



# **SmartLab Studio II XRD Measurement Plugin User Manual**

Rigaku Corporation

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## Notational conventions used in the manuals

This manual uses the following notational conventions:

### Notations for menus, commands, and dialog boxes

Notation	Explanation
<b>File</b> tab	Tab names are given in bold.
<b>Open</b> command under the <b>File</b> tab	Command names are given in bold, followed by the name of the menu on which that command is found.
<b>Open File</b> dialog box	The name that appears in the title bar of the dialog box is given in bold.
<b>OK</b> , <b>Cancel</b>	The names of command buttons and toolbar buttons in the dialog box are given in bold.
Context menu	This popup menu appears when you click the right mouse button.
Tool tip	When a mouse pointer is dragged over a toolbar button or a text box, a description is displayed for five seconds.
Active window	This is the window brought up to front of the screen or main window. An active window accepts entries of characters or figures and mouse operations.

### Notations for mouse operations

Notation	Explanation
Point.	Position the mouse pointer directly over the target object.
Click.	Press and immediately release the left mouse button.
Right-click.	Press and immediately release the right mouse button.
Double-click.	Press the mouse twice in rapid succession.
Drag.	Hold down the left mouse button and move the mouse.
Drag & drop.	Hold down the left mouse button down and move the mouse, releasing the mouse button at the target position.
Check/Uncheck the (check)box.	Click select(  or  ) /deselect(  ) the checkbox.

### Notations for keyboard operations

Notation	Explanation
<b>Enter</b> key	Key names appear as bold text.
<b>Alt + F1</b> keys	The plus sign (+) indicates that you should depress multiple keys simultaneously. For example, <b>Alt + F1</b> means to hold down the <b>Alt</b> key and press the <b>F1</b> key at the same time.
<b>Alt, W, S</b> keys	When multiple keys are shown separated by a comma (,), press the keys in the order shown. In the example at left, press the <b>Alt</b> , <b>W</b> , and <b>S</b> keys in this order.
Arrow keys	Keys labeled→, ←, ↑, and ↓.

## About the screen display

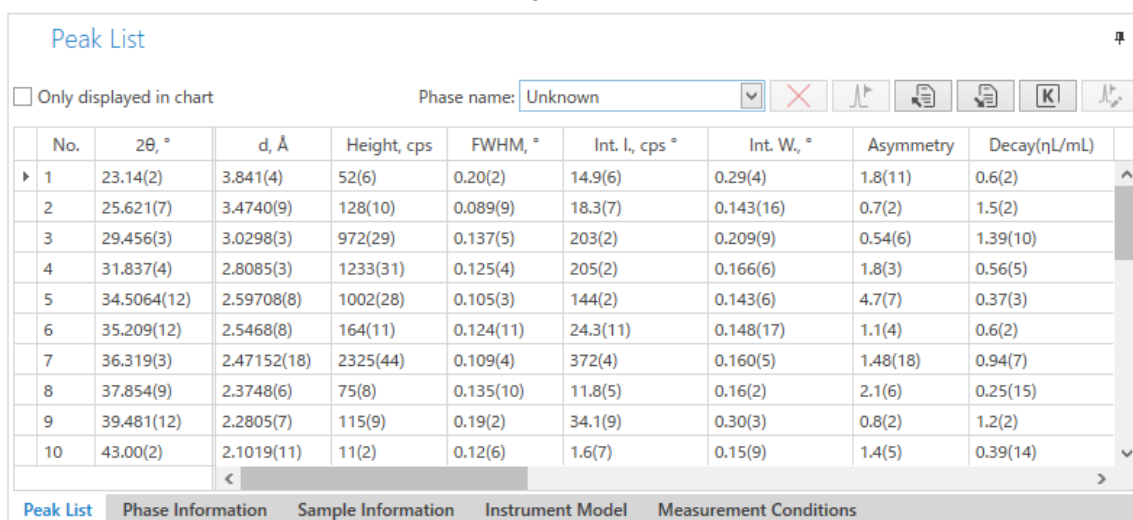
- The screen displays and display images describing execution results in this manual are examples recurring under the specific settings.
- In most cases, the descriptions in this manual are based on default conditions. Therefore, the actual windows and dialog boxes on your screen may differ from those shown in this manual.
- Also note that the screen images shown in this manual may differ slightly from the actual windows and dialog boxes on your screen.

## About the units

The units used in this software are in principle based on the International System of Units. The unit of length "Å", however, is sometimes used in this software because it is widely used as the unit of wavelength, chemical bond length, etc. Also note that  $1 \text{ Å} = 0.1 \text{ nm}$ .

## About the number display

SmartLab Studio II estimates the E. S. D. (estimated standard deviation) for each value obtained by the least squares refinement. The estimated standard deviation is enclosed in parentheses and attached to each value in the windows and dialog boxes of SmartLab Studio II.



