X-ray Imaging Beamline User Manual

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Contents

Chapter 1

Software Overview

This chapter will serve as an overview of the functionality of the `blcontrol` software. Figure 1.1 shows the full user interface that appears when the application is started. Each panel in the window is explained in its own section below.

1.1 Scan Settings

The scan settings panel is shown in Fig. 1.2. The top half contains fields for setting a sample name and ROI (region of interest) and a drop-down menu for choosing a scan type.

The sample name field is only used to identify the sample in any saved files. You can put whatever you like here or leave it blank.

The ROI setting allows you to choose a region of the spectrum between two energy values to be analyzed in real-time along with the total spectrum. If this value is set, the ROI will be highlighted in the spectrum plot and information about the portion of the spectrum will be displayed on the plot. The counts in the ROI will also be counted separately in any scans that are run.

The dropdown menu allows you to choose what type of scan to run, with the choices being "Single Spectrum," "Linear Scan" and "Grid Scan." Each scan type is covered in more detail below. When the scan type is changed, the lower portion of the panel will change to display the settings available for that scan type. For each scan type, press the "Start" button on the bottom of the scan settings panel to begin running the scan. The "Stop" button

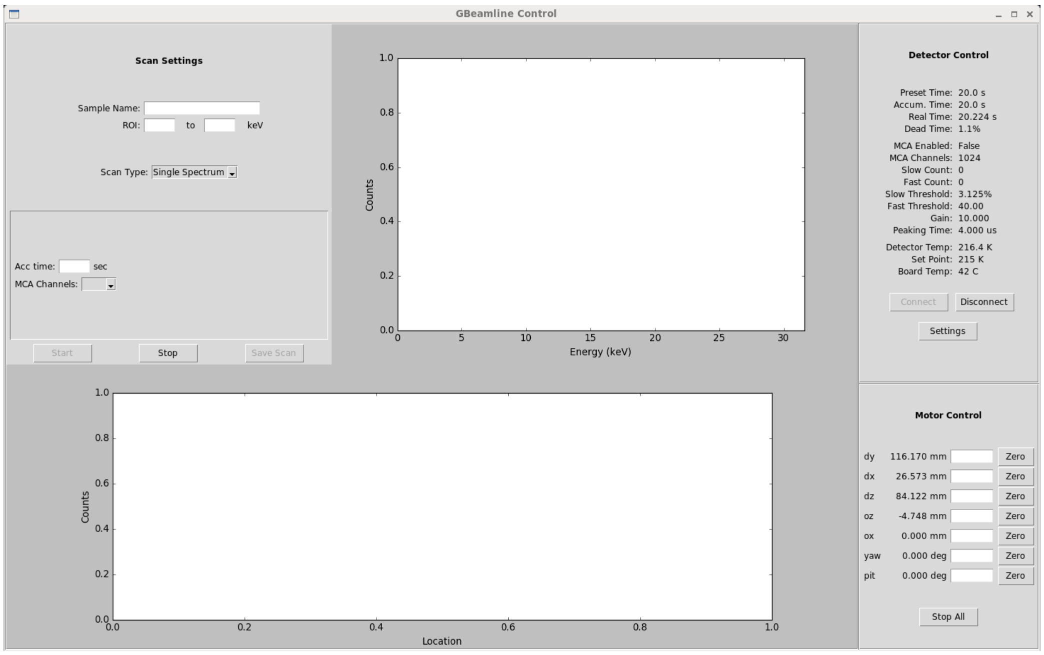

Figure 1.1: Screenshot of the full user interface on startup. The elements of the interface, clockwise from top left, are the scan settings, the single spectrum plot, the detector status readout, the motor control panel, and the scan plot.

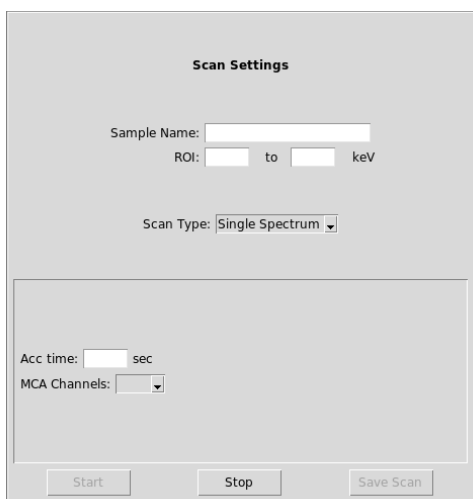

Figure 1.2: The scan settings panel, with scan type set to "Single Spectrum."

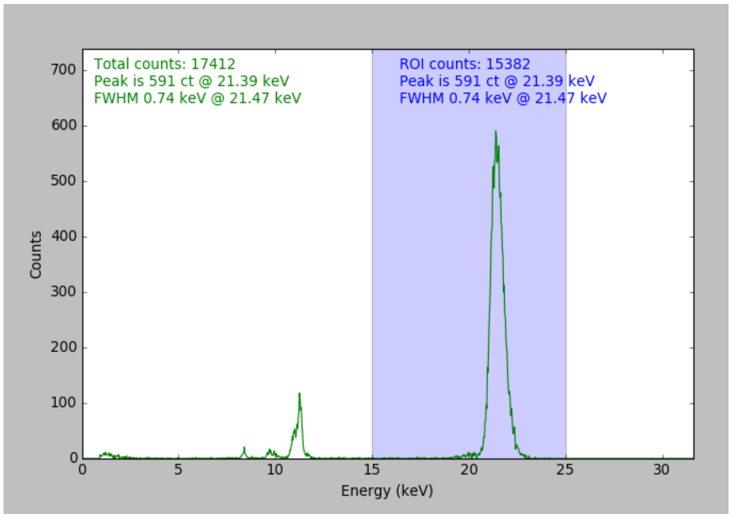

Figure 1.3: The spectrum plot display panel, during the collection of a single spectrum.

may be used to terminate the scan prematurely. Once a scan is finished or has been stopped by the user, the "Save Scan" button allows you to save the data from the most recent scan in a plaintext format. The saved scan file will include all of the detector status and settings data, and the current position of each connected stage.

1.1.1 Single Spectrum

Fig. 1.2 shows the layout of the scan settings panel when "Single Spectrum" is selected. For a single spectrum, there are only two scan-specific options: the accumulation time, in seconds, and the number of MCA channels to be used. The accumulation time can be any value, and the number of channels is selectable from a drop down menu. The detector allows the use of 256, 512, 1024, 2048, 4096, or 8192 channels.

When the spectrum acquisition is started, after a few seconds the spectrum will begin to display in the spectrum plot display panel, to the right of the scan settings panel. This plot will update in real time (with the update frequency depending on the number of channels) until the acquisition is complete.

An example image of the spectrum plot is shown in Fig. 1.3. In the upper

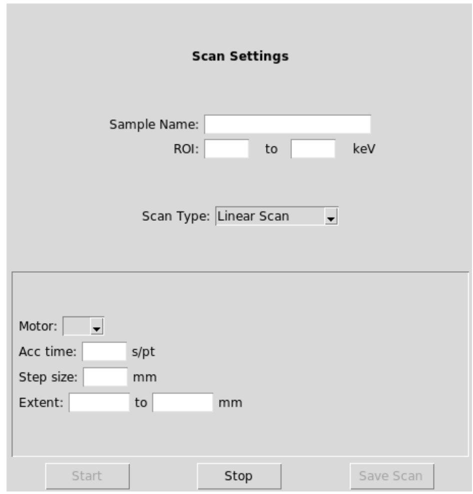

Figure 1.4: The scan settings panel when “Linear Scan” is selected.

left corner, the green text displays some information about the spectrum: the total number of counts, the number of counts and the location of the peak channel, and the full width at half maximum (FWHM) and center of the highest peak in the spectrum. For this spectrum, the ROI was set to 15-25 keV, and this region is highlighted in blue. The blue text in the upper right corner gives the similar information about the portion of the spectrum that is contained in the ROI. In this example, the highest peak in the ROI is the same as the highest peak in the full spectrum.

