Users Guide for HXMA Diffractometer Operation

Version 0.5

This document provides brief users guide for psi-8 diffractometer in HXMA.

Contents

1   Introduction of HXMA psi-8 diffractometer

HXMA psi-8 diffractometer has versatile configurations to accommodate various diffraction experiments. Available X-ray energy range is 5 keV – 40 keV.

1.1   Available equipments

Cyberstar scintillation detector

CCD X-ray detector

Vortex XRF detectors (four-element)

Closed loop cryostat (10 K – 450 K)

Analyzer crystals - HOPG(002), Si(111), Ge(111)
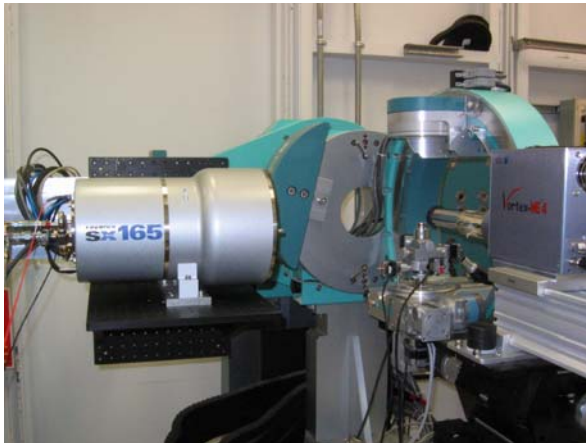
Figure 1.1

Diffractometer setup with CCD and Vortex detector

Figure 1.2

Psi-8 diffractometer detector arm with analyser setup.

1.2   Sample environments

1.2.1 Inert gas enclosure

To hold sample under inert gas (He or Ar) environment during X-ray scattering sample holder shown in figure can be used. Exposing sample to air during X-ray scattering measurement can build thin carbon layers on the sample surface. To prevent carbon buildup sample needs be placed under inert gas environment. There are two types of sample holder with sample surface either parallel or perpendicular to the phi stage. The sample holders have hole(s) for suction-holding of wafer samples. Also there are gas inlet and outlet.
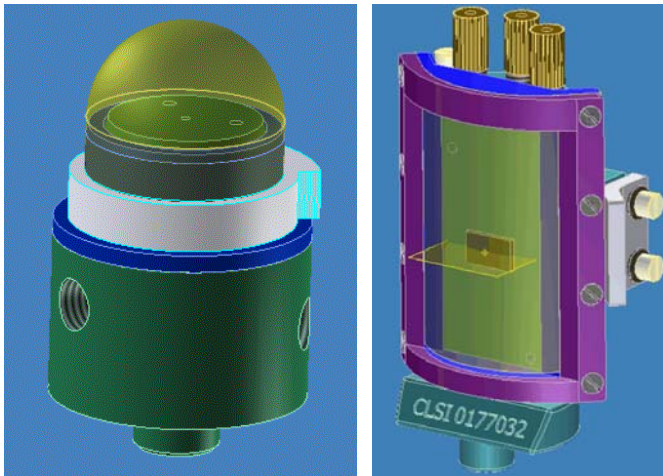
Figure 1.3
Horizontal (left) and vertical (right) inert gas environment sample holders.

1.2.2 Beryllium mini-dome from ambient pressure to UHV

A sample sensitive to the air or moisture can be handled with UHV Beryllium dome. The vacuum pressure in Be-dome can reach high-vacuum (1e-6 Torr) with TMP. Bakeout of Be-dome is required to achieve UHV.
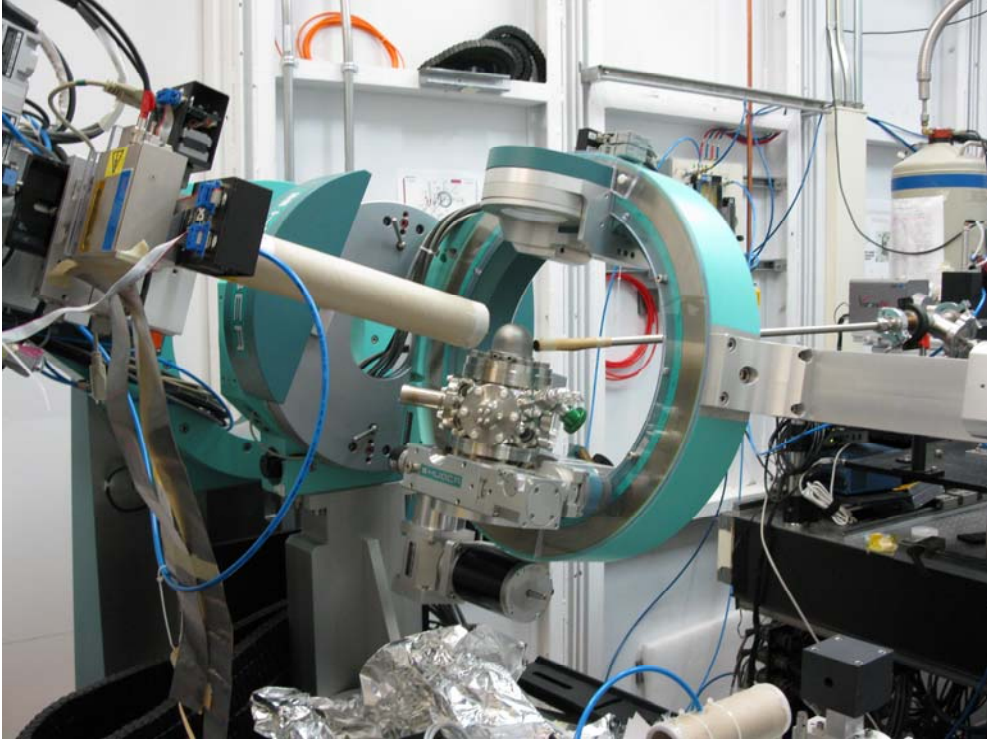
Figure 1.4 Mini beryllium dome mounted on the psi-8 diffractometer