No.	2θ, °	d, Å	Height, cps	FWHM, °	Int. I., cps	Int. W., °	Asymmetry	Decay(ηL/mL)
1	23.14(2)	3.841(4)	52(6)	0.20(2)	14.9(6)	0.29(4)	1.8(11)	0.6(2)
2	25.621(7)	3.4740(9)	128(10)	0.089(9)	18.3(7)	0.143(16)	0.7(2)	1.5(2)
3	29.456(3)	3.0298(3)	972(29)	0.137(5)	203(2)	0.209(9)	0.54(6)	1.39(10)
4	31.837(4)	2.8085(3)	1233(31)	0.125(4)	205(2)	0.166(6)	1.8(3)	0.56(5)
5	34.5064(12)	2.59708(8)	1002(28)	0.105(3)	144(2)	0.143(6)	4.7(7)	0.37(3)
6	35.209(12)	2.5468(8)	164(11)	0.124(11)	24.3(11)	0.148(17)	1.1(4)	0.6(2)
7	36.319(3)	2.47152(18)	2325(44)	0.109(4)	372(4)	0.160(5)	1.48(18)	0.94(7)
8	37.854(9)	2.3748(6)	75(8)	0.135(10)	11.8(5)	0.16(2)	2.1(6)	0.25(15)
9	39.481(12)	2.2805(7)	115(9)	0.19(2)	34.1(9)	0.30(3)	0.8(2)	1.2(2)
10	43.00(2)	2.1019(11)	11(2)	0.12(6)	1.6(7)	0.15(9)	1.4(5)	0.39(14)

The number in parentheses attached to the refined value has the following meaning.

1. When the number inside the parentheses has one figure digit  
Indicates that the last digit of the refined numerical value has a deviation about the number in parentheses. For example, in the case of "12.345(6)", indicates that the last digit "5" of the refined value "12.345" will have a deviation of "±6".  
That is, "12.345(6)" means  $12.345 \pm 0.006$
2. When the number inside the parentheses has two figure digits  
Indicates that the last two digits of the refined numerical value has a deviation about the number in parentheses. For example, in the case of "98.7(12)", indicates that the last two digits "87" of the refined value "98.7" will have a deviation of "±1.2".  
That is, "98.7(12)" means  $98.7 \pm 1.2$ .



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# 1 Overview

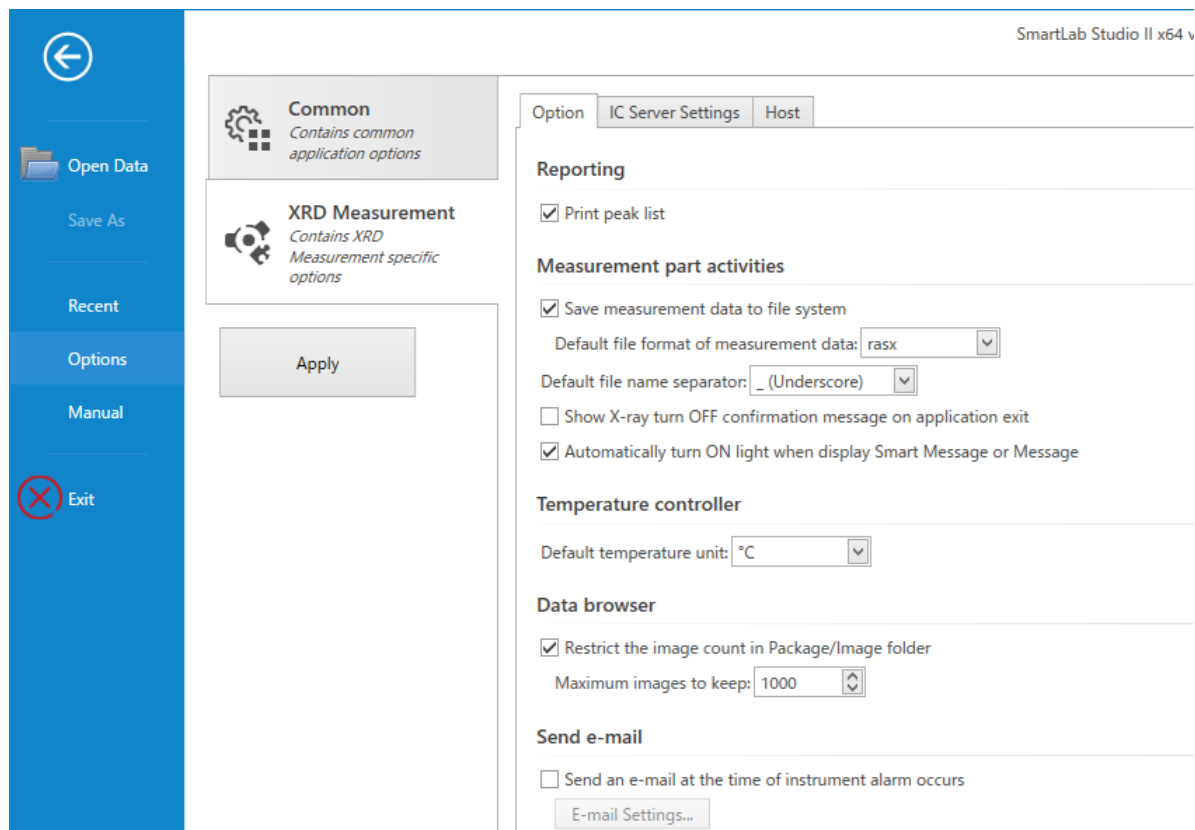
## 1.1 Functions of the XRD Measurement plugin

The XRD Measurement plugin enables user-friendly X-ray diffraction and X-ray reflectivity measurements, using X-ray diffractometers (in this instruction manual, the SmartLab automated multipurpose X-ray diffractometer is used as an example).