1.1.2 Linear Scan

A linear scan consists of moving a single stage over a distance in specified increments, and taking a spectrum at each position. This is useful during the alignment process, when you want to position each stage at the location that maximizes the count rate.

Fig. 1.4 shows the layout of the scan settings panel when “Linear Scan” is selected. A dropdown menu allows you to choose a motor to scan from the motors that are connected. The accumulation time field specifies the duration of the spectrum that will be taken at each position. Step size is the distance interval between each scan position. The default units are millimeters, but will change to degrees if a rotary stage is selected from the motor dropdown menu. Finally, the extent fields specify the beginning and ending points of

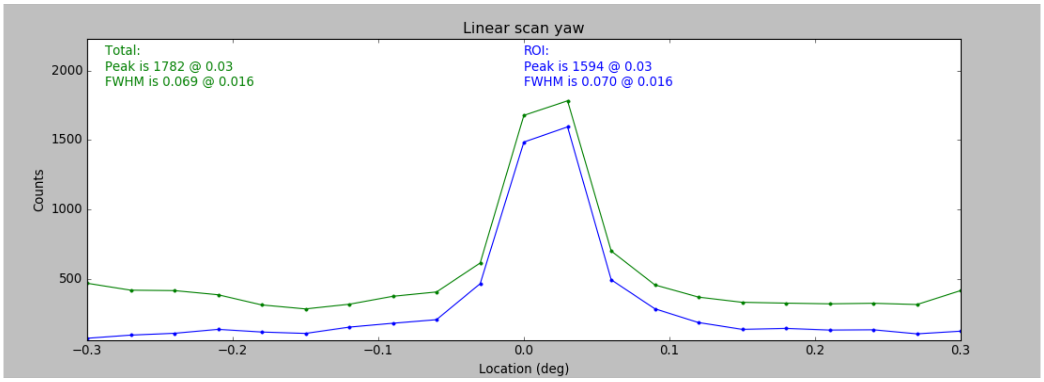

Figure 1.5: The plot displayed in the scan plot display panel, after a linear scan is run.

the scan. The extent is inclusive, meaning a spectrum will be taken at the beginning of the interval, and, if the interval is exactly divisible by the step size, a spectrum will be taken at the end of the interval as well. Together, the extent and the step size define the number of points in a linear scan. The approximate duration of the scan can be determined from the accumulation time at each point and the number of points, but note that some extra time will be needed for data transfer and stage motion.

While the scan is running, the spectra collected at each point will be displayed in the spectrum plot panel, similar to how it is displayed while collecting a single spectrum. During a scan, however, the number of MCA channels is limited to 256 to improve data transfer speed and decrease the size of the files generated from the scans. When the scan is finished, the stage will remain in the final location of the scan until moved by the user.

A plot will also be generated in the scan plot panel, as shown in Fig. 1.5. In real time during the scan, the plot will show the total number of counts collected at each location in green, and the number of counts in the ROI (if used) in blue. Information is also displayed about the highest peak for both the total count data and the ROI data.

1.1.3 Grid Scan

A grid scan is a 2D scan of the detector in the xy plane, which is useful for centering the detector on the axis of the optic. Fig. 1.6 displays the options for setting up a grid scan. The user specifies the accumulation time as in

Figure 1.6: The scan settings panel when “Grid Scan” is selected.

a linear scan. The step size is the distance between consecutive points in both the x and y directions. The grid size dropdown menu allows the user to specify the number of points to be collected, from 3×3 to 11×11 points (odd numbers only).

Unlike the linear scan, which allows the user to specify the start and end points of a scan, a grid scan is always centered around the position of the detector at the time the scan is started. When the scan is initiated, the detector will move to the first position, the lowest values of x and y, and proceed in a raster fashion until the scan is complete. First x is scanned all the way across in units of the step size, then y is incremented by one step and x is scanned in the opposite direction, and so on until the entire area has been scanned. As in the linear scan, the spectra appear in the spectrum plot panel as they are acquired.

The results of the scan are displayed in real time in the scan plot panel, shown in Fig. 1.7. Points are filled in as they are collected, and points not yet collected appear in gray. The total counts are plotted on the left, and the counts in the ROI, if used, are plotted on the right. Both plots display the calculated center of mass of the scans to aid the user in centering the detector. When the scan is finished, the detector will remain at the final point of the scan until moved by the user.

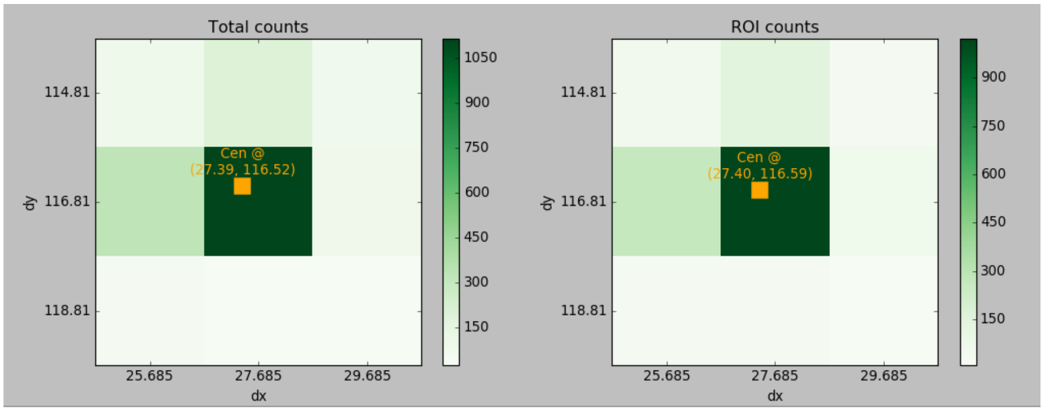

Figure 1.7: The plot displayed in the scan plot display panel, after a grid scan is run.

1.2 Motor Control

The user can move each stage independently using the motor control panel, shown in Fig. 1.8. For each connected stage, the current position is shown, followed by a new position field and a "Zero" button. To move the stage to a new position, enter the new position in the field and press Enter. The current position will update in real time as the stage moves. You can also move the stages using the hardware knobs. The zero button will set the current position of the stage to zero. The "Stop All" button, located at the bottom of the panel, can be used for an emergency stop of all stages.

If the power has been disconnected to one of the stages since the last use, it must be homed before the next use, otherwise the encoder will not have a valid position reference. If one or more of the motors is unhomed when the software is started up, the user will be prevented from moving that motor. A warning message will appear, the new position field for the affected stages will be grayed out, and the "Zero" button will be replaced by a "Home" button. Pressing the "Home" button will instruct the stage controllers to perform the homing routine automatically, but **you must make sure the area is clear for the motor to return all the way to the home position** before performing this step. This includes ensuring that the stages will not run into any obstacles while homing, and that the cables connecting the motors will not become tangled or overstressed. Also, **the current position will be lost when the homing routine is performed**. For these reasons, it is

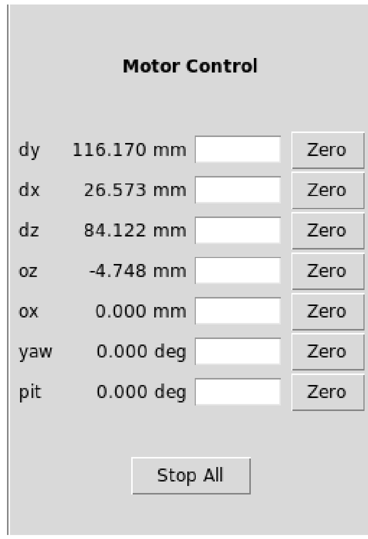

Figure 1.8: The motor control panel.

often preferable to home the motors manually, by using the knob on the controller to move them until the home sensor is triggered. This allows you to move the motors slowly, make sure there are no obstacles in the way, and mark the current position of the stages before beginning the homing process.