1.2.3 Low temperature with closed loop cryostat

Low temperature (10 – 450 K) sample environment can be achieved with closed loop cryostat.
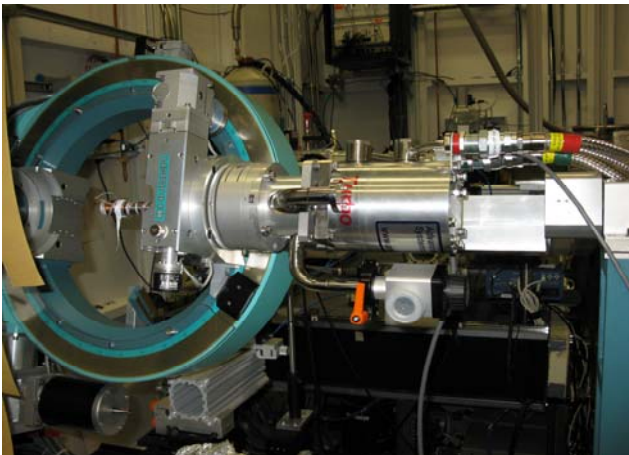
Figure 1.5

Cryostat installed on psi-8 diffractomter.
Beryllium radiation shield and shroud are removed.

1.2.4 High temperature

The mini Be-dome in combination with PBN heater sample can be heated upto 600 ℃ under ambient pressure and 800 °C in UHV.

1.2.5 Flow-cell/furnace type *in situ* reaction cell for powder diffraction

In-situ reaction cell has been provided to X-ray diffraction user community. The flow-cell/furnace design allows control of the sample temperature with possibility of reaching temperature of up to ~900 °C and also control of the atmosphere over the sample from rough vacuum to atmospheric flow to an overpressure.
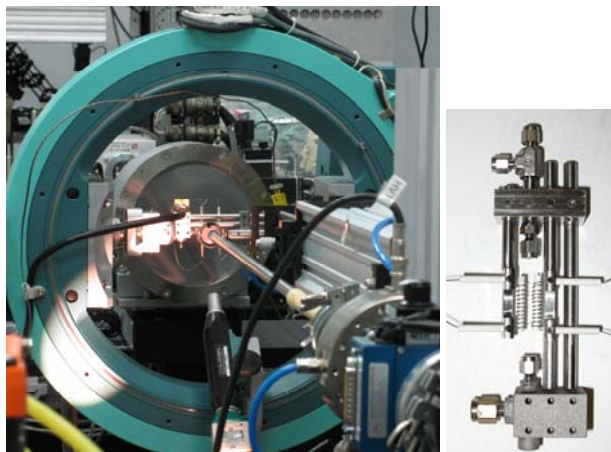
Figure 2. *In-situ* reaction cell mounted on psi-8 diffractometer with CCD detector.

1.3 Control

SPEC$^@$ has been used for diffractometer control, reciprocal scan, and data acquisition. Basic SPEC commands are described in separate document of "SPEC short manual for HXMA".

1.3.1 Step Motor control

Step-motor control is based on EPICS control.

Built-in EPICS motor control of SPEC is used through EPICS soft channels that bridges APS motor record and CLS motor record. This is because SPEC support EPICS motors based on APS motor record which is different from CLS motor record.

1.3.2 X-ray fluorescence detectors

Spectra from X-ray fluorescence detectors (single-, four-element Vortex$^@$) are handled though mca EPICS control. Region of interests and other detector parameters are primarily set in mca EPICS. SPEC reads ROI setting from EPICS and also ROI's can be set by SPEC. Mca spectra are saved in separate data files. Main SPEC data file records ROI's as counters along with other parameters needed for dead-time correction.

1.3.3 CCD detector

SPEC scans with X-ray CCD detector (Mar165) has been provided by indirect control. Area detector EPICS control is used for CCD image acquisition. The CCD image can be saved to CCD control linux PC only. Through the EPICS control, SPEC set CCD image file name which reflect scan number and points in SPEC data file.

SPEC also controls exposure time and put comments to CCD image file head. The comments include angle positions of diffractometer and incident X-ray energy. ROI's within CCD can be set with EPICS or by SPEC. Background subtracted integrated intensities within ROI's are recorded as counters in SPEC data file. CCD shutter control relies on time delay set by SPEC, and beamline fast shutter uses gate signal from scaler to control exposure time.

2   Where to start

2.1   Starting software SPEC

SPEC can be started from any Linux OPI computer at the beamline. It is recommended for user to make new folder for each beamtime (or each project).

Go to the folder where data will be saved and type

> runSPEC

The command will start SPEC for psic diffractometer.

If four-circle geometry is required, type

> runFOURC

Using psi-8 diffractomter as four-circle geometry means not including nu, mu angles are at their zero positions and not included in reciprocal space calculation.

Redefining standard macros can be possible through spec.mac. SPEC loads spec.mac in starting directory as last macro to read-in. Any standard macro redefined in spec.mac can be effective if SPEC starts from the directory containing spec.mac.

If macros are not work properly due to macros loaded by previous users, fresh start of SPEC is possible by typing

> runSPEC –f

For more option of starting SPEC type

> runSPEC --help

2.2 Pre-Checking

HXMA supports various experimental techniques which require quite different beamline configurations. Checklist for diffractometer can be found in Appendix.

