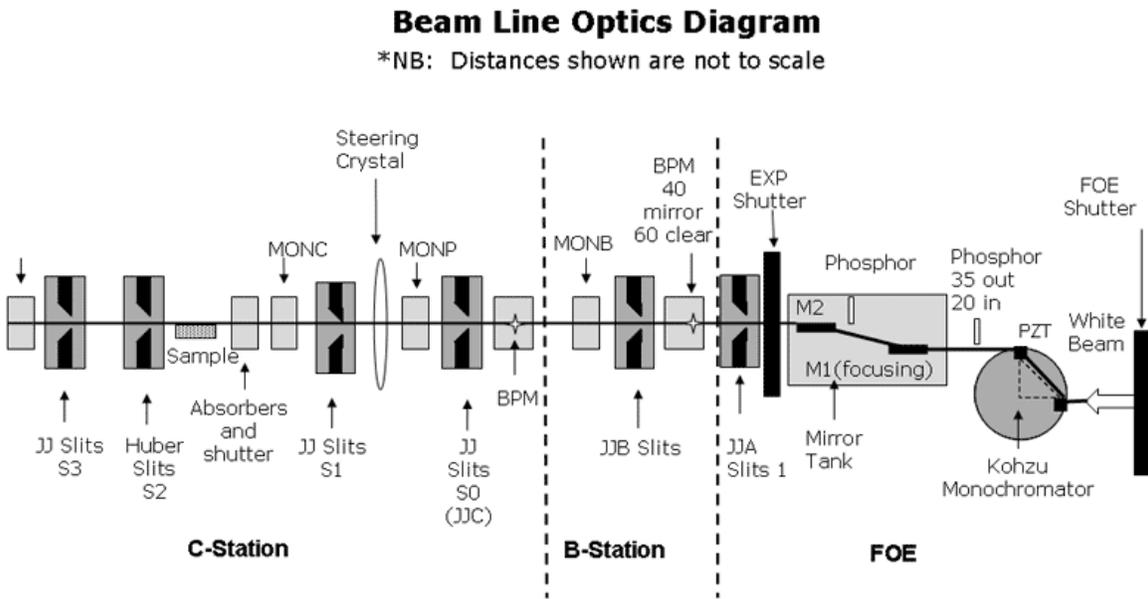


Liquid Surface X-ray Scattering User Help

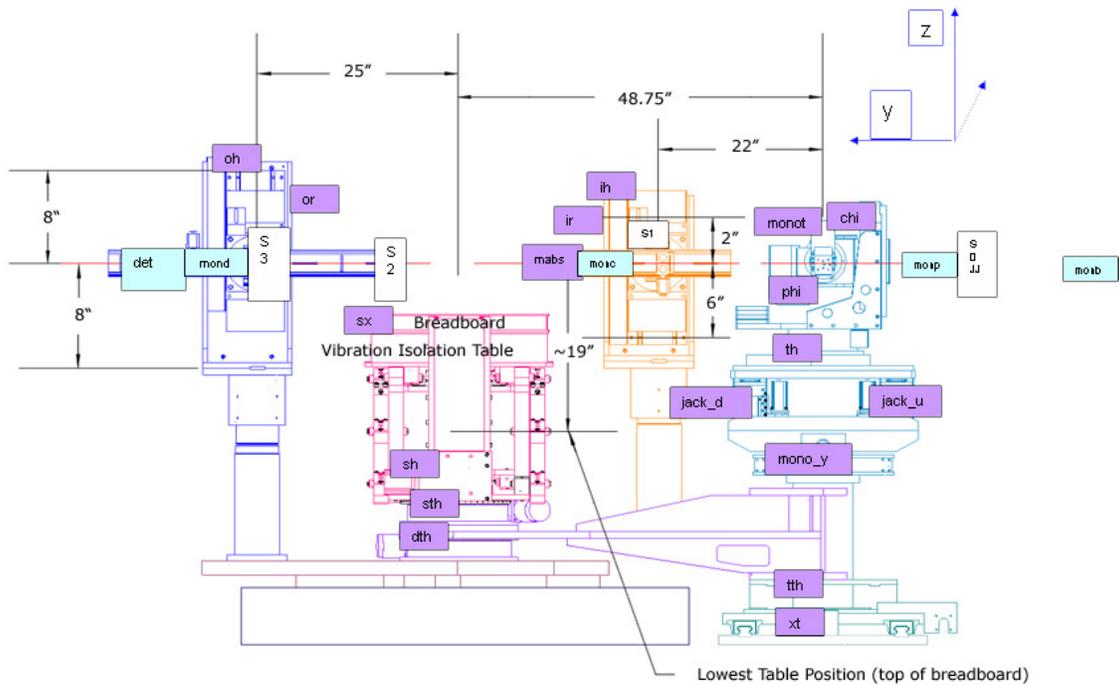
- 1. Instrumentation Schematics**
 - a. Beamline Optics Diagram
 - b. Liquid Surface Spectrometer Layout (with motor names)
- 2. Software**
 - a. EPICS (MEDM windows for users)
 - b. SPEC Commands in Brief
 - c. IDL Cheat Sheet
- 3. Geometric Alignment for the Liquid Surface Spectrometer**
 - a. Determining Geometry Parameters and Zero Angle Correction
 - b. SPEC Cheat Sheet for the Geometric Alignment of the Liquid Surface Spectrometer
- 4. Detectors**
 - a. Ion Chamber
 - b. Scintillator detector (Cyberstar 1000)
- 5. Troubleshooting**