1.3 Detector Control

1.3.1 Detector Status

Figure 1.9 shows the detector control panel. The top portion of the panel displays constantly updated status information from the detector. The preset time is the total duration for which the detector will accumulate the current spectrum. “Accum. Time” is the amount of active accumulation time elapsed so far in the current spectrum, and “Real Time” is the amount of real (clock) time elapsed so far. The difference between the two is the dead time, which depends on the count rate and the currently set peaking time in the detector's pulse shaping electronics. More information about peaking time can be found in the DP5 User Manual [2, p. 8].

“MCA Enabled” and “MCA Channels” give the current status of the detector's multi-channel analyzer. “Slow Count” and “Fast Count” are the

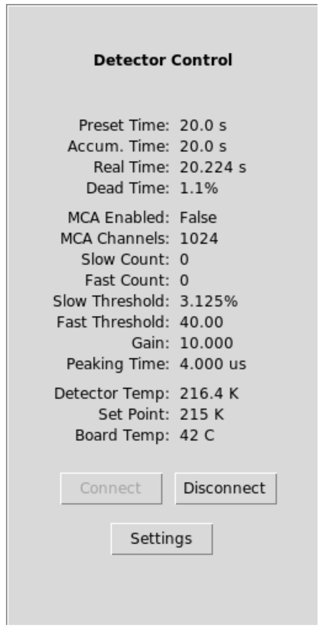

Figure 1.9: The detector status panel.

sum of all counts in the slow and fast channels, respectively, and "Slow Threshold" and "Fast Threshold" are the currently set thresholds for the lower level discriminator for the respective channels. The DP5 User Manual discusses the differences between the slow and fast channels [2, p. 7-8]. The slow channel threshold is given in percent of the full energy range, and the fast channel threshold is a number between 0 and 511.93, where 512 is the full energy range (see [1, p. 162] for more information on the fast channel threshold). The total gain of the amplifier, which governs the energy range of the MCA, is listed next. The status readout concludes with the total gain of the preamplifier, the peaking time, the current detector temperature and the set point of the detector cooler (in Kelvin), and the current temperature of the electronics board (in degrees Celsius). The detector should be cooled to below 225K. Lower temperatures are better for reduced noise.

Below the status readout are three buttons for interacting with the detector. The primary purpose of the "Connect" and "Disconnect" buttons is to re-establish communication if the detector stops responding or delivering status updates. The detector communication port is opened and ready to be used when the software is started.

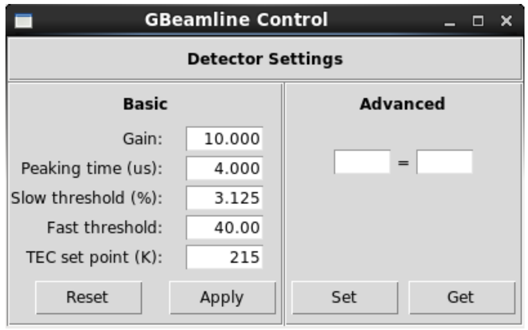

Figure 1.10: The detector settings popup window.

1.3.2 Modifying Detector Settings

The “Settings” button in the detector control panel opens the “Detector Settings” window, allowing the user to modify certain detector parameters. This pop-up window is shown in Fig. 1.10. On the left (“Basic”) side, a number of commonly used settings are listed along with their current values. To update one of the settings, modify the value in the text field and then press the “Apply” button. If you have modified one or more of the values in the text fields but you do not want to apply these changes, press the “Reset” button to reset all values to their previous settings.

The right side of the settings window, labeled “Advanced,” allows the user to edit any of the ASCII configuration values for the DP5. All ASCII commands and the allowed values for each are listed in the DP5 Programmer’s Guide [1]. This function should not need to be used regularly, and caution should be used when modifying the ASCII configuration.

To obtain the current value of an ASCII configuration parameter, enter the 4-character name of the parameter in the left text field and press the “Get” button. The parameter value will appear in the right text field. To change the value of a parameter, enter the parameter name in the left text field and the new value in the right field (after the “=” sign). After setting a new value, it is good practice to press “Get” again to verify that the desired value has been set correctly.

1.4 Configuration Files

Two configuration files are used by the `blcontrol` software. Both are found in the `blcontrol/config` directory. The file `bldata.txt` contains the zero positions for each stage in units of steps from the home sensor. It should not need to be edited by the user, even when installing a new stage. The software will automatically write to this file when the zero position is changed by the user.

The second file is called `blconf.txt`. It is used by the software to read various settings for the detector and motors, but it is not editable directly in the software. When a stage or detector is modified or added to the system, it will be necessary to edit `blconf.txt` to include the specifications for the device, using a text editor. Note that if the configuration file is modified, the software will need to be restarted for changes to take effect. It is good practice to create a backup of your configuration before making modifications so that you have a working version to revert to if something breaks.

Sec. 1.4.1 shows a recent version of this file for illustrative purposes—the values listed there may not necessarily be valid for the current iteration of the system. Each section heading is described in Sec. 1.4.2. Note that `#` indicates comments, `;` indicates inline comments, section headings are indicated by `[...]`, and configuration values are listed as `key=value`. Even if a device is not currently connected to the beamline assembly, it can still have configuration information listed in `blconf.txt` for future reference.

1.4.1 Example `blconf.txt`

```
# Beamline configuration file for motors and detectors
# Last updated 10 April 2018

[Motor Names]
36144=yaw
36142=pit
36153=dx
34795=dy
36592=dz
36900=ox
50852=oy
36610=oz
```

```
37203=rot3

[Motor Res] # Deg/step or mm/step, from zaber.com
# Note: on motor spec sheets the resolution is given in mm or deg
# per microstep at the default microstep resolution, which is 1/64.
yaw=0.015
pit=0.015
dy=0.003048
dx=0.003048
dz=0.03175
ox=0.006395
oy=0.006096
oz=0.0079375
rot3=0.01

[Max Current]
# Amps
yaw=0.95
pit=0.95
dy=0.5
dx=0.5
dz=0.55
ox=0.55
oy=0.95
oz=1.2
rot3=1.100

[Travel]
# mm
yaw=
pit=
rot3=
dx=50.8
dy=152.4
dz=150
ox=150
oy=40
oz=254
```

```
[Stage Port]
usbsn=AL00BUSL
serialport=/dev/ttyUSB0
timeout=5 ;seconds
baudrate=9600

[Detector Port]
timeout=10
serialport=/dev/ttyS0
baudrate=115200

##### Detector Calibration #####
# energy = (channel number)/((calib factor)*(hardware gain)*(num channels))
#  + offset
# calib_factor units are 1/keV
# offset units are keV

[14845 Calib]
#as of 10 April 2018
calib_factor=0.00315691059703
offset=-0.0439739471587

[14711 Calib]
#updated 12 sept 2016 with spectrum data from 9 sept 2016
calib_factor=0.000772012270785
offset=-0.302908357512

[2607 Calib]
#as of 20 April 2017
calib_factor=0.000564960446259
offset=-0.104852853501
```

1.4.2 Configuration File Headings

Motor Names

In this section each motor is listed by serial number and given a name which will be used to identify it in the software and the rest of the configuration file. A new `key=value` pair should be created for any new stage that is introduced to the system, and the resolution, maximum current, and travel should be defined in the following systems.