2.2.1 Hardware limit switch

Hardware limit switch positions can be changed depending on experimental type. It is users' responsibility to set hardware limit switch to protect diffractometer and equipments.

2.2.2 Disable unnecessary detectors

X-ray fluorescent detector and X-ray CCD detector need to be disabled if they are not used. Often these detectors were enabled from previous run. If EPICS for these detectors are not ready, SPEC can be crashed or hanged-up. If corresponding EPICS is running (started by previous users but not terminated) then there will be unnecessary waiting time in count or scanning.

> mca_off

> ccd_off

2.2.3 cyberstar window setting

Users need to properly set SCA window of scintillation detector (cyberstar, see 3.3). The window needs to be set according to the incidence X-ray energy. Also the window setting needs to be changed if gain or high voltage of detector is changed.

2.3 Sample alignment

Proper alignment of sample is crucial for diffraction measurement. Beamline provides motorized sample goniometer (X, Y, Z, θx, θy) for inert gas environment sample holders or capillary tube.

Closed loop cryostat alignment needs to be done manually.

2.4 MOSTAB

Most of anomalous scattering measurements (involving energy scan) **Mo**nochromator **Stab**ilization (MOSTAB) is vital part to keep height of incidence X-ray constant. MOSTAB controls piezo for theta angle of monochromator second crystal based on the normalized difference of outputs from split ionization chamber or quadruple pin-diode BPM.

3   Using detectors

Pin diode, ionization chambers and cyerstar detectors are configured as default counters when spec starts.

3.1   Pin Diode (ip)

ip0: measure flux scattered off from Kapton film in the beampipe end.

It can be used to monitor flux incoming to the sOE hutch.

 ip1: used for energy calibration.

Standard metal foil can be placed before the pin diode.

Ip2: on detector arm filter box, used for bulk peak measurements.

3.2   Ionization Chambers (IC's)

i0: the first IC that monitors flux incoming to the defining slits.

i1: IC after beam defining slits, used to normalize signal (monitor counter).

i2: IC on detector arm.

Use *ic_info, ic_sens* and *ic_offset* to display and change gain and offset of SR570.

3.3   Scintillation detector (cyb)

It is cyberstar detector on the detector arm.

Use *cybermenu* to set up parameters for the cyberstar detector.

High voltage, gain, window range can be set through *cybermenu*.

cyberscan can be used to scan SCA window to select proper window and reject XRF and higher harmonics.

Known settings:

Energy (keV)	Gain	Window low	Window high

3.4 Using X-ray fluorescence (XRF) detectors with spec

SPEC can take mca data if the EPICS control for MCA detector is up and running.

Typical step to follow:

Start EPICS control for mca detectors to use (see instructions of **starting EPICS control** below).

Start GUI for mca, get spectrum from standard or sample, and set ROI's.

To use four element Vortex detector (if it is not configured yet), use macro **on_4ele**.

cf) In SPEC, use macros **setup_mca** for more flexible MCA setup.

Check ROI's with macros **mca_rois**.

Type **save_rois on**. Any scan will save ROI's to spec data file. Use **save_rois off** to disable ROI saving.

Type **MCAscanpt** before any scan macro, for example **MCAscanpt dscan eta -1 1 10 1**

To disable four-element Vortex use **off_4ele** and **save_rois off**.

Macros relevant to MCA setup and usage are:

setup_mca-> interface to configure multiple epics MCAs in spec.

show_mca -> display the configured epics MCAs nicely.

mca_rois -> to automatically check the created ROIS in each MCA and display their parameters.

save_rois ->to turn on/off the feature of saving MCA_ROIS(defined in roi_pv[], and filled when mca_rois is called) **to spec data file.**

rm_mca -> remove one or all configured MCAs,also remove all rois related to that MCA

rm_roi -> remove one/all configured MCA ROIS.Can also rmove all rois related to one MCA by calling rm_roi mca_nme

getandsave_mca-> to start counting and save MCAs and save their spectra in spec file.

MCAscanpt->to save the MCA spectra in a separate file on each scan point of whatever scan(MCAscanpt anyscan macro)

MCAscanend-> to save the MCA spectra at the end of a scan (MCAscanend any scan macro)

EPIC control for the XRF detectors needs be started beforehand.

3.4.1 Starting EPICS control of four-element Vortex detector

Make sure IOC (computer) IOC1606-017 is turned on and connected to the network (10.106). If something doesn't seem to be working, see ???.

Connect all cables associated with the detector and electronics (see the detector related instructions in Hardware below)

3. Set up a video camera to watch the front panel of the XMAP crate

4. Turn on the XMAP electronics.

5. Double-click the "Start XMAP IOC" icon on the desktop, or type "runXMAPIOC". This should present a window with a numbered menu of detectors, one of which you can enter by name or by associated ID number.

Enter the detector (e.g. 4-Element or 1 for the 4-element Vortex detector).

You will be asked for a password. Use either the hxma account password. Leave the window open (closing it will shut down the control application)

6. On the video monitor, wait for the lights to stop flashing (it should settle into a 1Hz blink).

7 Start the control GUI by double clicking on the "XMAP4" or "XMAP1"

desktop icon (see Software->GUI)

Open the "ADC Trace" window for each element: **DXPs->DXP Control**, then in the "DXP Control" window, **More->ADC Trace**

set the "us per bin" to 100

make sure you see a sawtooth pattern that resets about 3-5 times per second.

Open the **Baseline Plots** and make sure all are fairly symmetric and that they are centered very near zero

Back on the DXP Control window, make sure "Energy Peaking Time" is set appropriately.

3.5 Using X-ray CCD camera with spec

MarCCD saves images on local linux PC and it is not possible to save to serve driver.

Still SPEC can "control" MarCCD through EPICS control.