1. Instrumentation Schematics

1a. Beamline Optics Diagram



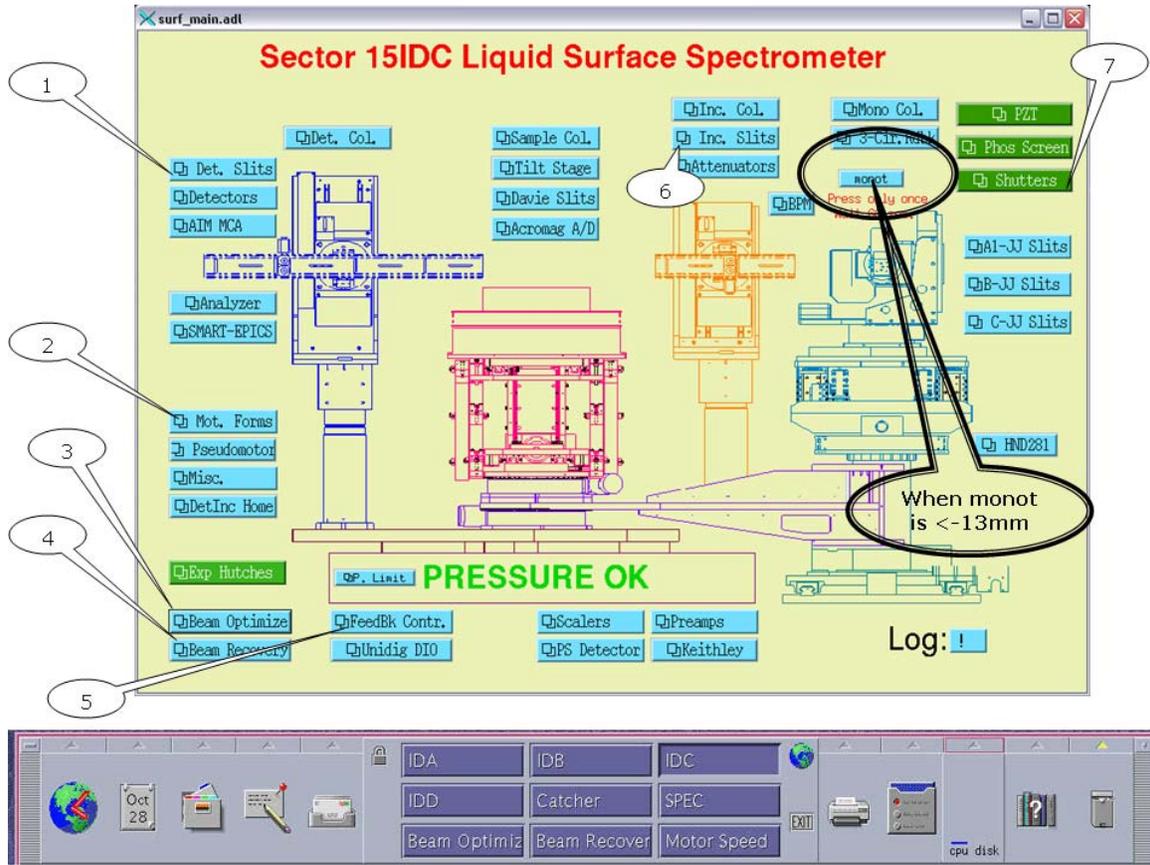
1b. Liquid Surface Spectrometer Layout



2. Software

2a. EPICS (MEDM windows for users)

