

Rigaku Smartlab Standard Operating Procedure

Manager:

Dr. Dmitri Barbash
Senior Research Scientist

Contact:

Drexel University
Bossone 112
3141 Chestnut Street
Philadelphia, PA 19104
Office: 215-571-4611
Mobile: 267-918-3188
dvb36@drexel.edu

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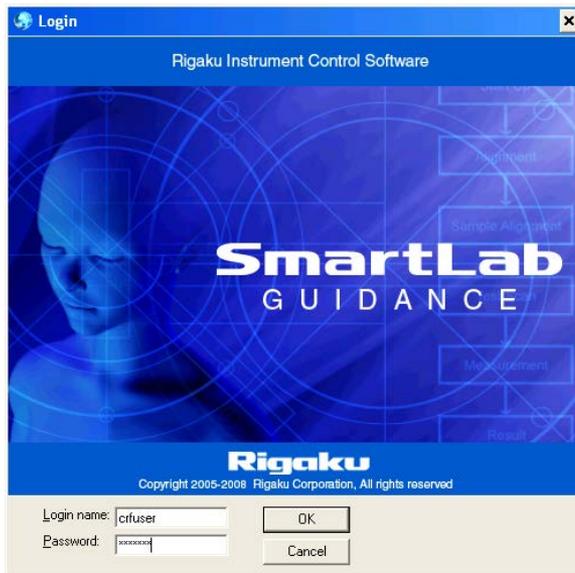
These notes are meant to serve as an aid to assist users who have been trained and certified by MCC Staff. If ever you are unsure about the correct operation of the instrument or any of its components, please consult a MCC staff member before continuing. Never use equipment that you are not trained and approved to use.

Before using the MCC, please review the MCC User Handbook available through our website.

SmartLab XRD SOP

- Open ILab credential before the first training session.
- Discuss with you PI what kind of the samples and possibly mode (PB or BB) you will be using XRD or possibly both.
- BB (Bragg-Brentano) is the classical powder mode for the polycrystalline samples. PB (Parallel Beam) mode utilizes high resolution beam for highly oriented samples e.g the thin films and epitaxial film samples.
- BB and PB mode supplement from Rigaku is attached to this training.

Locate and Open SmartLab Guidance icon from the Desktop.
Program might be open so you skip this step



Log in name: crfuser
Password: crfuser

Note: credentials to the computer is the same (in case you have an issue with SmartLab Guidance and you need to restart the computer.)

Program opens in the following format. Selecting the right package BB or PB based on your sample.

1-3. Perform the Optics Alignment, Sample Alignment and Measurements.



Locate the right package for your measurements

The screenshot displays the SmartLab Guidance software interface. The main window title is "SmartLab Guidance - crfuser(System User)". The interface includes a menu bar (File, Edit, Tasks, View, Control, Process, Options, Window, Help), a file tree on the left, a control panel with buttons for "Save as...", "Set default conditions", "Startup...", "Shutdown...", and "Run", and a status table at the bottom left. The status table lists various parameters and their current values.

Item	Status	Offset
Theta/2-Theta	0.0000 deg	-
2-Theta	0.0000 deg	-0.111
Omega	0.0000 deg	-0.096
Phi	0.0000 deg	0.000
2-ThetaChi	0.0000 deg	0.000
Z	-0.09606 mm	-
Rx	0.0000 deg	-
Ry	0.0000 deg	-
Attenuator	Open	-
Incident slit	2.209mm	-
Receiving slit # 1	1.314mm	-
Receiving slit # 2	0.300mm	-
Shutter	Close	-
Tube voltage	-	-
Tube current	-	-
HV # 1	621.0 V	-
PHA baseline # 1	510.00 mV	-
PHA window # 1	950.00 mV	-
Count mode # 1	Differential	-

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GUIDANCE
Rigaku Instrument Control Software

BB (Bragg-Brentano) package is chosen here

The screenshot displays the SmartLab Guidance software interface. The main window title is "SmartLab Guidance - crfuser(System User)". The interface includes a menu bar (File, Edit, Tasks, View, Control, Process, Options, Window, Help), a tree view on the left showing various measurement packages, and a central control panel. The "General (Bragg-Brentano focusing)" package is selected in the tree view. The control panel shows a sequence of steps: "1 Optics Alignment (BB)", "2 Sample Alignment (BB)", and "3 General Measurement (BB)". The status bar at the bottom indicates "For Help, press F1".