The "control" means file name of CCD image can be set by SPEC.

Also SPEC can insert some information to head of CCD image file (16 bit tiff format).

3.5.1 Hardware and timing control

Current CCD image acquisition is based on scaler, fast shutter and time delay.

Scaler output is hard wired to the uniblitz fast shutter so that fast shutter opens only when scaler is activated (counting). If CCD is enabled (ccd_on) SPEC takes extra step to give enough time for CCD readout. When count (ct or any scan) starts SPEC sends command to start CCD. Then, scaler is activated and faster shutter opens. After specified counting time set by SPEC is elapsed scaler deactivated and fast shutter closes. SPEC waits predefined delay time to move to next point of scan or print counting results.

CCD starts   Scaler activated   Scaler deactivated   CCD ends   count ends

|--------------------|:::::::::::::::::::::::::::::::|------------------------|------------------|

Fast shutter open   Fast shutter close
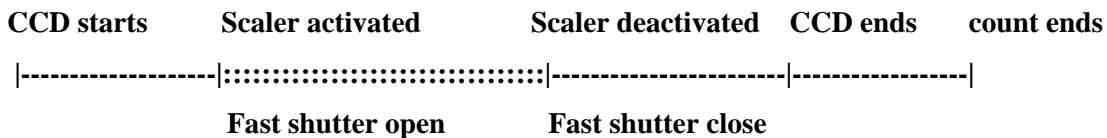
3.5.2 Prechecking

Following two steps are required/checked to use CCD through SPEC.

- "Remote Control" in data acquisition from marccd linux PC.
- Starting CCD EPICS IOC

Details can be found in 9.2 Quick Start

3.5.3 Enable/disable CCD

ccd_on will enable CCD image acquisition through spec macro *ct.*

ccd_off will disable CCD.

3.5.4 CCD setup

ccd_setup : select CCD to use (only one choice for now) and start setup.

1) CCD PV name   **ccd1606-002:cam1**

2) Detect Dist.

3) CCD next file sequence

4) CCD on (1) / off (0)

5) CCD file on (1) / off (0)   # Before start *ccdscan*, turn off CCD file.

6) CCD shutter delay time   # Use default value

7) CCD read delay time   # Use default value

8) CCD polling rate   # Use default value

9) CCD filename

10) Fixed EPOCH # in Filename # Put 0 for filename without EPOCH

11) MONITOR counter number

12) CCD_Status counter number

13) The 6 motors to record

14) Using timingbox or not   # Use default value

15) Add additional log file

16) CCD verbose mode on

17) CCD ROI MinX

18) CCD ROI MinY   # ROI rectangular box with corners of

19) CCD ROI SizeX   (MinX, MinY) and (MinX+SizeX, MinY+SizeY)

20) CCD ROI SizeY

21) CCD ROI expansion in X   # 21, 22 for ROI background estimation

22) CCD ROI expansion in Y

23) CCD Binning X   # Use default value

24) CCD Binning Y   # Use default value

3.5.5 Scan with CCD

scanccd [any scan macro of SPEC]

Perform any scan macro with CCD images saved at each scan point.

CCD files will be saved as

CCD_filename.scan_number.point_number.file_sequence.tif

For example,

```
scanccd dscan eta -10 10 100 2
```

will generate 101 CCD file with 2 sec exposure at each scan point.

CCD filename might look like **ccdtest.S003.N0012.012.tif** for 12th scan point if

"9) CCD filename" was set as "ccdtest,

the scan is the third scan,

 and "3) CCD next file sequence" was set to 1 before scanccd starts.

3.6 Configuring additional detectors

It is assumed that the additional detectors are temporary in nature.

3.6.1 Adding IC to counters.

Use *u_column_add* macro which is based on *cdef* of *spec*.

The counter can be removed by *u_column_remove*.

\#   *u_column_show*: display user defined data columns

\#   *u_column_add*: add one new entry of user defined column

\#   *u_column_remove*: delete one or(a set related to one key identifier)

\#   column/columns

\#   *u_column_clear*: clear all user defined columns

3.6.2 Adding cyberstar detectors

Default cyberstar detector (*cyb)* is configured in counter setting.

This is to add extra cyberstar detector(s), which will be used for non-permanent basis.

Use u_column_add and

then use cyberunitsetup

Example) *cyberunitsetup* 1 0 1 3 2 4 10 5 0.1

   This defines the second cyberstar unit as an SCA (type 0) model PPU5CH (model 1), configured with address 3, on SPECs serial device 2 with 4 seconds timeout. The unit has 5 channels, from 10 to 14. The default window size for scanning is 0.1 V. This means that scans on the motor cyb will scan the lower threshold and adjust the upper threshold to give a window of 0.1 V.

Then use *cybermenu* .

4 Energy macros and scans

HXMA uses two-crystal monochromator with fixed exit height. The second crystal of the monochromator has three motors (not the same as three-motor mono available in SPEC); rotation, translations along the downstream and vertical offset. Monochromator is somewhat similar to four-motor (monu, mond, montrav, and monoff) monochromator in SPEC classification with some differences.

Monochromator energy is changed through EPICS control. Limits of X-ray energy is 5 keV to 24 keV for Si(111) mono-crystal and 7 keV to 40 keV for Si(220) crystal. High energy cut-off by focusing mirror is about 30 keV. X-ray energy between 30 keV and 40 keV is available without focusing.

Several energy changing macros are available depending on a tracking of second monochromator crystal positions.

mve changes energy with two motors of the second crystal are changed to properly track X-ray diffracted from the first crystal and maintain fixed exit height.

amve changes energy (*mve*) and moves analyzer theta and two-theta to corresponding Bragg condition of analyzer crystal.