IDC Liquid Surface Spectrometer Main Page



SPEC Command Window

The screenshot shows a control interface with several windows:

- surface_detectors.adt**: A window with four detector monitors (A, B, C, D) and an Oxford Cryostat. Each monitor displays 'Counts' and 'SPEC' values.
 - Monitor A: 611756
 - Monitor B: 399996
 - Monitor C: 300000
 - Monitor D: 313
 - Oxford Cryostat: 644
- Console**: A window with a text area containing the text: "SPEC command window (if freezes, get a new Console from cpu)".
- Remote Shutter**: A window with buttons for "Remote Shutter Front End Shutter" and "Exp. Shutter", both with "Open" and "Close" options.
- attenu**: A window with a numerical display showing "40" and "1", and "Open" and "Close" buttons.
- Feed Back Set**: A window with a list of feedback settings, including "1 Turn Feedback off" and "2 DAC Voltage".
- System Info**: A panel with buttons for "This Host", "system info", "Console" (circled in red), and "Find Host".
- Taskbar**: A bottom bar with buttons for "IDA", "IDB", "IDC", "IDD", "Catcher", "SPEC", "Beam Optimiz", "Beam Recover", and "Motor Speed".

Annotations and callouts:

- 1. Detectors**: Points to the surface_detectors.adt window.
- Monoc: normalization detector:**
 - 1: keep count rate between 5k cps and 500k cps
 - 2: keep dark current <100cps
 - 3: Check N₂ supply
- 5. Surface Feedback**: Points to the Feed Back Set window.
- 6. attenuator**: Points to the attenu window.
- 7. Remote Shutter**: Points to the Remote Shutter window.

A **SPEC plot window** is also mentioned in the top right, but its content is not clearly visible.

Beam Optimization Window

3. Beam Optimization

To optimize the beam when
 1) Intensity drifts
 2) Intensity feedback is off
 3) after recovering from a beam dump

Beam Dump Recovery Window

4 Beam Recovery

After the beam comes back from a dump, follow the procedure to recover the beam

Surface Motor Speed

2. Motor Speeds

Check or change the speeds circled in red; the setting indicated are for sample scans which are slower than in alignment

Note: do not change Max speed and Base speed

PV Name	Mnemonic	Max Speed	Speed	Base Speed
		(UNIT/S)	(UNIT/S)	(UNIT/S)
15IDC:m58	chi	4.00000	2.00000	0.50000
15IDC:m59	phi	8.00000	4.00000	1.00000
15IDC:m57	th	3.00000	2.00000	0.50000
15IDC:m60	monot	1.00000	1.00000	0.10000
15IDC:m18	mono_y	1.00000	0.5017	0.10000
15IDC:m20	jack_u	1.00000	0.9998	0.10000
15IDC:m19	jack_d	1.00000	0.9998	0.10000
15IDC:m26	tth	0.30000	0.0300	0.0010
15IDC:m17	base_x	1.00000	1.00000	0.50000
15IDC:m52	ih	0.50000	0.50000	0.0099
15IDC:m53	ir	1.00000	0.10000	0.0100
15IDC:m61	sh	0.50000	0.1000	0.0100
15IDC:m21	sth	0.50000	0.50000	0.10000
15IDC:m54	oh	0.50000	0.50000	0.0099
15IDC:m55	or	1.00000	0.10000	0.0100
15IDC:m23	dth	0.50000	0.1000	0.0050
15IDC:m41	xtalro	1.00000	1.00000	0.0010
15IDC:m42	xtalii	0.50000	0.50000	0.0010
15IDC:m25	sx	1.00000	0.25000	0.10000
15IDC:m56	tilt	1.00000	0.50000	0.0100
15IDC:m45	BPMLin	2.00000	2.00000	0.05000



2b. SPEC Commands in Brief

General Help

prdef *command* - prints the command usage. Or, just type command without any arguments.

history or **!** allow you to look at past commands (eg. “!d” looks at all past commands starting with d)

onsim/offsim – In simulation mode: no motors move, no permanent changes made, calculations only.

ca (e.g. ca 0 0 1) Calculates all angles and heights for specified qx,qy,qz

wh Lists positions of the 10 real motors.

wm *motor* lists complete info for up to 6 motors. (Example: wm oh)

Scans

DET=monc - sets the detector to ion chamber, monc

plotsselect - choose desired input (Example: plotsselect monc)

setplot - Allows you to plot data in real time or after scan is completed.

ascan (*motor* *start** *finish** *intervals* *time*)

Task: Scans absolute position of specified motor. *mm or degrees.