Reflection SAXS (medium resolution PE)
General Measurement
General (Bragg-Brentano focusing)
General (Bragg-Brentano focusing) D/h
General (medium resolution PB/P5A)
General (medium resolution PB)
General (high resolution PB-Ge(220)K2)
General (high resolution PB-Ge(400)K2)
General (ultra-high resolution PB-Ge(22)
General (ultra-high resolution PB-Ge(44)
In-Plane General (medium resolution PE)
In-Plane General (high resolution PB-Ge(220)K2)
In-Plane General (high resolution PB-Ge(400)K2)

SIC2b.scp c:\Dmitri\>

Save as... Set default conditions

Startup... Run

Shutdown...

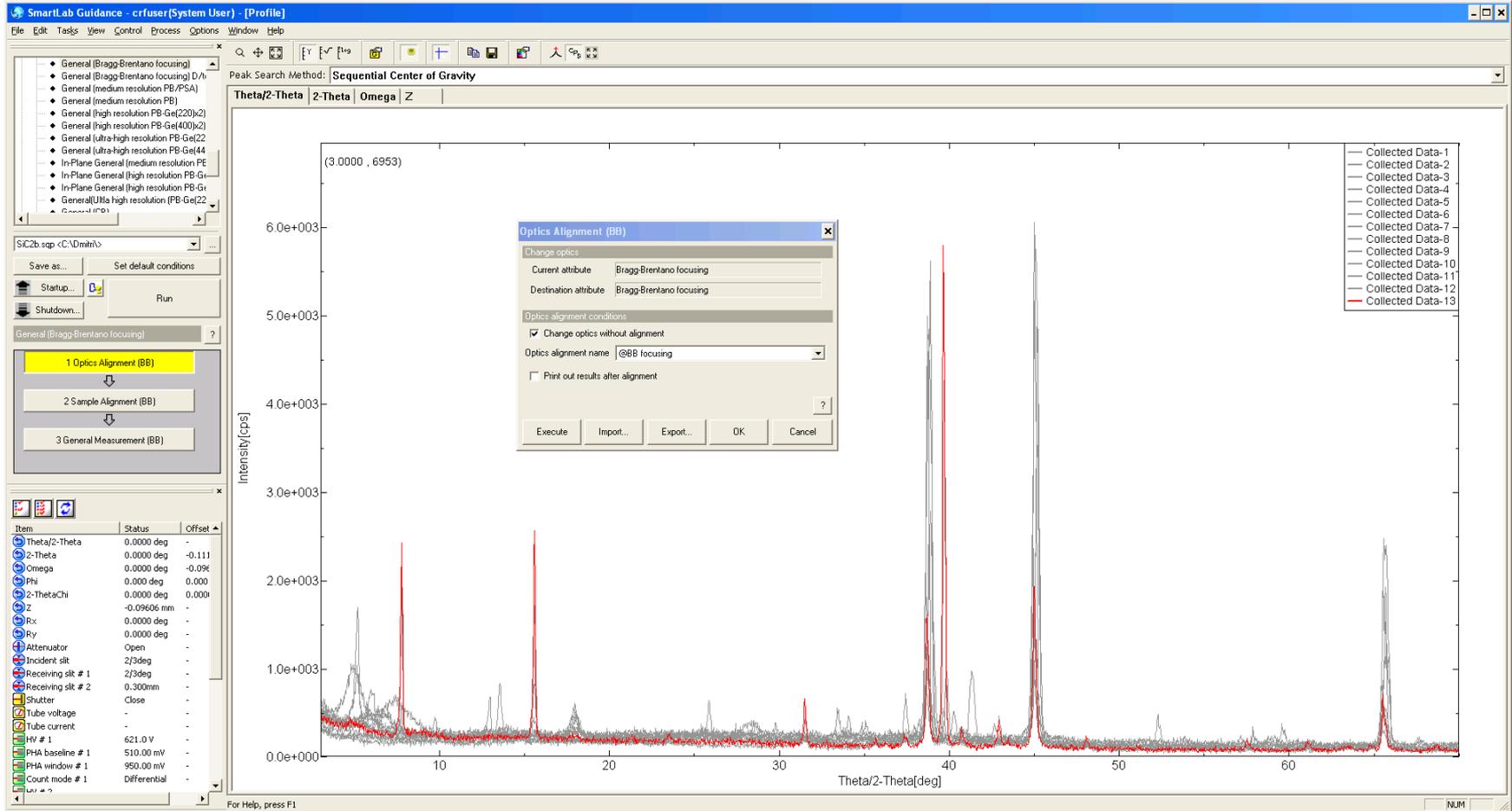
General (Bragg-Brentano focusing) ?