FHmve changes energy with only vertical offset of the second crystal is changed to maintain fixed exit height. Since horizontal position of the second crystal is not changed scan energy range should be limited less than 2 keV.

5   Using analyzer crystal

Analyzer crystals are typically used to reduce background count especially to cut florescence (inelastic) X-ray from sample.

Also, using analyzer crystal is equivalent to use very tight slit for a good angular resolution.   Although moderate angular resolution can be achieved with Soller slit, Soller slit is not implemented for the moment.

Available analyzer crystals are pyrolytic graphite(002) , Ge(111), Si(111), and Si(004).

Analyzer crystal	d-space (Å)	Bragg angle degree 10 keV	width μrad @10 keV	width degree @10 keV	Reflectivity
PG(002)	3.355	-			
Ge(111)	3.2662725	10.9409	58.939	0.00338	
Si(111)	3.1354161	11.4035	27.597	0.00158	
Si(004)	1.357675	27.1685	13.343	0.000764	

5.1 Aligning analyzer crystal
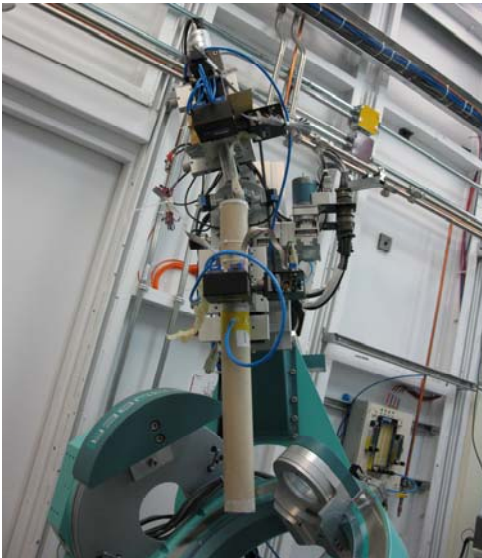
It should be done after psi-8 diffractometer is aligned (See **7.1 diffractometer alignment procedure**).

Make sure slit in the detector arm defines zero beam, that is $del = mu = 0$.

Move analyzer two theta (*atth*) to zero and open s2 silts (*s2hgap* and *s2hgap*) wide enough.

Move analyzer crystal from beam path (for example **mvr** *az -5).*

Find straight through beam with analyzer two theta scan.

dscan atth -1 1 30 .3

Move to peak position and define *atth* as zero (the peak position should be close to zero).

Bring in analyzer crystal to beam path and cuts beam to half by repeating

dscan az -1 1 20 .3

dscan ath -1 1 30 .3

5.2 Analyzer macros

sa `analyzer_crystal`

Setting the analyzer to use. It will list the defualt analyzers and ask the user to choose one of them (by name). The user can enter a custom name and d-constant of a crystal of their own choosing. Use variable `d_ana  d_ana_n`

amve `energy`

Change energy to `energy` and move *ath* and *atth* to corresponding Bragg condition of analyzer crystal.

aEscan start end step dwell_time [fixQ]

Escan with proper analyzer tracking. At each energy ath and atth move to satisfy Bragg condition of analyzer crystal.

6 Miscellaneous Hardwares

6.1 XIA filter box

Standard configuration for XIA filter boxes is two XIA filter boxes before sample (and monitor counter) and one after sample (before analyzer crystal). The first two filters can be mainly used to reduce flux to sample so that radiation damage to the sample can be minimized. The filter after sample is to protect cyberstar detector.

6.1.1 Control of the XIA filter box

The XIA filter box is controlled through "S2E1606-001.cs.clsi.ca" port 4. The address of first filter box is set to 0.

Example of *spec* command:

1774.PSIC> *sock_put("s2e1606-001:4004", "\!PFCU00 S\r\n")*

1775.PSIC> *p sock_get("s2e1606-001:4004")*

```
%PFCU00 OK 0101 DONE;
%PFCU00 OK PFCU v1.0 (c) XIA 1999 All Rights Reserved
CHANNEL IN/OUT (FPanel  TTL  RS232) Shorted? Open?
        1     OUT    OUT    OUT  OUT      NO    NO
        2      IN    OUT    OUT   IN      NO    NO
        3     OUT    OUT    OUT  OUT      NO    NO
        4      IN    OUT    OUT   IN      NO    NO
RS232 Control Enabled: YES
RS232 Control Only: NO
Shutter Mode Enabled: NO
Exposure Decimation:    1
DONE;
```

Table 3: PFCU command summary

Command	Description	Arguments
2	PF2S2 Mode Enable shutter commands	None
4	PF4 Mode Disable shutter commands (initial default)	None
C	Close shutter	None
D	Exposure Decimation	Decimation value (1 to 65535)
E	Exposure	Exposure Time / (Decimation*10 ms) (1 to 65535)
F	Fault Status	None
H	SHutter Status	None
I	Insert Filter	Up to 4 filter numbers 1, 2, 3 or 4 (in any order)
L	Lock: ignore non-RS232 controls	None
O	Open shutter	None
P	Position Inquiry	Control Source (RS232,Panel,TTL) (optional – no argument gives overall setting)
R	Remove Filter	Up to 4 filter numbers 1, 2, 3 or 4 (in any order)
S	Status Display	None
U	Unlock: enable non-RS232 Control	None
W	Write Filter Position	0 or 1 for each filter
Z	Clear Short Error condition	None

6.1.2 Macros for XIA filter box

fb_setup `[counter-mne] [min-count]`

> `counter-mne` is the mnemonic of the counter to be used

> `min-count` is the minimum acceptable count for the counter specified. If the user enters a negative number, it will be interpreted as a percentage of the counter's current count

fbc

> this will update the coefficient matrix for the current energy

fbu

this will provide the log10 of the attenuation coefficient for the current filterbox combination, if an argument is provided then it will display the attenuation coefficient for the combination provided

fb_on

this will enable the automatic filterbox configuration during scans

fb_auto

this finds a suitable filterbox combination to bring the counts to the threshold

Slit control

There are three slits directly related to the psi8- diffractometer: beam defining slit, guide slit, and scattering slit. Currently XIA slits are used for all three slits.