Motor Res

This section lists the resolution if each motor in real units, degrees per step for rotary stages and mm per step for linear stages. These values are taken from the specifications for each stage listed on `zaber.com`. As indicated in the comments, the values in this configuration are in units/step, while the values listed on the Zaber website are given in units/microstep.

Max Current

These are the maximum allowed values for the running and holding currents for each motor from the specification sheet. The units are Amps.

Travel

This section lists the travel for each motor, in mm. Rotary stages have no limit on travel (they are allowed to move past the home sensor), so this value is left blank. This section also tells the software which units to use—a stage with no travel defined is a rotary stage and therefore will use degrees instead of mm.

Stage/Detector Port

Settings for the communication port to the Zaber stages are listed under `Stage Port`. The serial number of the USB-to-serial converter allows the software to find the communication port automatically, or it must be specified by the `serialport` variable. The timeout is user-definable and the units are seconds. `baudrate` is the rate used when opening the port, and it must match the baud rate that the stages are set to accept (this should not be modified under normal circumstances).

The options for `Detector Port` are similar, except there is no USB serial number because the detector communication is serial only.

Detector Calibration

This part of the configuration file consists of multiple sections, one for each detector that is used in the beamline. The comments give the units of each calibration variable and the instructions that the software uses to convert from channel to energy using the calibration variables. Whenever a detector is calibrated, the section corresponding to that detector's serial number must be updated to reflect the new values of `calib_factor` and `offset`. A new section should be created for any new detector that is used in the system, and it must have the heading `[***** Calib]`, where `*****` is the serial number of the detector. Comment lines should always be given for each detector to indicate when it was last calibrated. For more information on calibrating the detectors, see Sec. 4.2.

Chapter 2

Stages

2.1 Overview

The stages used in this beamline are from Zaber Technologies, Inc., and have built-in drivers, controllers, and encoders. They can be controlled via software or by turning the knobs located on the side of the motor housing. In general they need very little setup before use, and many of the relevant information has already been covered in Chapter 1. The following sections will cover the procedure for setting up a new stage in the beamline.

2.2 Setting up a new stage

2.2.1 Setting to correct protocol

The first step to using a brand new Zaber stage is to ensure that the communication protocol and baud rate are set properly to communicate with the `blcontrol` software and with each other. There are two communication protocols for the Zaber stages, Binary and ASCII. The software communicates using the binary protocol because some of the stages aren't capable of using the ASCII protocol, and we use a baud rate of 9600 which is the default for the binary protocol.

The easiest way to change the communication protocol is by using the Zaber Console software, which runs on Windows only. It can be installed from the Zaber website at `https://www.zaber.com/wiki/Software/Zaber_Console`. Once it is installed, connect the stage to the PC. You may have to use a serial connector instead of USB if the Windows PC doesn't have the correct drivers for a USB-to-RS232 converter. Open the software, open the serial port, and press the "Find Devices" button. Choose the option to convert all devices to Binary protocol at 9600 baud. Once this process is complete, you can disconnect the stage from the Windows PC and install it in the beamline.

2.2.2 Editing configuration file

The structure of the configuration files is discussed in detail in Sec. 1.4. For a new stage, it is necessary to define a few parameters in the configuration file before it can be used with the software. Give the motor a short name under "Motor Names," and then this name will be used to set the configuration values in the following sections. Following the instructions from Sec. 1.4, create entries for "Motor Res," "Max Current," and "Travel," following the specification sheet for the new device. Save the configuration file, and you are ready to start up the software and use the new stage. Note that the new stage, and any stages that were unplugged from power during the installation of the new stage, will likely have to be homed before use. See Sec. 1.2 for details on homing the stages.

2.2.3 Editing stage firmware settings

A list of all the settings that can be edited in the stage firmware can be found in the Zaber Binary Protocol Manual[9]. Most of the settings will not need to be changed, but you may want to edit the running and/or holding currents if the motors seem to be getting hot. These can be changed in the Zaber Console software on Windows.

Chapter 3

X-ray Source

3.1 Overview

The sources used in the beamline are microfocus X-ray tubes from the Jupiter 5000 series by Oxford Instruments. Currently three source target materials are available: W, Cu and Cr. Because the Bremsstrahlung (continuous spectrum) is used for measuring the spectral response of the optics, the choice of source will depend on which target material does not have spectral lines in the energy range of interest. The sources are powered by a Spellman XLG high voltage power supply [8] which has been internally modified to provide the correct filament current to the Jupiter 5000 tubes.

The geometry of the X-ray tube sources is shown on the data sheet [6]. It is important to note that the X-rays are generated at a point 1.22 inches behind the front flange surface of the tube, so any measurements relative to the source need to take this into account.

The following sections discuss the operation of the Jupiter 5000 X-ray tube sources. Section 3.2 covers the procedure for starting up the source under normal conditions. If the source is new, or hasn't been used in more than three months, then it must be started up using the conditioning procedure outlined in Section 3.3. Finally, Section 3.4 discusses how to safely shut down the X-ray source.

3.2 Normal startup procedure

1. Mount the x-ray tube to the aluminum stand with the copper collimator. Affix the thermocouple wire to the outside of the x-ray tube, near the center, with tape. Start up cooling fans by plugging the 12V power supply into the power strip.

2. Ensure that the on/off switch on the x-ray power supply is in the off position. Connect the blue filament cable to the BNC input on the x-ray tube. Insert the high voltage cable into the x-ray tube and screw down the connector. Connect the ground wire to the screw next to the high-voltage input and screw down snugly.

3. Double check that all shielding is in place, including copper pipes, brass optic housing, and leaded glass at the detector end of the beam. Use brass foil to cover any gaps in the shielding. Also make sure everyone in the room is wearing proper dosimetry.

4. Turn on the power supply by moving the switch to the on position. The front panel should read **0.0 mA, 0.0 kV**, and the HV OFF button should light up.

5. Press and hold the HV OFF button to display the preset current and voltage. When the HV is enabled, it will power up to this preset value. The value can be adjusted by turning the mA and kV knobs while holding down the HV OFF button. Set the preset current to 0.0 mA and the preset voltage to 10.0 kV. This is the minimum voltage rating for the Jupiter 5000 x-ray tubes. Note that no actual output is being produced at this stage.

6. Press the HV ON button to power up the supply to the preset voltage. The HV ON button should illuminate and the front panel should read 0.0 mA, 10.0 kV. Using the Geiger counter, check the beamline area for radiation leakage, especially in places where two pieces of shielding come together (such as the holes in the brass optic housing). If any radiation leakage is detected, or any warning lights illuminate on the front panel of the power supply, turn off the output by pressing HV OFF. Record the time and tube temperature reading in the logbook.

7. Increase the output voltage to **20.0 kV**. Sweep the beamline area again using the Geiger counter. Record the time and tube temperature.

8. Increase the output current to **0.025 mA**. Sweep the beamline area again using the Geiger counter. Record the time and tube temperature. Wait 30 seconds after increasing the current before proceeding to the next step.