1 Optics Alignment (BB)
2 Sample Alignment (BB)
3 General Measurement (BB)

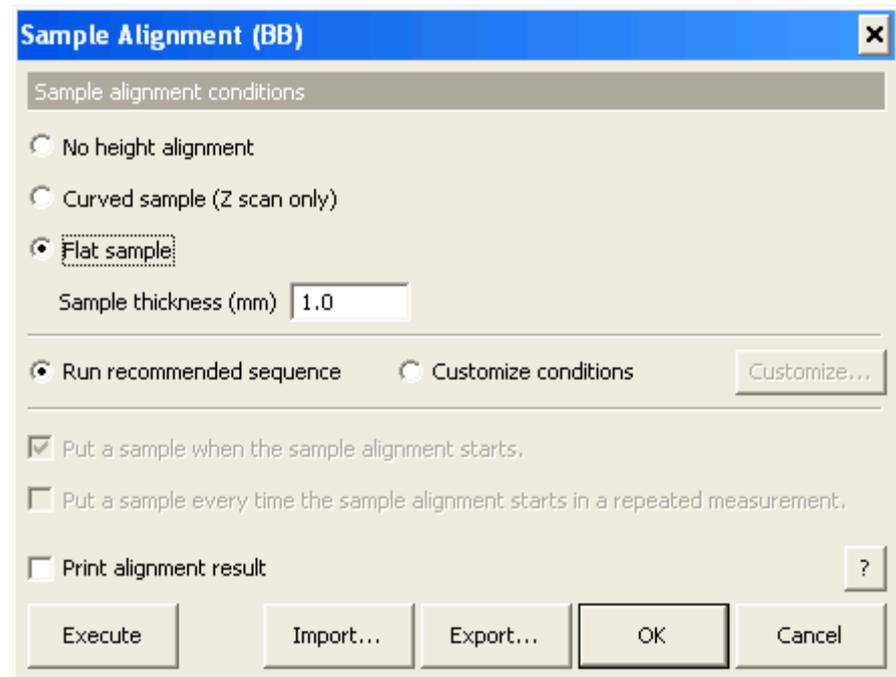
Item	Status	Offset
Z	-0.09606 mm	-
Rx	0.0000 deg	-
Ry	0.0000 deg	-
Attenuator	Open	-
Incident slit	2.209mm	-
Receiving slit # 1	1.314mm	-
Receiving slit # 2	0.300mm	-
Shutter	Close	-
Tube voltage	-	-
Tube current	-	-
HV # 1	621.0 V	-
PHA baseline # 1	510.00 mV	-
PHA window # 1	950.00 mV	-
Count mode # 1	Differential	-
HV # 2	-	-
PHA baseline # 2	-	-
PHA window # 2	-	-
Count mode # 2	-	-
HV # 3	-	-
PHA baseline # 3	-	-