Beam defining slit is located before sample and normally monitor counter is located right after the slit.

Guide slit and scattering slits are located after sample.

The slits are referred as horizontal and vertical even though it is not quite correct for psi-diffractometer. Horizontal is along gamma direction and vertical is along delta direction.

6.1.3 Slit setting

Please note the quote from E. Vlieg for surface diffraction,

" Most of the time, the detector arm will have two sets of slits: one set close to the sample (slit1) and one in front of the detector (slit2). In the in-plane direction, slit1 and slit2 together define the active sample area. The value of slit1 is the most important one for the active area, while slit2 is more important for the angular acceptance. In order to minimise the effects of the coupling between real and angular space, it is a good idea to have slit2 slightly larger than slit1. Typical values are 2 mm for slit1, and 3 mm for slit2. In the out-of-plane direction (*l*-direction), only slit2 is important. Slit1 (if implemented) should be kept wide open in that direction."

6.1.4 Macros for slit

[under construction]

7 Data reduction and analysis program

7.1 Measurement from point detector

To extract structure factor from experimental data, several corrections should be applied. For scattering intensities measured through rocking scan with point detector, typical steps to pull out structure factors are; following

- Obtain integrated intensity from a rocking scan.
- Apply corrections of Lorentz-Polarization factor, area, and truncation rod acceptance length to the integrated intensity
- Average over symmetry equivalent rods

Users can use ANA-ROD program
(http://www.esrf.eu/computing/scientific/joint_projects/ANA-ROD/) for data reduction and/or CTR analysis.

HXMA provides data reduction programs (made with awk language and CPLOT) for integrating intensities and applying corrections.

offspec.awk

correct_phi.awk (correction for nonspecular rod)

correct_eta.awk (correction for specular rod)

After averaged over symmetry equivalent rods, other programs (for example, ROD) can be used for structure analysis. Users also can use their own CPLOT programming for non-linear fit (*.5.c).

8 Diffractometer Alignment Procedure

Purpose: To make incident X-ray passes the diffractometer center **AND** *eta, del, mu,* and *nu* base plates parallel to the X-ray at their zero angles (in user unit).

After step 8.1, 8.2, 8.3 ***align_diff*** macro can be used for automatic diffractometer alignment. Please refer step 8.4, 8.5, 8.6 for manual alignment.

See also step-by-step guide, CLS HXMA Psi-8 Alignment Procedure.

8.1 Mounting centering tool

REMOVE VORTEX AND ANY OTHER PROBES OR DETECTORS. MOTION OF THE CENTERING TOOL CAN HIT STUFFS AROUND SAMPLE/ SAMPLE STAGE.

Centering tool is one directional slit mounted on extending structure from the *phi* stage. The mounting does not require removing sample goniometer. But sample height (*samz*) need to be lowered to clear the X-ray pass.

8.2 Pre-checking of motor dials

  If this is not a minor correction, motor dial positions must be checked before the align procedure starts.

For *nu, mu, eta*: **mvd** *motor 0* will move specified motor to zero angle in dial.

For *chi*: **mvd** *chi 90* will move chi to 90 degree.

  Check *nu, mu, eta, del* and *chi* positions.

  If the angle position is not zero or 90 (including dials in motor and reducing gear), turn motor axis to bring every dial to zero.

  In stationary mode, power of a diffractometer motor is turned off automatically. If you manually turned the motor axis, please record the amount in diffractometer log book. The record can be help beamline scientist to adjust maximum motor speed which does not loose step.

8.3   Stationary ion chamber setup

Place ion chamber on microprobe table and adjust its position so that the direct beam can get into ion chamber.

Adjust ion chamber gain properly.

8.4   Diffractometer vertical height alignment

Install centering tool on the *phi* stage.

Set ion chamber on microprobe table (usually it is prekb) as detector (i.e. *DET=prekb*).

mvd *chi 180* : move *chi* to 180 degree in dial unit.

Scan *phi* to find peak. You find peak at ϕ_0.

Then move *phi* to $\phi_0 + 180$, and scan *phi* to find peak. Let's call this new peak position as ϕ_1.

Now $\phi_1 = \phi_0 + 180$ then diffractometer has correct height. You can forward to horizontal position alignment.

If $\phi_1 \neq \phi_0 + 180$, then move *phi* to $(\phi_0 + \phi_1)/2$ and do vertical table scan.

Find peak by vertical table scan:

d2scan vtbu start_rel end_rel vtbd start_rel end_rel step time.

for example) **d2scan** *vtbu* 0 50 *vtbd* 0 50 50 1

Raise or lower table to peak position. Now the X-ray is passing diffractometer center.

Forward to horizontal position alignment section.

8.5   Diffractometer horizontal position alignment

mvd *chi 90* : move *chi* to 90 degree in dial unit.

Scan *phi* to find peak. You find peak at ϕ_0.

Then move *phi* to $\phi_0 + 180$, and scan *phi* to find peak. Let's call this new peak position as ϕ_1.

If $\phi_1 = \phi_0 + 180$ then diffractometer has correct height. You can forward to horizontal position alignment.

If $\phi_1 \neq \phi_0 + 180$, then move *phi* to $(\phi_0 + \phi_1)/2$ and do vertical table scan.