9. Increase to the desired voltage in increments of 10 kV, checking for radiation leakage, recording the time and temperature, and waiting 30 seconds between each increase. Do NOT exceed 50 kV. Lower the voltage and/or the current if the temperature nears 45C. Do NOT allow the temperature to exceed 49.5C.

10. Once the desired voltage is reached, test the flux by taking a 30 second test spectrum with the detector. If more flux is needed, the current may be increased in increments of 0.025 mA. Check for radiation leakage, record the time and tube temperature, and wait 30 seconds between each increase. If the detector dead time reaches 5% or higher or the temperature rises too much, decrease the current. Do NOT exceed 1 mA. You should generally not need to exceed 0.1 mA to obtain sufficient flux.

11. The x-ray source is now powered up and ready for the alignment process to begin. While the source is powered on, do not reach onto or over the benchtop. Every 15 minutes or so, record the temperature of the tube, make sure the current and voltage is stable, check for error messages on the front panel of the power supply, and sweep the beamline area for radiation leakage.

3.3 Tube conditioning procedure

This procedure must be used when starting up a new tube or a tube that has been in storage for longer than three months. During a period of storage, residual gasses can accumulate in the x-ray tube vacuum, and applying a high voltage without first conditioning the tube can cause arcing, which can lead to permanent damage to the tube [7].

1. Follow steps from Section 3.2 up to step 6 to start up the tube at **0.0 mA, 10.0 kV** and check for radiation leakage.

2. If any instability is noted on the mA meter, allow it to stabilize to display 0 mA. Operate at this condition for at least 15 minutes.

3. Increase the beam current to **0.2 mA** and sweep the beamline area for radiation leakage with the Geiger counter. Note the tube temperature and any instability in the mA meter. Maintain this setting for 5 minutes or longer, until no instability is noted on the mA meter.

4. Increase high voltage in 5 kV steps at 5 minute intervals until **25 kV** is reached. After each increase, note the tube temperature and check for radiation leakage. Hold 5 minutes at these conditions.

   Note: if any instability (especially loud popping) is observed, lower the kV setting to the previous step. Allow mA to stabilize at least 5 minutes before increasing settings again.

5. Increase beam current to maximum current rating, **1.0 mA**. Note the temperature, current stability and radiation leakage. Hold for 5 minutes.

6. Continue to increase high voltage as in step 4, in 5 kV steps every 5 minutes until the maximum rated voltage, **50 kV**, is reached. Note the tube temperature and check for radiation leakage and instability after each increase. Do not allow the tube temperature to exceed 49.5C. Allow at least 5 minutes at full power to insure that the tube is operating correctly.

7. Slowly reduce the current to 0.025 mA, then slowly reduce the voltage to the desired operating voltage. Note the tube temperature and check for radiation leakage. Proceed with step 10 onward from Section 3.2.

3.4 Shutdown procedure

1. Slowly dial current down to **0.0 mA**. Wait 10 seconds.

2. Slowly dial voltage down to **10.0 kV**. Wait 10 seconds.

3. Press the HV OFF button. Wait until the current and voltage readings are stable at **0.0 mA, 0.0 kV**.
4. Once current and voltage are stable at zero, turn the power switch on the power supply to the off position.
5. Allow tube temperature to cool to room temperature, then unplug 12V power supply to disable cooling fans.

Chapter 4

Detectors

4.1 Overview

The beamline software is compatible with Amptek detector assemblies which use the DP5 Pulse Processor and MCA board[2], including the XR-100[5] and the X-123[4, 3] models, both of which come in silicon drift (SDD) or cadmium telluride (CdTe) detector varieties. The XR-100 and X-123 models are very similar, except the digital pulse processor and power supply in the XR-100 are separate from the detector and preamplifier, while in the X-123, everything is integrated into a single package.

The SDD and CdTe detector are useful for different situations and energy ranges of interest. The SDD has overall better resolution and lower noise, and is more efficient than the CdTe detector at low energies. The CdTe detector has a lower resolution and is more prone to noise at lower energies, but it is much more efficient at high energies. As a rule of thumb, the SDD should be used for measuring energies below about 25 keV, and the CdTe for energies higher than 25 keV.

Any of the detector models from Amptek listed above can be mounted onto the detector stage assembly, powered up as specified in the manual, and connected to the computer via RS-232. The `blcontrol` software should automatically connect to the detector when next powered up; if not, try modifying the `serialport` configuration variable in `config/blconf.txt`.

The detectors are rather fragile and it is important to handle them with care. In particular, they are very sensitive to any sort of mechanical shock, so it is important to not drop them during mounting, or allow them to run into any other elements of the beamline during alignment. The beryllium window on the end of the detector housing is also easily damaged. It is recommended to keep the red protective cap or a tungsten cap with no pinhole on the end of the detector when it is not in use. The detector diode is held under vacuum behind the Be window and cooled by a thermoelectric cooler (TEC). The detector has best performance (best resolution and least noise) when kept at a temperature below 225K. If the set point is below 225K but the TEC is unable to cool the detector to this temperature, this could indicate damage to the TEC or loss of vacuum, and the detector will likely need to be serviced by the manufacturer.

4.2 Calibration

Each detector needs to be calibrated every few weeks or after a long period of disuse. To calibrate the detector, we measure sealed sources with known spectral lines and correlate the MCA channels of these lines with their energies.

4.2.1 Collecting calibration spectra

Any source with spectral lines in the energy range of interest can be used for calibration. At the time of this writing, we are calibrating all detectors with three sealed sources: ^{55}Fe, which has spectral lines at 5.9 and 6.5 keV; ^{57}Co, with a line at 14.4 keV; and ^{137}Cs, which has a line at 32.2 keV.

For calibration, a long spectrum (at least 10 minutes) will be acquired with every source following the steps below.

1. Start up the software and adjust the detector gain so that all peaks from the sources you are using will be within the detector's energy range.

2. Using tape, affix one of the sources to the mylar on the end of the Cu pipe near the detector. Using the knobs on the stages, move the detector so that the Be window is close to the source.

3. In the software, acquire a short spectrum (30 seconds to 1 minute) to ensure that the source peaks are visible and the detector dead time is not too high (should be ¡5%). You should use a large number of

channels to get the best possible resolution—8192 is best. If necessary, move the detector and take another short spectrum.

4. Acquire a long spectrum with the same number of channels for at least 10 minutes, and then save it.

5. If the peaks in this 10 minute spectrum are still not very well resolved, take another spectrum for 10 minutes or more. All spectra from a given sample can be added together for better statistics during the analysis.

6. After saving the spectrum from the previous source, remove the source and repeat steps 2-5 with a new source. Make sure to use the same gain and the same number of channels for each source. The acquisition time can vary from source to source. Repeat with all sealed sources.

7. When finished with the sealed sources, put them away in the lead source holder and place the holder in a locked cabinet.

4.2.2 Calibration data analysis

The script `blcontrol/scripts/calib.py` assists with the detector calibration by fitting the peaks in each source spectrum, and then fitting each of these peaks to a line which defines the detector calibration parameters. The energy as a funciton of channel number, $E(C)$, is found by fitting the source peak channels to a function of the form

$$E(C) = \frac{C}{\alpha \times G \times N} + E_0 \tag{4.1}$$

where G is the hardware gain and N is the total number of channels. α and E_0, called the calibration factor and the offset, respectively, are fitting parameters. Figures 4.1 and 4.2 show examples of the plots output by the calibration script. The script will also print the calculated values of the calibration factor and offset. You should inspect the outputs to ensure that the values printed are sensible. Then,to enable the calibration, paste these values into the appropriate location in `blconf.txt` for the detector that you are calibrating.