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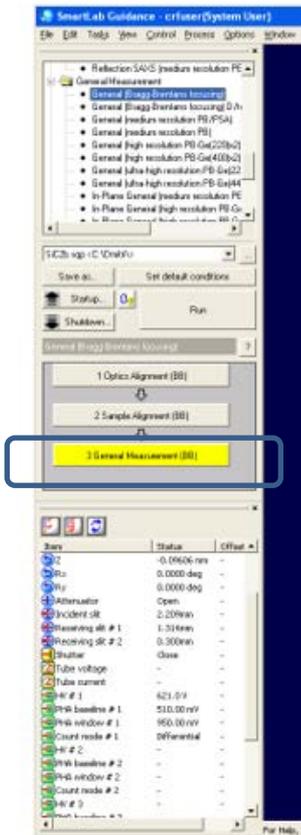
NUM



Perform the Sample alignment Step 2



Sample Measurement with the acquisition parameters



General Measurement (BB)

Save measurement data

File name: C:\XRD Data\Chris\COVID\W4C3_LiF_HCl_20wtequiv_5days_sonic_s ...

Sample name:

Memo:

Manual exchange slit conditions: Soller/PSC (deg) 5.0, IS L (mm) 10.0, PSA (deg) Open, Soller (deg) 5.0, Read current slits

Monochromatization: K beta filter method, Diffracted beam monochromator method

Detector mode: 1D

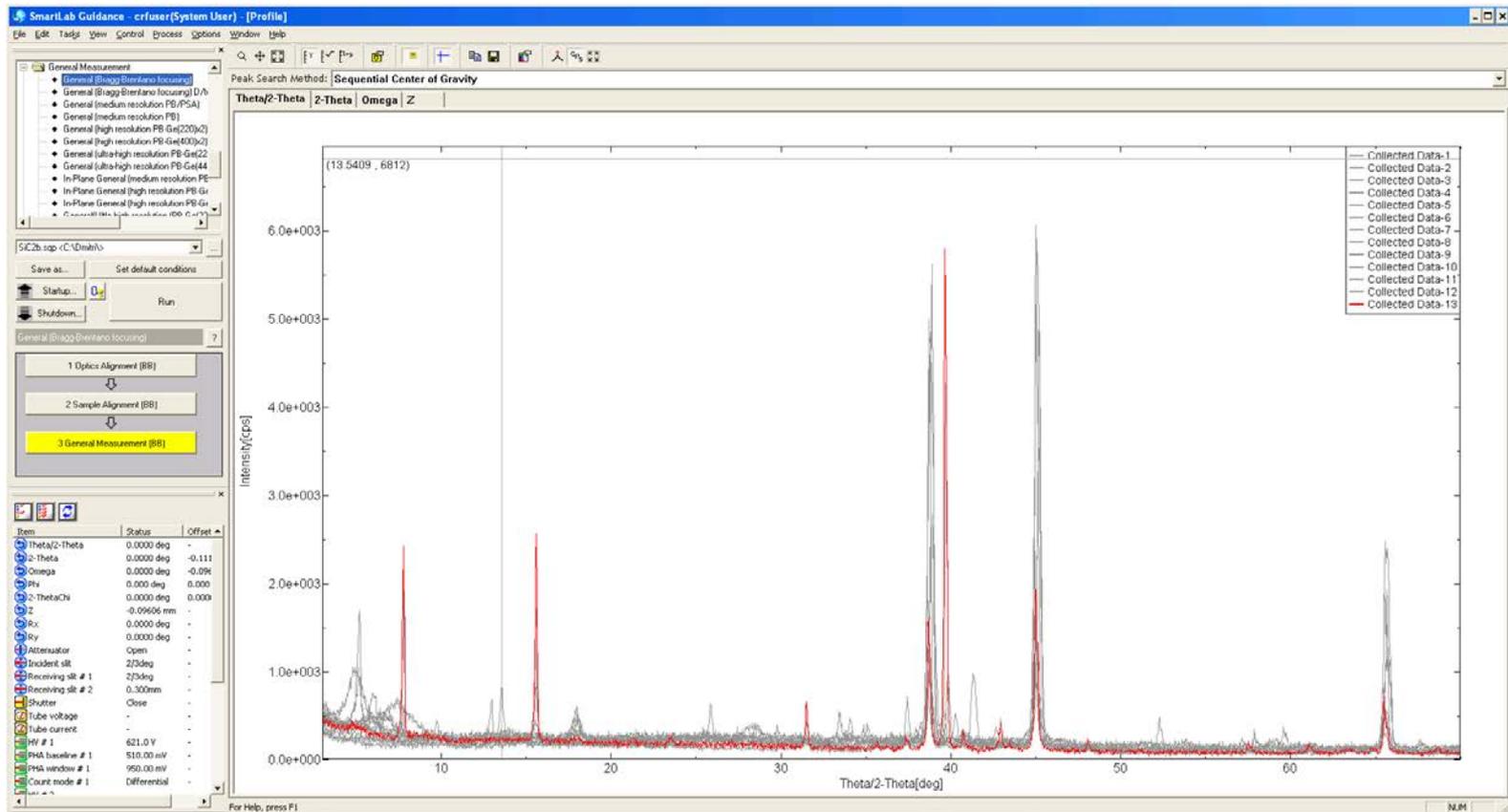
Exec.	Scan axis	Mode	Range	Start (deg)	Stop (deg)	Step (deg)	Speed Duration time	IS deg	RS1 deg	RS2 mm	Attenuator	Comment	Options	Voltage (kV)	Current (mA)
<input type="checkbox"/>	Theta/2-Theta	Step	Absolute	5.0000	80.0000	0.0200	0.50	2/3	2/3	0.300	Auto		Set...	0	0
<input checked="" type="checkbox"/>	Theta/2-Theta	Step	Absolute	3.0000	70.0000	0.0300	0.50	2/3	2/3	0.300	Auto		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30
<input type="checkbox"/>	Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	2/3	2/3	0.300	Open		Set...	40	30