Find peak by vertical table scan:

d2scan htbu start_rel end_rel htbd start_rel end_rel step time.

for example) **d2scan** *htbu* 0 5 *htbd* 0 5 50 1

Move table to peak position. Now the X-ray is passing diffractometer center. Forward to diffractometer table tilting adjustment section..

8.6 *Diffractometer table tilting adjustment*

Now X-ray passes diffractometer center. However the incident X-ray might not parallel to rotation base of *nu/mu* or *del/eta* at their zero position.

We use different approach for yaw (nu/mu) and pitch (del/eta) adjustment.

For yaw (nu/mu), user unit of angles can be set to zeros instead of table rotation. But it is based on assumption that you did **Pre-checking of motor dials** (section 2.2) properly.

After diffractometer centering, move *phi* by 45° to clear beam path and scan *nu* to find peak (with *prekb*).

Then move *nu* to the peak angle, say v_0.

Now set *nu* to zero, by typing *set nu 0*.

It makes peak-position in user unit zero and dial unit is still v_0.

Now move *mu* to v_0 and set to 0.

        mvd mu v_0; **set** mu 0

User unit of *nu* and *mu* are set to zero at peak position.

For *del/eta*, table pitch (vertical tilting) must be adjusted.

9 Epics control of MarCCD (from HXMA wiki page)

9.1 Introduction

These are the configuration, startup, and basic usage notes for the MarCCD EPICS control software. The software is based on the **synApps 'areaDetector'** application. This control application connects directly to the MarCCD application and can write image files in TIFF format as per user specification.

These instructions can be found at http://wiki/index.php/HXMA_MarCCD_Detector.

9.2 Quick Start

On the MarCCD workstation, log in as user 'marccd'.

Double-click on the "**MarCCD**" icon.

On the MarCCD GUI, select **Acquire->Remote Control...**

On the Remote Control window, confirm or set the following

Server Environment: NETHOST=localhost

Server Command: /home/marccd/contrib/marccd_server/marccd_server_socket

Server Arguments: 2222

Server Log: /home/marccd/log/remote_server.log

Press **Start** on the Remote Control window, then **Dismiss** the window.

Go back to the data acquisition workstation

Double-click on the "**MarCCD_IOC**" icon.

Double-click on the **MarCCD_GUI** icon.

Select marCCD Drivers->marCCD #1 General, or change settings with marCCD Drivers->marCCD #1 Specific.

Start taking data

9.3 Usage

Most of the MarCCD EPICS control GUI is informational. The following are the more commonly used controls.

9.3.1 Image Files

The image files are only available in TIFF format, using 16-bits per channel (i.e. 48-bit color/grayscale). The **File format** (not to be confused with **Filename format**) will display "netCDF" and should be ignored.

Note: due to the EPICS version of the controls being named similarly as the vendor's software, there can be some confusion as to whether the EPICS software can write image files. It doesn't do this. It can READ the image files written by the vendor's software for analytical purposes, but it is not set up to re-write it.

9.3.2 Single Shot Exposure

In the **Area Detector** screen, select **marCCD Drivers->marCCD #1 General**. That should launch the general purpose **marCCD Detector Control** window. Alternatively, you can launch the expert controls with

marCCD Drivers->marCCD #1 Specific, which puts most of the controls in a single view with extra status displays.

In the **Collect** section:

Set the **Exposure time** (in seconds)

Ensure the following:

Acquire period is set to 0

 # images is set to 1

Image mode is set to "Single"

frame type is set to "Normal"

Overlap type is set to "Sequential"

Array Callbacks is set to "Enable"

In the **Readout** section:

Set **Binning** for each axis according to your requirements.

Ensure that **Frame shift** is set to 0

In the **File** section:

In the general control window, press the **Driver file I/O** button. That will launch the files control window. The expert window has the same controls built in.

Set **File path** to the directory you want all of your images saved to.

Set **File name** to the **root name** of the files you want your images saved to.

Set **Next file #** to the starting value you want your sequence of images numbered from.

Set **Auto increment** to "Yes"

Set **Filename format** to a string as follows:

To specify the directory and root part of the file, start with "`%s/%s`".

To specify the file number, at least use "`%d`".

You can specify the number of digits with a number between `%` and `d`. This really isn't useful unless you also specify zero padding, below.

You can specify zero padding by putting a zero in front of the number, e.g. "`%04d`, which would result in files numbered "0001, 0002,... 0999, 1000".

Between the filename root and the file number, and after the file number, you can add just about any set of characters.

Since the files are in TIFF format, it is highly recommended that the Filename format end with "`tif`".

Examples: assuming you set the File path to /tmp, File name to test, and Next file # to 5:

for a file that you want to look like "`/tmp/test-0005.tif`", the Filename format should be "`%s/%s-%04d.tif`"

for a file that you want to look like "`/tmp/test05.tif`", the Filename format should be "`%s/%s%02d.tif`

Set **Auto save** to "Yes"

To actually generate an image, go to the **Collect** section and press **Start**.

The various displays in the **Status** section will inform you of the status of the exposure.

9.3.3 ROIs (Regions-of-Interest)

In the **Area Detector** screen, select **marCCD Plug-ins->ROI #1**. That should launch the **ROI1** window.

Set **Enable** to **Yes**

Set Callbacks block to Yes

You can examine individual ROI information and modify the ROI's settings with **Individual ROIs** menu.

Set Use this ROI? to Yes

Make sure **Data type** is set to **UInt16**

Set Compute statistics to Yes

Set **histogram?** to **Yes** if you are interested in seeing the quasi-distribution of pixel intensities. At first, set the parameters as follows:

Set **Size** to 65535.