Example: ascan oh -0.2 0.2 20 1

dscan (*motor start* finish* intervals time*)

Task: Scans relative position of specified motor. *mm or degrees.

Example: dscan oh -2 2 10 1

shscan (*halfwidth intervals time*)

Task: moves sample and detector heights together.

oscan (*halfwidth intervals time*)

Task: Moves detector in a “circle” around the sample.

Comments: Involves simultaneous motion of the or and oh motors

P CEN – prints the center position of a scan.

umv tth CEN - moves motor to center position of last scan

set tth 7.406 - resets tth motor so that current position reads 7.406

Other Useful Macros

ct (*time or monitor_counts*)

Task: Counts for a set period of time (positive) or to monitor counts (negative).

mv (*motor angle/position*)

Task: Moves motor to absolute position specified.

Example: mv tth 50

Comments: **mvr** moves motor by a relative amount from current position.

umv updates motor position to screen as motor moves.

umvr Moves motor by relative amount, updates motor position in real time.

umi (*alpha beta*) and **umk** (*qx, qy, qz*)

Task: Change spectrometer alpha and/or beta angles. Many motors involved!

Examples: umi 0.2 0.0 umk 0 0 0.2

Slit Macros

wslits Displays slit widths

s1v 0.1 0.1 (*mm below and above center position*)

Task: Opens slits to +/- 0.1mm about a center position

s2vscan 1 0.2 10 1 (*total_scan_range slit_gap intervals time*)

Task: Scans the height of slit2, maintaining a constant opening of 200 microns.

Operating Linear Detector

mcavert (*time or monitor counts*)

Task: Collects data from the linear detector

2c. IDL Cheat Sheet

1) Make sure that chemmat28 is connected to the computer in use

2) Go to ‘preferences’ and check below

startup file: chemuser\MIDL\startup_mm.pro

Path setting: c:\RSI\IDL\lib
Z:\Chemuser\MIDL

General Info

Important: All the data processing routines used here employ the concept of a “current file”. The current file can be changed at any moment by adding a **/new** to any of the statements. This will prompt the user to identify, interactively, the new file (with the previous one being “forgotten”). Note that one should not use **/new** unless it is needed since there is a time overhead at reading a file.

Keywords: The actions taken by the various routines can be modified using keywords and some of these keywords are common to many of the routines. In the interest of brevity these keywords are listed here, instead of being repeated, over and over again, in the descriptions of the individual routines. A reminder to new IDL users, IDL keywords come in two varieties, the “switch keyword” which is either “set” (by invoking its name preceded by /) or “not set”, such as the **/new** mentioned above, and keywords which move values into and out of routines (these may be further subdivided into input and output keywords). The following is a partial list of common keywords used here. The routines used in the examples will be explained later

columns An input keyword used by various routines which need to pick specific data columns from the data block in a scan in a Spec file. **columns** accepts as input a 2 or 3 element integer input, with the first number representing the x-column (the scan variable), the second, the y-column (usually detector reading) and the optional third one representing the normalization column (usually *monc* output). The columns can be numbered either from left (starting at 0 and going up) or from right (starting at -1 and going down). For example, in the call:

scan_show, columns = [0,-1]

the x-values are read from the first (from left) column, the y-values are read from the last column and no normalization is done. In the call

scan_read, columns = [2,-1,-2]

the x-values are read from the third column (typical in reflectivity scans), y from the last and normalization from the one before the last.

/new As mentioned above, this is a switch which forces reading in a new spec file.

/output Switch, used by all the routines which generate screen graphic output. When **/output** is set, a copy of the screen graphic is sent to the current printer. The size of the printout can be controlled using additional switch keywords (active only in conjunction with **/output**). These are:

/full	obvious
/half	ditto
/quarter	ditto
/blin	intermediate between half and quarter.

The size keywords are sticky, meaning that whenever one is used, it'll determine the size of all subsequent plots until the next time the size is changed.

result This is an output keyword, enabling one to write the data processed by various routines into an IDL variable. For example the routine **patch_z** (described later) is used to patch together reflectivity scans and display the result on the screen, as in
patch_z, 45, 47, 50

(the numbers are scan numbers, explanation later). When called instead as

patch_z, 45, 47, 50, result = whatever

the result of the patching is put in the variable **whatever** and is available for further processing.

Important: The data is present in the variable in our standard data format. This is a 3-column array, where the columns, in order, contain x-values, y-values and y-errors.