Drive the 4 axes to the current zero positions after the measurement completed.

Calculated scan duration : 00:18:37

Execute Import... Export... OK Cancel

Example of the performed scan



PB (Parallel Beam) Medium Resolution Package is chosen here

The screenshot displays the SmartLab Guidance software interface. The title bar reads "SmartLab Guidance - crfuser(System User)". The menu bar includes "File", "Edit", "Tasks", "View", "Control", "Process", "Options", "Window", and "Help".

The left-hand panel shows a tree view of measurement packages. The "General (medium resolution PB)" package is selected and highlighted in blue. Other packages listed include "Reflection SAXS (medium resolution PE)", "General Measurement", "General (Bragg Brentano focusing)", "General (Bragg Brentano focusing) D/h", "General (medium resolution PB/P5A)", "General (high resolution PB-Ge(220)k2)", "General (high resolution PB-Ge(400)k2)", "General (ultra-high resolution PB-Ge(22)", "General (ultra-high resolution PB-Ge(44)", "In-Plane General (medium resolution PE)", and "In-Plane General (high resolution PB-Ge)".

Below the tree view, the file path is "G:\D exp <C:\VRD Data\Zhengtao\Yaobo\...", and there are buttons for "Save as...", "Set default conditions", "Startup...", "Shutdown...", and "Run".

The main area shows a workflow diagram with three steps: "1 Optics Alignment (PB)", "2 Sample Alignment", and "3 General Measurement". The "3 General Measurement" step is highlighted in yellow.

At the bottom left, there is a table with columns "Item", "Status", and "Offset".

Item	Status	Offset
Z	-0.09606 mm	-
Rx	0.0000 deg	-
Ry	0.0000 deg	-
Attenuator	Open	-
Incident slit	2.209mm	-
Receiving slit # 1	1.314mm	-
Receiving slit # 2	0.300mm	-
Shutter	Close	-
Tube voltage	-	-
Tube current	-	-
HV # 1	621.0 V	-
PHA baseline # 1	510.00 mV	-
PHA window # 1	950.00 mV	-
Count mode # 1	Differential	-
HV # 2	-	-
PHA baseline # 2	-	-
PHA window # 2	-	-
Count mode # 2	-	-
HV # 3	-	-
PHA baseline # 3	-	-

The bottom right corner features the "SmartLab GUIDANCE" logo and the text "Rigaku Instrument Control Software". A "NUM" button is visible in the bottom right corner.