Set **Minimum** to 0.

Set **Maximum** to 65535.

Set **ROI start** and **ROI size** as you need. It is **highly** recommended that ROI #1 be set to (0,0) and (2048,2048) respectively, that you pay attention to the **Statistics** section, particularly the **Maximum** reading for overflows.

For multiple ROI information in tabular format select from the **Combined ROIs** menu.

9.3.4 Multiple Frame Exposures

It might be useful to set **Overlap mode** to **Overlap** when doing multiple exposures in succession. This allows an exposure to begin while the previous file is being written. If you do use this feature, AND you do not need ROIs, it would be advisable to set **Array callbacks** to **Disable** if **Overlap mode** is set to **Overlap**. Callbacks will block the overlap feature. If you want reliable ROIs, you have no choice but to keep **Array callbacks** enabled.

9.4 Start-Up

The details of starting up the MarCCD system can be found here.

9.4.1 Hardware

The hardware system is fairly complex. Setup, configuration, and operating instructions should only be performed by experienced personnel, thus are beyond the scope of this

document. If the MarCCD workstation, the cryogenics system, or the detector is not powered up, inform the beamline staff.

Regarding the workstation, it is not integral to the operation of the detector hardware. It usually can be rebooted with little or no impact to the detector or cryogenics.

HOWEVER, the workstation should **NOT** be unnecessarily rebooted. It is still possible to lock up the detector this way.

Finally, the workstation **IS** integral to data acquisition, since it acts as the data and control server for the EPICS control software.

9.4.2 Software

On the MarCCD workstation, log in as user 'marccd'.

Double-click on the "**MarCCD**" icon.

this should launch the MarCCD GUI and a terminal window

the GUI is what users would normally use locally, and can be monitored for remote usage

the terminal window reports the status of the system's hardware.

On the MarCCD GUI, select **Acquire->Remote Control...**

On the Remote Control window, confirm or set the following

Server Environment: NETHOST=localhost

Server Command: /home/marccd/contrib/marccd_server/marccd_server_socket

Server Arguments: 2222

Server Log: /home/marccd/log/remote_server.log

Press **Start** on the Remote Control window.

Dismiss the Remote Control window.

Go back to the data acquisition workstation

Double-click on the "**runMarCCD_IOC**" icon.

There should be a fair amount of text and should end with a prompt such as "`ccd1606-002>`".

Double-click on the **MarCCD_GUI** icon.

The EPICS control window should appear.

9.5 Shutdown

in the MarCCD IOC window, type exit

in the MarCCD GUI, select Acquire->Remote Control...

Press "Stop".

You will be prompted with "Do you want to abort data collection Immediately?"

Answer "No,..."

Dismiss the Remote Control window

shut down the MarCCD EPICS control GUI (NOT the main MarCCD control GUI).

Don't forget to close the EPICS controls "main" window, also.

10 Appedix

10.1 Table 1. List of spec motors

spec name	Controller	spec conf.	description
del	EPICS	psic	I1039
eta	EPICS	psic	I1040
chi	EPICS	psic	I1041
phi	EPICS	psic	I1042
mu	EPICS	psic	I1038
nu	EPICS	psic	I1037
htbu	EPICS	psic	I1035
htbd	EPICS	psic	I1036
vtbu	EPICS	psic	I1025
vtbd	EPICS	psic	I1026
samx	EPICS	psic	I1090
samy	EPICS	psic	I1091
samz	EPICS	psic	I1092
ath	EPICS	psic	I1043
atth	EPICS	psic	I1044
tune	EPICS	common	
ev		commom	Energy changeable with track-on
s0hgap	XIAHSC	common	408
s0hcen	XIAHSC	common	
s0vgap	XIAHSC	common	407
s0vcen	XIAHSC	common	
s1hgap	XIAHSC	psic	415
s1hcen	XIAHSC	psic	
s1vgap	XIAHSC	psic	434

s1vcen	XIAHSC	psic	
s2gap	XIAHSC	psic	409
s2hcen	XIAHSC	psic	
s2vgap	XIAHSC	psic	410
s2vcen	XIAHSC	psic	

10.2 Table 2. Motor parameters

motors	Resolution Step per degree/mm	Sign of user*dial	Steady-state speed [Hz]	Base speed [Hz]	Acceleration time [sec]	Backlash [steps]	High limit
del	8000	1	8000	800	250	200	
eta	8000	1	8000	800	250	200	
chi	-8000	1	8000	400	250	200	
phi	-4000	1	16000	800	250	200	
mu	-8000	1	2000	200	125	200	
nu	-8000	1	2000	200	125	200	
htbu	800	1	50	20	125	50	
htbd	800	1	50	20	125	50	
vtbu	16000	1	2000	2000	125	50	
vtbd	16000	1	2000	2000	125	50	
samx	200	1	200	200	125	50	
samy	200	-1	200	200	125	200	
samz	200	-1	200	200	125	50	
ath	4000	1	8000	200	1000	100	
atth	-4000	1	8000	200	1000	100	

10.3 Table 3. RS232 port assignment of Nport

Port assignment of 16-channel serial-to-Ethernet device"S2E1606-001.clsi.ca"

Port number	Device	spec	Note
1	XIA slit	s1vgap, s1vpos s1hgap, s1hpos s2vgap, s2vpos s2hgap, s2hpos	
2	Cyberstar X2000 controller	cyb	counter
3			
4	XIA S2F2 shutter		
5	Lakeshore temperature controller		EPICS control is optional.
6			
7			
8			
9	SR570	ic0	counter
10	SR570	ic1	counter
11	SR570	ic2	counter
12			
13			
14			
15	ESP 301		
16	Eurotherm 2416	t_euro, europv	counter