The list above is by no means exhaustive, but it'll do for now.

Note: All the routines generating graphic output accept all the usual IDL graphics keywords as well

To read in a SPEC file

SPEC file can be read in in a variety of ways, usually the most convenient is using **scan_info**. This routine provides information about a chosen scan in the current file, or, optionally, the file itself. Example:

```
IDL>psyms, 0      (define symbols, optional)
IDL>pcols        (define plot colors, optional)
```

These (optional) commands need to be issued only once per session.

```
IDL>scan_info, 0, /new      (gives file info for new file)
IDL>scan_info, 0          (gives file info for the current file)
```

Typical output from the above looks like

```
IDL> scan_info, 0
```

```
Filename      :      P:\MIDL\Surface\Data\11.14.03
```

```
Date/time     :      Thu Nov 13 23:29:16 2003
177 scans present
```

Listed local parameters:

```
Chi In_Ht In_Rot Sample_H Det_Th Out_Ht Out_Rot Phi
```

an_Sam_H cpm ns dtoffset Theta

IDL>scan_info,26 (basic info for scan 26)

Typical output looks like

IDL> scan_info, 26

Filename : P:\MIDL\Surface\Data\11.14.03
Scan header : S 26 hklscan 0 0 -0.0055 -0.0045 0.250001 0.250001 3 -3.2e+06
Date/time : Fri Nov 14 02:07:44 2003
11 columns, 4 rows

G_L1 : 559.441 ; G_L2 : 1237.806 ; G_L3 : 645.580

Q_vector = [0.000000, -0.005499, 0.250001]

Peak location : -0.00483333 ; Peak intensity : 105520.
COM = -0.00485209 ; FWHM = 0.000499316 ; CEN = -0.00533265
LAMBDA = 1.1269

Scan info accepts a number of keywords, as follows:

/pars Switch, when set a list of tracked parameters with their value is displayed.
/slits Switch, when set the list of all the slit values is displayed.
/full Switch, when set all the gory details of the scan, as written in the file, are shown.

Reading SPEC Scans

Data from any *single* scan can be read into an IDL variable using the function **scan_read**. The basic syntax is

IDL>res = scan_read(s#, columns = col)

where **s#** is the number of the scan wanted and **col** is a 2-3 element vector (see keyword **columns** in "General Info"). Optionally, one may live out **columns**. In such case IDL will ask for the column numbers, interactively.

The function returns the read data in the standard [x,y,y_error] format. **scan_read** accepts a number of keywords, most of them not of interest for the general user. The ones worth knowing are:

/err Switch, when set the return variable contains [x, y_error/y,0] (the third column is zeroed).
header Output keyword, can be used to return the header of the data block. For example

```
IDL> res = scan_read(18,col=[0,-1,-2],head=header)
IDL> print, head
```

H K L Epoch monb monp mond mca Seconds monc det

Displaying SPEC Scans

Data from single scans or groups of scans can be displayed using **scan_show**. The basic syntax is

```
IDL>scan_show, s#, columns = col
```

with **s#** and **columns** same as above.

It is possible to display multiple scans at once, for example the command

```
IDL>scan_show, 5, 8, 15, 12, 2, columns = [0,-1,-2]
```

Will display on a single plot the data from the five scans numbered 2,5,8,12,15 (the order in which the numbers are provided doesn't matter), using the first, last and before last columns for [x,y,e_error], for all scans (it is, of course, the users responsibility to make sure that all scans are of compatible type and the column assignment is valid for all of them).

More generally, whole ranges of scan numbers can be combined, as in

```
IDL>scan_show, '6-13, 16, 18-22', columns = col
```

In this case all the scans from #6 through 13, scan #16 and the scans from 18 through 22 will be used. Note that the scan number entry in this case is a single character string, not numeric.

As a last possibility, actual scan data in our standard data format (a [3,n] array) can be provided. For example, one can have

```
IDL>a = scan_read( 4, columns = col)  
IDL>b = scan_read( 32, columns = col)
```

```
IDL>scan_show, a, b
```

Note that **columns** entry is not required in this case. This mode of use is valuable when one wants to display together scans from different SPEC files, or processed data (not original scans).