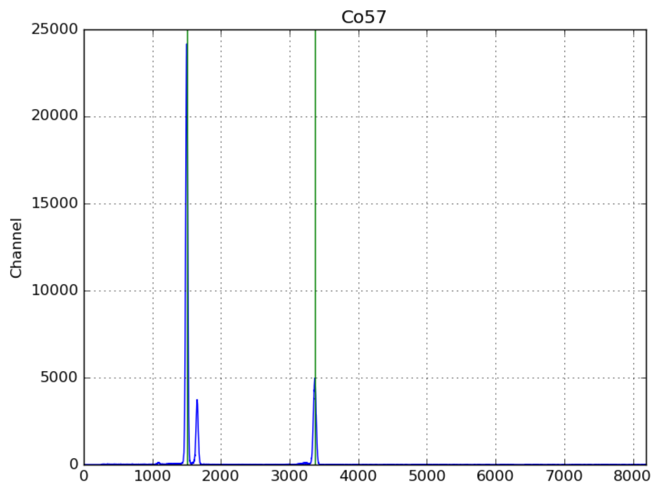

Figure 4.1: An example of a calibration spectrum from ^{57}Co, with the peaks highlighted.

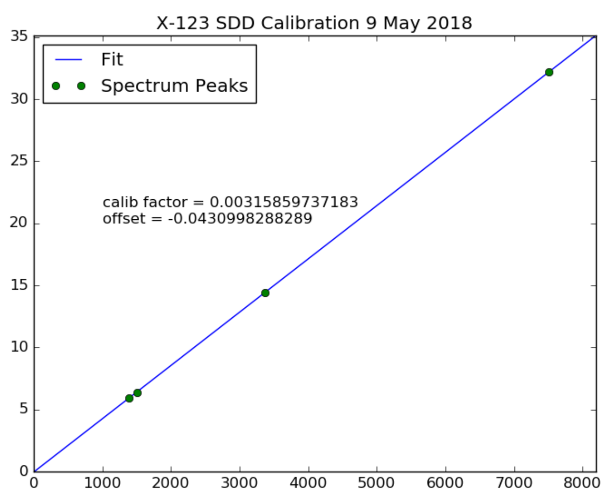

Figure 4.2: This plot shows a linear fit to the peak channel as a function of energy for multiple calibration sources, calculated by the script `calib.py`.

Chapter 5

Alignment and Data Aquisition

This chapter covers the steps for aligning a point-to-point focusing optic in the beamline, and then collecting the data which will later be analyzed to determine the optic's resolution and reflectivity with respect to energy. This procedure is valid for bare nickel/nickel-cobalt optics as well as multilayer-coated optics. A basic familiarity with the BLControl software is assumed here, so please read Chapter 1 first if you have not done so already.

During the alignment process, there are a few things that you will need to regularly check (every 15 minutes or so) and make note of in the log book:

- X-ray tube temperature: make sure it does not rise above 45°C
- Detector temperature: should be below 230K for taking data
- Radiation leakage: sweep the beamline periodically with the Geiger counter to check
- Helium (if using) pressure and flow rate—see Section 5.2 for details

In addition, while the x-ray source is on, you should always be wearing chest and ring dosimetry.

5.1 Setup and visual alignment

Before starting the alignment, mount the detector and plug it in if necessary. Make sure the detector and the motor controllers are connected to the computer. Then, start up the software as described in Section 1. During the initial alignment, leave the red cap or blank tungsten pinhole on the end of the detector to protect the beryllium window from damage.

Take note of the detector temperature and set point, displayed in the "Detector Control" panel. If the detector has just been plugged in, it may need 10-15 minutes before it cools to below 220K, at which point it can be used.

The first step in the alignment process is to roughly align the optic and detector by eye using visible light.

1. Start up the software. Make sure all motors appear in the "Motor Control" panel, and that the detector is cooling.

2. Remove all brass and copper pieces of shielding from the beamline and set them aside. Be careful not to bump any of the copper pipes into the detector.

3. Place the optic into the housing, and put the housing onto the v-block in the optic mount. If measuring in a magnifying configuration (i.e. the optic is closer to the source than to the detector), then the small end of the optic should point toward the sorce.

4. Using the optic z stage ("oz"), move the optic so that the inflection point is at the correct source-to-optic distance, as indicated in the optic design. Note that this distance is to the x-ray source spot, which is actually 1.22 inches behind the front flange of the x-ray tube[6]. Set this oz location to zero in the software.

5. Move the detector z stage to the center of its travel. By moving the stage assembly on the table, put the front window of the detector at the correct focal length as specified in the optic design, again keeping in mind that the x-ray source should be measured 1.22 inches behind the x-ray tube flange.

6. If the x-ray tube is currently mounted on the aluminum bracket, remove it and carefully set it aside. Attach the fiber optic holder to the aluminum bracket, with the copper collimator on the front. Insert the fiber optic output into the holder and turn on the white light source.

7. Replace the brass housing around the optic. If necessary, move the source or optic mounts so that the holes in the brass housing are centered with respect to the white light. Then, using the optic x and

Figure 5.1: Setup and visible light alignment

y stages ("ox" and "oy"), adjust the optic position so that it is centered with respect to the holes in the housing. Set these "ox" and "oy" positions to zero in the software.

8. Holding a sheet of paper between the optic and the detector, locate the single-bounce focal spot. Adjust the pitch and yaw stages until the single-bounce focus appears symmetric. See Fig. 5.1 for reference images. Once pitch and yaw are aligned, set their positions to zero in the software.

9. Holding a sheet of paper in front of the detector, locate the double-bounce focal spot. Adjust the position of the detector in the x and y directions ("dx" and "dy") until the focal spot coincides with the front window of the detector. Try to keep the dx stage close to the center of its travel– you may need to move the detector stage mount around on the table to achieve this.

10. Replace the copper pipes, starting with the pipe closest to the source. After placing each pipe, use a piece of paper at the end of the pipe to locate the beam of visible light, and adjust the position of the pipe so that the beam is centered. The pipes may not end up exactly parallel to the tabletop.

11. Remove the white light source and mount the x-ray tube. Take care not to move the source mount in the process, as doing so could alter the alignment. Use brass foil to cover any remaining gaps in the shielding. Remove the protective cap from the detector window.

5.2 Helium

In this section, we will start the flow of helium through the copper shielding pipes to reduce the attenuation of the x-rays (since helium has a much longer attenuation length than air). This is only necessary if you want to measure low energies (below about 5 keV), so for most multilayer-coated optics you can skip to Section 5.3.

Note that if you are using helium, your count rate will probably be considerably higher than what you are used to in air for a given tube current. You will probably need to reduce the current accordingly so that the detector dead time remains below 5%.

1. Seal any connection points in the copper pipes to create a mostly air-tight seal. Carefully wrapped duct tape many overlapping layers with few wrinkles) works fine for this.

2. Connect any tubing that runs from one pipe to another, so that helium can flow from one end of the beamline to the other.

3. Connect the helium tank to the tubing on one end of the beamline. You may want to use a needle valve between the tank and the copper pipe to give you greater control over the helium flow rate.

4. At the other end of the beamline, you should have one open section of tubing. Fill a beaker or other container with water and insert the open end into the water. When helium is flowing, it will bubble through the water and allow you to visualize the flow rate.

5. Open the helium tank. Using the tank regulator and the needle valve if present, adjust the output pressure until you see about one bubble every few seconds on the other end of the beamline. This should correspond to < 5 psi of output pressure. If the pressure is too high, then stop the helium flow and check for leaks, especially at the points where two copper pipes come together (add more duct tape if using).

