: MPTIF (supported by PyPIE-v3.4.5 and later versions, or other format you like) → **Save as "To Disk"** (Note: saving to the network is slow and could cause image acquisition to lose synchronization; therefore do not save data to the network directly.)
6. Move STXM **Detector X** to about -83000 µm. Open the STXM shutter, and you can see a zone plate (ZP) projection on the sCMOS. Check the ZP projection center Y pixel number and move Detector X to

make it close to 1024. (Note: the sCMOS image is rotated by 90 degrees, X and Y directions are flipped with each other.) The ZP center X pixel is not movable, and it is located around 1080 pixels.

7. Normally, you need to adjust OSA X and Y now by jogging 1 µm in either direction to get the OSA aligned.
8. **Image Adjustment** tab → **Range**, you can increase the beamline slits size slightly to make the image intensity between 30000 and 50000 in the **HDR** mode. You may increase the STXM slits size to 50/50 for C and N K-edge. Other edges should be less than 30/30 in general. Under any circumstances, if you see sCMOS image intensity is more than 50000 (**HDR** mode), or if waterfall patterns wipe out the sCMOS, close the STXM shutter or beamline valve immediately.
9. **Trigger** tab → **Off** (for live video mode) → **Standard** (for STXM-Ptychography data acquisition)
10. Set up a STXM scan on the STXM image. In the **Sample Image Scan** tab → image **point by point** mode, **Defocus spot size** 2500 nm (or any other spot size **from 100 nm to 6 µm**), step size: 500 nm (**spot size x 20%**), scan size 5.0x5.0 µm (or any other size), 11x11 points (other popular points include 5x5 (minimum), 7x7, and 9x9), STXM dwell time 310 ms (sCMOS exposure time 300 ms, 10 ms extra buffer time). (Note: the sCMOS exposure time and the STXM dwell time can be adjusted based on image intensity, and as low as 50 ms can be applied.)
11. After the sCMOS data file name and frame number are set, start sCMOS acquisition by clicking the "**Capture**" button, then click STXM scan "**Start**".
12. After the ptycho scan, acquire a background image on the MOSAIC software with the STXM shutter "**Auto**". Change Trigger Mode to "**Off**", change the saving file name to A260606072**bg** (for example), set a frame number, such as 5, and capture the background multi-tif image file.
13. After the above ptycho scans, click "**Move-CMOS-data_to_loki-shortcut**" on the desktop of the ptychography data acquisition computer.
14. Analyze ptycho data on the user or staff ptycho reconstruction computer.
15. Back to normal STXM: move **Detector X to Zero** with the STXM shutter "**Auto**".
16. Return to image scan (**Line by Line**), typical: 10x10 µm, 100x100 points, dwell time 1 ms. Change other beamline parameters to previous settings for normal STXM, such as slits size.
17. If the sCMOS will not be used for more than 4 hours, you should turn off the power. Then, you can vent the STXM tank.