1)To view individual spec scan results, say for scan #27—has to be a dsan or ascan,

```
IDL>scan_show, 27, col=[0,-1,-2], psym=-8,/output,/quart&wshow  
(col=[x,y,monc], output for printer, optional)
```

2)To read a scan 9 data into IDL for data analysis

```
IDL>res=scan_read(9,col=[0,-1,-2])
```

Patching together spec scans taken with different absorbers, scaling appropriately

(1) for GID

IDL>patch_xy, '100-107, 109', /force (linear scale)

IDL>patch_xy, '100-107, 109', /force, /ylog (log scale)

Note that scan numbers must be listed in the order of increasing theta values

(2) For reflectivity

IDL>patch_z,95,96,97,[-98,99,-100],res=a,/output,/quarter(negative is for background scan whose count is 1/2 count of the specular scan

plot options:

/new/ylog,xran=[0,1],yran=[1,2]..

Detector linear fit

IDL> detfit, 126, /pil, tit= 'Have a nice day!', /new (\$\$\$\$ should print scan file title)

CCD related (temp)

1) dth scans

IDL> lee_dth_scan, '3-7', ran=[1,3],step=.5

Using g_11, g_12, g_13

g_11,[154,155,156]

g_12,[154,155,156]

g_13,[154,155,156]

;=====Demonstration:

Listings in CARS5\users\chemuser\MIDL\Surface\Data>Listings.txt

File 08.20.03 contains Q_xy set of scans, # 25-33

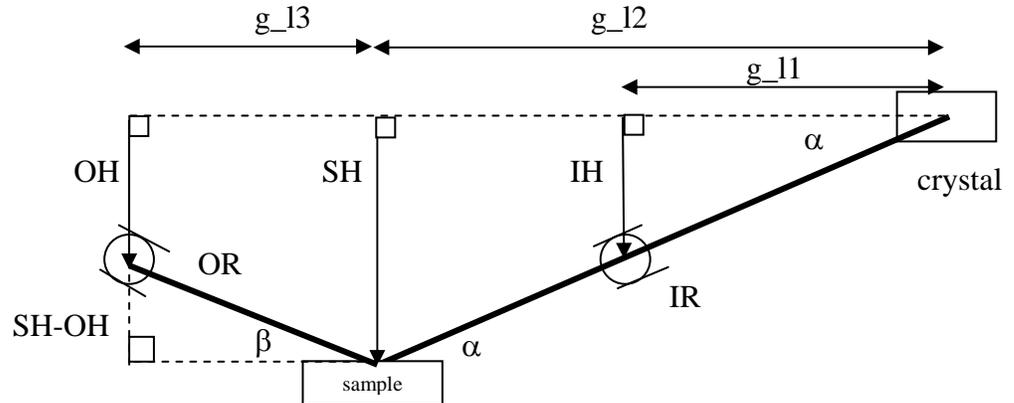
File 11.16.03 contains Q_y set of scans, # [71-76,77-82,83-88]

File 11.14.03 contains Q_z set of scans,

#, 59,60,61,62,63,64,65,[66,-67,-68],[69,-70,-71],[72,-73,-74]

3. Geometric Alignment for the Liquid Surface Spectrometer

3.a Determining Geometry Parameters and Zero Angle Correction



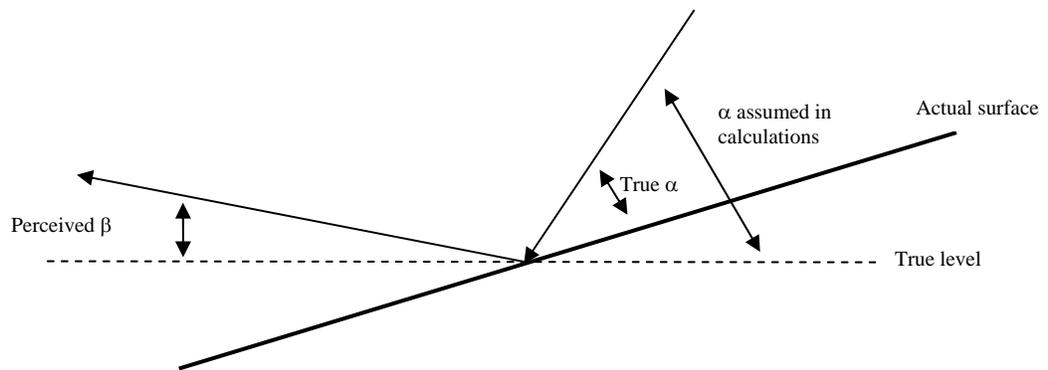
Find g_{11} . For this parameter only, you don't need to have the sample in place. It's essential that beam is centered on the steering crystal. Select four different α angles and record IH for each angle (perform iscans here; these involve simultaneous motion of both the incident height and rotation). Vary α by up to 5 degrees. Use MONC to measure intensity. In IDL, perform a linear fit to determine g_{11} . The y-intercept should be very close to zero.

$$IH = (g_{11}) \tan(\alpha)$$

$$IH \sim (g_{11}) (\alpha)$$

Therefore $g_{11} = \text{slope of IH versus } \alpha$

Zero Angle Correction insures that beam is parallel to the interface. This should be a very small correction since the beam and the interface are very close to horizontal to begin with. See the figure below.