6. Once you have a decent flow rate at a sufficiently low pressure, you can move on to Section 5.3. While using helium, you need to keep an eye on the flow rate, output pressure, and amount of helium remaning in the tank. Check and record these values every 15 minutes or so while the helium is flowing, and adjust the output pressure if the flow rate becomes too high or if bubbles stop appearing.

5.3 Initial X-ray alignment

In this section, we align the optic in pitch and yaw, and the detector in the x and y directions (i.e. perpendicular to the optical axis).

1. Start up the x-ray source, as detailed in Section. 3.2. The source voltage should be set so that the max energy is at least 5 keV above the energy range of interest (e.g. the location of the multilayer peak). All shielding should be in place at this time. Make sure to check periodically for radiation leaks and note the X-ray tube temperature.

2. Without setting an ROI, perform a 3×3 grid scan to find the center of the beam, and move dx and dy to this location.

3. If the optic has a multilayer, take a 30 second spectrum to find the multilayer peak. Set the ROI to encompass this peak. It should be wide enough to still encompass the entire peak, even if it shifts 1 or 2 keV in either direction during alignment, but should not encompass any "stray peaks" at lower energy.

   Note: If the optic does not have a multilayer, then no ROI needs to be set. From now on during the alignment process, if an ROI is set, then the ROI peak or center of mass from a linear or grid scan should be used, as opposed to the peak or center of mass of the total counts.

4. Perform a linear scan of *pit*, $\pm 0.3°$ (18 arcminutes) in steps of $0.03°$. 3-5 seconds of counting time per point should be sufficient. Move *pit* to the center of the peak, and set it to zero.

5. Repeat step 4 for *yaw*.

6. Scan *ox* ± 1 mm in steps of 0.2 mm. Move *ox* to the center of the peak and set it to zero.

7. Repeat step 6 for *oy*.

8. Repeat steps 4 and 5 for $\pm 0.2°$ in steps of $0.02°$, then repeat steps 6 and 7.

9. Repeat steps 4 and 5 for $\pm 0.1°$ in steps of $0.01°$, then repeat steps 6 and 7.

10. Using a brass sheet to block the beam and shield your hand, place the 3 mm diameter pinhole on the end of the detector. Perform a 3×3 grid scan, with the step size the same as the pinhole diameter, and move to the center of mass.

11. Scan and re-zero *pit* and *yaw* again $\pm 0.1°$ in steps of $0.01°$, then scan and re-zero *ox* and *oy* ± 1 mm in steps of 0.2 mm (as in step 9).

12. Repeat steps 10 and 11 with 2 mm and 1 mm diameter pinholes. Increase count time if necessary for better statistics. You may also reduce the size of the linear scans and use smaller steps to help refine the peak location, as long as the peak fits entirely within the bounds of the scan.

    Note: If the grid scan is still very symmetric with a 1 mm pinhole, you can continue to step down to a 0.5 mm or even 0.25 mm pinhole. The smallest pinhole that will be used depends on the resolution of the optic being measured, but generally you should go as small as possible while the 3×3 grid scans are still symmetric and have a well-defined beam center.

13. With the smallest pinhole in place, continue to repeat the alignments of *ox*, *oy*, *pit* and *yaw* (linear scans) and *dx* and *dy* (grid scan). Repeat this cycle until the positions are no longer changing by more than $0.001°$ or 0.01 mm.

This alignment may change slightly if the source is turned off, as the focal spot within the tube can be in a different position each time it is powered on. If the source is power cycled at any point, just repeat step 13 to verify the alignment.

5.4 Focus finding and HPD measurement

Now that the optic is aligned with respect to the x-ray beam, and the detector is aligned in the xy plane, we will locate the focal point in the z direction and calculate the resolution of the optic.

This section can be time-consuming, and you may want to skip it if you only care about the optic's spectral response and don't need to know the resolution (or already have good enough resolution data from a previous measurement). You are likely to be close enough to the focal distance that the spectrum data will be the same whether you find the exact focus or not. However, if you skip this step, you will have to repeat the entire alignment process to get resolution data in the future, so it's best to do it now if you think you might want it.

During this procedure, you are moving the detector back and forth along the beam direction. Therefore, you must be careful to ensure that the detector does not run into the copper shielding pipes. If you need to reposition the pipes to make room for the detector to move, turn off the x-ray source first, and make sure you don't hit the optic with the pipes while moving them.

1. Your current dz position should be at the nominal focal length of the optic (measured manually during visual alignment) and should be set to $dz = 0$. If not, set it to zero now.

2. With the smallest pinhole in place, re-center the detector using a grid scan. Then take a spectrum of about 30 seconds (you can alter this depending on your count rate) at the current position. Note in the log book how many counts are in your ROI.

3. Change the pinhole to the next size up and repeat the spectrum for the same amount of time. Again note the ROI counts in the log book. Repeat this step with progressively larger pinholes, up to 5 mm diameter.

4. Following the instructions in Section 6.1.1, calculate the HPD at the current position.

5. Move to $dz = 20$ mm. Repeat steps 2-4. If the HPD improves (i.e. decreases), continue another 20 mm in this direction. If it worsens, try the opposite direction. Continue moving in steps of 20 mm until a minimum in the HPD is found. Return dz to the position where the HPD is minimized.

   Note: If you run out of travel on the dz stage, you can return dz to the center of travel and move the entire stage assembly forward or backward on the tabletop. Your position reference will be lost, so you will need to re-center the detector in x and y and re-find the minimum HPD in z.

6. Move dz 10 mm in the direction of the next lowest HPD, and repeat steps 2-4. If the HPD is lower, stay at this dz position, otherwise return to the position of the minimum.

7. Repeat step 6 for a move of 5 mm, and then for a move of 2.5 mm.

8. Using the lowest measured value of the HPD, calculate the optic's spatial resolution as outlined in Section 6.1.

5.5 Spectrum data collection

1. If you performed the focus finding alingment in Section 5.4, then move dz to the location of the best measured HPD. Remove any pinhole from the detector and re-center by performing a 3×3 grid scan in 5 mm steps.

2. Collect a long spectrum (typically 10 minutes or more, depending on count rate) with no pinhole on the detector. When the acquisition is complete, make sure to save the spectrum file.

3. Turn off the x-ray source and remove the optic from the beamline. Place a 3 mm pinhole on the detector. Re-start the source to the same current and voltage as before.

4. Collect a long spectrum without the optic for the same amount of time as in step 2. If, after one minute or so, the dead time of the detector is over 5%, stop the acquisition, change the pinhole to a smaller diameter to reduce the count rate, and restart. Once the long spectrum is complete, make sure to save the spectrum file in the same directory as the file from step 2. Make sure to record which file is which (optic vs. no optic) and what size pinhole you used for the no optic spectrum.

Chapter 6

Data Analysis

6.1 Optic Resolution

6.1.1 Half-Power Diameter

The optic's half-power diameter (HPD) is found by fitting the count data to the following function, which is the integral of a gaussian:

$$f(d) = A(1 - \exp\left(-\frac{(d - d_0)^2}{4b}\right) + f_0 \tag{6.1}$$

where d is the diameter of the pinhole, $f(d)$ is the count rate at that diameter, and A, d_0, b, and f_0 are fitting parameters. The HPD is then given by the value of d where $f(d)$ is equal to half of its maximum value:

$$d_{1/2} = d_0 + 2\sqrt{b \log\left(\frac{2A}{f_0 + A}\right)} \tag{6.2}$$

A script to perform this fit and produce an accompanying plot is found at `blcontrol/scripts/HPD.py`. The `find_HPD` function defined in the script takes two lists as input, a list of the pinhole diameters, and a list of the corresponding number of counts recorded in the ROI using that pinhole. It will fit a function like and produce a plot that shows the fitted function and the calculated HPD. You can use this function by importing it and running it from the Python interpreter in a terminal.