First, move sample out the way and scan oh with nominal α equal to zero. Set oh center to zero. Then move spectrometer to some small angle ($qz=0.05$) and move sample into place. Don't pick too small of an angle since there is a risk that you will detect transmitted beam in addition to the reflected beam. Perform an shscan to center the sample. Perform an oscan with the detector slits open fairly wide. In this way, minor curvature in the sample surface will deflect the beam away from the true specular direction, but will still be captured by the detector. If the slit is open too wide, you may capture transmitted beam. Perform macro zero_angle to take the measured β and estimate a correction to α (half the difference in β). The correction can be based on a single angle α .

Measured β Offset

Small and random
Constant with increasing angle
needed
Increasing with increasing angle
needed

Calls for...

A smiling face, Good!
Correction to zero angle correction
Correction to geometry parameter

Find g₁₂. Perform sample height scans for a number of different α 's (like 0.03, 0.05, 0.10, 0.15) and determine the sample height (negative number) corresponding to the center of each scan. Determine g₁₂ in same manner as g₁₁.

Find g₁₃. Perform an oscan for four different α 's and determine OH for each angle. Perform a fit, using the value of g₁₂ that you determined in the previous step.

$$\tan\alpha = (\text{SH}-\text{OH}) / (g_{13})$$

$$\alpha = (\text{SH}-\text{OH}) / (g_{13})$$

$$\text{but, SH} = (g_{12})\tan\alpha = (g_{12})(\alpha)$$

$$\text{so, } \alpha = [(g_{12})(\alpha) - \text{OH}] / (g_{13})$$

$$\text{OH} = (g_{12} - g_{13})(\alpha)$$

Therefore, for linear fit to graph OH versus α , the slope = $(g_{12} - g_{13})$

3.b SPEC Cheat Sheet for the Geometric Alignment of the Liquid Surface Spectrometer

(Align the beam to be parallel with the surface of the sample and determine g₁₁, g₁₂ and g₁₃)

A) Alignment for g₁₁

- SURF> g_trck=0;pa (to disable oh or sh)
- SURF>s1v 0.01 0.01,s1h 1.5 1.5
- SURF>DET=monc; plotselect monc
- SURF>umk 0 0 0
- SURF>dscan ih -0.3 0.3 20 1
- SURF>umv ih CEN;set ih 0
- SURF>umk 0 0 0.05
- SURF>dscan iscan -0.5 0.5 20 1
- SURF>umk 0 0 0.1
- SURF>dscan iscan -0.5 0.5 20 1
- ...continue (Repeat the iscan to an angle as far as your experiment requires.)
- SURF> g_trck=1;pa (enable oh or sh)
- Use IDL to obtain g₁₁ value (see IDL cheat sheet), input g₁₁ in SPEC, and then check the alignment at a few angles.

B) Zero_angle procedure

- (mv sh to cut incident intensity by 1/2 and set sh 0)
- SURF>s1v 0.01 0.01; s1h 1.5 1.5;s2v 1 1;s2h 2 2;s3v 1 1;s3h 2 2
- SURF>DET=det;plotselect det
- SURF>abs 41
- SURF>umv sh -2
- SURF>dscan oh -1.5 1.5 20 1
- SURF>umv oh CEN;set oh 0
- SURF>umi 0.35 0.35
- SURF>wh

- j. SURF>abs 20
 - k. SURF>shscan 0.4 20 1
 - l. SURF>umv sh CEN; set sh NOM
 - m. SURF>dscan oh -1.5 1.5 20 1
 - n. SURF>abs 40
 - o. SURF>zero_angle
 - p. Record mi value on the screen to note the correction for alpha.
 - q. Repeat from a) to n)
- C) Alignment for g₁₂ and g₁₃
- a. SURF>s1v 0.01 0.01; s1h 1.5 1.5; s2v 1 1; s2h 2 2; s3v 1 1; s3h 2 2
 - b. SURF>DET=det; plotsselect det
 - c. SURF>abs 41
 - d. SURF>umi 0 0
 - e. SURF>umv sh -1
 - f. SURF>dscan oh -1.5 1.5 20 1
 - g. SURF>umv oh CEN; set oh 0
 - h. SURF>umk 0.35 0.35
 - i. SURF>wh
 - j. SURF>abs 20
 - k. SURF>shscan 0.7 20 1
 - l. SURF>umv sh CEN; set sh NOM
 - m. SURF>oscan 1.5 20 1
 - n. SURF>umi 1 1
 - o. SURF>wh
 - p. SURF>abs 10
 - q. SURF>shscan 1.2 20 1
 - r. SURF>umv sh CEN
 - s. SURF>oscan 1.57 20 1
 - t. SURF>umi 2 2
 - u. SURF>wh
 - v. SURF>abs 0
 - w. SURF>shscan 2.4 20 1
 - x. SURF>umv sh CEN
 - y. SURF>oscan 1.5 20 1
 - z. SURF>umi 3 3
 - aa. SURF>wh
 - bb. SURF>abs 0
 - cc. SURF>shscan 2.4 20 1
 - dd. SURF>umv sh CEN
 - ee. SURF>oscan 1.5 20 1
 - ff. Continue the measurements until shscan measurement is impossible.
 - gg. Use IDL to find g₁₂ and g₁₃ (see IDL cheat sheet), input them in SPEC, and then check the alignment at a few angles.

4. Detectors

4.a Ion Chamber Detectors

Ion chamber setup

(esp. monc, the beam normalization detector on the Incident Arm)

- 1) Preamp Offset: Keep dark count (no beam) lower than 100
- 2) Preamp Sensitivity: Select gain so the count rate is >5000 counts/second and $<500,000$ counts/second (to keep the error $<2\%$)
- 3) Use N_2 for photon Energy between 8-30keV. Check N_2 supply everyday (or Ion chamber's count is wrong)
- 4) Ion chamber high voltage: For photon energies less than 25keV use a voltage of 2 kV. For higher energies, use 1.5 kV

How to calculate absolute current output from ion chamber

Ratemeter (if set to "1x") gives an output of 100,000 cts/s for every volt out of preamp. The preamp converts current from the ion chamber to a voltage.

(high sensitivity; $5\text{nA/V} \Rightarrow$ only 5 nA required to produce 1 volt output.

Low sensitivity; $5\text{ microA/V} \Rightarrow$ a much larger current required to make same 1 volt output)

For example:

2,300,000 cts/s gives 2.3 volts. If the preamp sensitivity is set to 5 microamps/volt, this means that 11.5 microamps are produced by the

4.b Scintillator Detector (Cyberstar 1000)

- Use MCA to check the window, gain and HV settings
- Check linear range
- Check hutch noise (put lead tape in front of S2 with beam on)

5. Troubleshooting

- 1) IF monb and monp count rates are normal but monc rate is abnormally low, check monot position on TV for “Newport Control”—last number of the four numbers on the TV. If monot is equal to ~ -13.5 , go to MEDM panel “LIQUID SURFACE SPECTROMETER” in Sun window IDC (see graph 2.a.1), and click the “**monot**” button on the right. After ~ 1 minute, monot should go to the position marked on at the TV monitor. If monot fails to go to the designated position but at a position > -11 , then use SPEC to mv monot 0.
- 2) If monb and monp count rates are fluctuating, there are two possible reasons. One may be due to the malfunction of the intensity feedback, and the other may be due to the instability of the synchrotron beam. Turn the intensity feedback off to see if the fluctuation persists. If it does then the synchrotron beam is unstable. Call the floor coordinator to complain. Otherwise call the beamline scientists.
- 3) If monc count rate fluctuates but monp and monb are normal, check phi (third number) or chi (second number) on the TV to see if they fluctuate. If they do then move phi or chi back and forth a few times. These are servo motors so they hunt all the time and sometimes may get into a bad spot.
- 4) After a refill, turn off the feedback and go to MEDM panel “SURFACE BEAM CONTROL” in Sun window Beam Optimization (graph 2.a.3). Follow the instruction from 1-8 on that panel.
- 5) If the intensity feedback is drifting constantly, follow the instruction in 3) for beam optimization after a refill.
- 6) After a beam dump, pull out MEDM panel “Dump Recovery” in Sun Window Beam Recovery (graph 2.a.4). Follow the instruction from 1-5. Then use Beam Optimization to optimize the beam intensity.
- 7) If Surf Froze, open a new console (see graph 2.a.2) and change to your working directory, then start surf.