6.1.2 Resolution

To calculate the spatial resolution from the HPD, we must account for the magnificaiton factor of the optic and the finite size of the source. We assume that the source spot size and the optic spatial resolution add in quadrature to contribute to the measure HPD. Therefore, if the source size is d_{src} and the magnification factor is M, then the optic's spatial resolution r can be approximated by

$$r = \sqrt{\left(\frac{d_{1/2}}{M}\right)^2 - d_{\text{src}}^2} \tag{6.3}$$

where $d_{1/2}$ is the measured HPD from Sec. 6.1.1.

Given the spatial resolution, the angular resolution θ of the optic is easily estimated using the source-to-optic distance, u:

$$\theta = 2 \arctan\left(\frac{r}{2u}\right) \tag{6.4}$$

6.2 Reflectivity

6.2.1 Calculation

On the most basic level, the reflectivity of the optic at a given energy is simply the ratio of the number of photons reflected from the optic to the number of photons incident on the optic. This is called the *double-bounce reflectivity* because the photons are reflected once from each of the two ends of the optic. The *single-bounce reflectivity* is the reflectivity after a single reflection from the optic, and corresponds to the reflectivity of the multilayer coating. If we assume that the multilayer is exactly the same on both ends of the optic, and thus they have the same single-bounce reflectivity, then we have that $R_{\text{double-bounce}} = R^2_{\text{single-bounce}}$. Of course, the multilayer will not be exactly the same on each end of the optic, but it's a useful approximation so that we can compare the optic to multilayers on flats and other samples.

When we take the long optic spectrum after aligning the optic, we are directly measuring the number of photons reflected from the optic. The input to the optic is related to, but not the same as, the spectrum we take from the source after removing the optic. It is not the same because the collecting area of the optic is different from the collecting area of the detector, and because the detector is farther from the source than the optic is, and the flux drops off as $1/r^2$. Taking these into account, the input spectrum $I_{\text{input}}(E)$ is related to the source spectrum taken in Sec. 5.5, $I_{\text{src}}(E)$, by

$$I_{\text{input}}(E) = \left(\frac{A_{\text{optic}}}{A_{\text{detector}}}\right)\left(\frac{u+v}{u}\right)^2 I_{\text{src}}(E), \tag{6.5}$$

where A_{optic} and A_{detector} are the respective collecting areas of the optic and detector, u is the distance from source to optic, and v is the distance from optic to detector. Then taking the ratio of I_{optic}, the optic output spectrum, to I_{input}, yields the double-bounce reflectivity, and taking the square root of this yields the single-bounce reflectivity.

A Python script to perform this computation, `reflectivity.py`, is provided in `blcontrol/scripts`. The most convenient way to run the script is by copying it to the directory where the optic and source spectrum data files are located. The variables at the beginning of the script will need to be edited for the parameters used, and then it can be run from the terminal using `./reflectivity.py`. The script produces a text file and a plot of the calculated reflectivity in each of the MCA channels.

6.2.2 Modeling

To model the reflectivity of the optic, we consider the path of a ray emanating from the source, reflecting from each end of the optic, and impinging on the detector. It is characterized by energy E and the angle ϕ that it makes with respect to the axis of the optic. We assume that the intensity of the source is constant in ϕ so that $I(\phi, E) = I_0(E)$ where $I_0(E)$ is simply the spectrum of the source. The ray reflects from one end of the optic (we'll assume it's the h-end, but it's the same in either orientation) at a graze angle θ_h which is a function of ϕ: $\theta_h = \theta_h(\phi)$. The multilayer on this end has a reflectivity as a function of energy and graze angle $R'_h(\theta_h, E) = R_h(\phi, E)$ that is determined by the properties of the multilayer, including the d-spacing, Γ, and microroughness. After reflecting from the h end, the intensity $I'(\phi, E) = R_h(\phi, E)I_0(E)$. The ray then impinges on the e-end of the optic which has a reflectivity function $R_e(\phi, E)$, and the intensity $I''(\phi, E) = R_h(\phi, E)R_e(\phi, E)I_0(E)$. The ray then continues to the detector. Thus if we divide through by the source spectrum, the two-bounce reflectivity of the optic as a whole is

$$R_{\text{opt}}(\phi, E) = R_h(\phi, E)R_e(\phi, E). \tag{6.6}$$

Of course, the detector is not sensitive to the angle of incidence of the incoming rays, only the energy. So we integrate over all values of ϕ which produce a valid ray that will reflect from the optic. These limits of integration ϕ_1 and ϕ_2 can be determined from the design geometry of the optic. The area element dA in this case is the area of the ring on the h-end of the optic where the rays with angles between ϕ and $\phi + d\phi$ will reflect. Then divide by the total area of the h end. All together, this looks like:

$$R_{\text{opt}}(E) = \frac{\int_{\phi_2}^{\phi_1} R_h(\phi, E) R_e(\phi, E) dA}{\int_{\phi_2}^{\phi_1} dA}. \tag{6.7}$$

In practice, actually calculating dA and doing the integral is not worth the hassle. We can get a pretty good approximation simply by averaging over ϕ. We would also like to use the actual graze angles θ_h and θ_e as variables, as this is what we will need to input into IMD. We will integrate from the edge to the intersection, keeping in mind that a ray that reflects near the edge on one end will reflect near the edge on the other end, and similarly for a ray near the intersection. Thus,

$$R_{\text{opt}}(E) = \frac{1}{\int_{\phi_{\text{int}}}^{\phi_{\text{edge}}} d\phi} \int_{\phi_{\text{int}}}^{\phi_{\text{edge}}} R_h(\theta_h, E) R_e(\theta_e, E) d\phi. \tag{6.8}$$

Equation 6.8 is used as the basis for the numerical model that is computed using IMD and Python. IMD is used to calculate R_h and R_e, and a Python script performs the integration.

To calculate the reflectivity in IMD, first define the multilayer stack for the h-end of the optic, with an appropriate d-spacing, Γ, and microroughness. Also include the Pt and NiCo substrate if necessary. Then, under Independent Variables in the IMD window, define the range of energies and graze angles. The graze angles for the h-end are defined in the mandrel design parameters, and we proceed from the edge to the intersection. The number of energy values you use should be comparable to the number of MCA channels used to collect the data, and 20 graze angle values is usually sufficient. Calculate the reflectivity in the menu Calculate → Specular Optical Functions and Fields, and then save the `.imd` file. Close the plot and export to a `.sav` file from the menu using File → Export Results to IDL Save File.... Repeat this process for the e-end of the optic, using the same energy values and the same number of graze angles, but using the values defined for the

e-end in the mandrel design. When finished, you should have a `.imd` and a `.sav` each for the h end and the e end of the optic which represent their respective reflectivity functions.

The Python script to perform the integration is found at `blcontrol/scripts/model.py`. It parses the `.sav` files, performs the multiplication of the reflectivity functions, and averages over the graze angles. The script also uses a Gaussian smoothing filter to simulate the finite energy resolution of the detector. It then plots the square root of R_{opt}, which is the single-bounce reflectivity, along with the measured single-bounce reflectivity for comparison. You can use this plot to go back and tweak various model parameters such as the d-spacing, microroughness, and density of each end of the optic, and the energy resolution of the detector, to see how they affect the model.

Chapter 7

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