The SmartLab Studio II software automatically selects the appropriate optics system and sets measurement conditions after the user chooses an analytical purpose and enters basic sample conditions. Processes of optics and sample alignment and data measurement are provided as “Package measurement”, allowing the user to acquire data easily for various types of analyses simply by changing optical devices and mounting samples as guided by onscreen prompts. The optical devices used with SmartLab are equipped with sensors to allow the SmartLab Studio II software to detect and recognize the optical device type. This prevents incorrect selection of slits or analyzer and assures that measurements are performed under ideal conditions.

## 1.2 Setting the XRD Measurement plugin

The settings for the XRD Measurement plugin are located on **File – Options – XRD Measurement** tab on the Ribbon.



The settings are divided into three tabs.

Option	This tab provides settings regarding reporting and measurement Part Activities.
IC Server Settings	This tab provides settings regarding the IC server.
Host	This tab provides settings regarding the host communication. (the settings for the systems linked with the host computer only)

The settings that can be made on each tab are explained in the following subsections.

### 1.2.1 Option tab

Settings regarding reporting and measurement Part Activities can be set on this tab.

Option IC Server Settings Host

**Reporting**

☒ Print peak list

**Measurement part activities**

☒ Save measurement data to file system

Default file format of measurement data:

Default file name separator:

☐ Show X-ray turn OFF confirmation message on application exit

☒ Automatically turn ON light when display Smart Message or Message

**Temperature controller**

Default temperature unit:

**Data browser**

☒ Restrict the image count in Package/Image folder

Maximum images to keep:

**Send e-mail**

☐ Send an e-mail at the time of instrument alarm occurs

[E-mail Settings...](#)

#### Print peak list

Select this checkbox to include peak search results when printing measurement data (only when peak search was performed).

#### Save measurement data to file system

Select this checkbox to save measurement data always to the file system when saving measurement data from Part Activities.

#### Default file format of measurement data

Select either **rasx**, **ras**, or **asc** as default file format of measurement data when saving data from Part Activities.

#### Default file name separator

Select **\_ (Underscore)** or **- (Hyphen)** as a delimiter between a file name of measurement data and character string automatically added.

#### Show X-ray turn OFF confirmation message on application exit

Select this checkbox to show a confirmation message asking whether to turn off X-rays or not before shutting down the application.

#### Automatically turn ON light when display Smart Message or Message

Select this check box to let the light turn on automatically when SmartMessage or any other message is displayed.

#### Default temperature unit

Select either **°C** or **K** as the default temperature unit used in XRD Measurement.

**Restrict the image count in Package/image folder**

Restricts the number of the images obtained in 2D measurement, to be displayed in the **Package** of the **Data Browser** in order to prevent decline in responsiveness and malfunctioning caused by exceeding of the PC's memory capacity when many images are measured.

**Maximum images to keep**

Sets the number of the images, obtained with 2D measurement, displayed in the **Package** of the **Data Browser**.

**Send an e-mail at the time of instrument alarm occurs**

Select this checkbox to send instrument alarm information to the address set in the **E-mail Settings** dialog box when the instrument alarm occurs.

**E-mail Settings**

Opens the **E-mail Settings** dialog box. This dialog box is used to set the e-mail address for sending notification when the instrument alarm occurs.

### 1.2.2 IC Server Settings tab

Settings regarding the IC server can be set on this tab.



Option IC Server Settings Host

☒ Connect the IC Server

IP address (default is "localhost") :

localhost

#### Connect the IC Server

Select this checkbox to connect the currently running SmartLab Studio II with the IC server. Normally, this checkbox is selected.

#### IP address

Enter the IP address of the PC for running the IC server. If the IC server runs on the same PC that is used for SmartLab Studio II, enter **"localhost"**.



**CAUTION:** In this version, do not change the default settings (checkbox selected, IP address set to "localhost").





## 2 Starting up the SmartLab Studio II

Before using the SmartLab Studio II, turn on the power of the SmartLab control PC and the SmartLab main unit.



**CAUTION:** For details on how to turn on the SmartLab main unit, refer to the Quick start guide.

- (1) Double-click the **SmartLab Studio II** shortcut icon on the desktop. The login window appears.



- (2) Enter the user name (login name) and password in the **Login** and **Password** boxes, respectively, and click the **Login** button.



**CAUTION:** • Set your password when you log in for the first time.

- To log in in audit trails & ER/ES system mode, select the **Audit Trails & ER/ES System** check box on the login screen.

The SmartLab Studio II will launch and the main window will appear. (Wait 30 to 60 seconds until it opens.)



- (3) Click the **XRD Measurement** tab to display the XRD Measurement plugin panel.

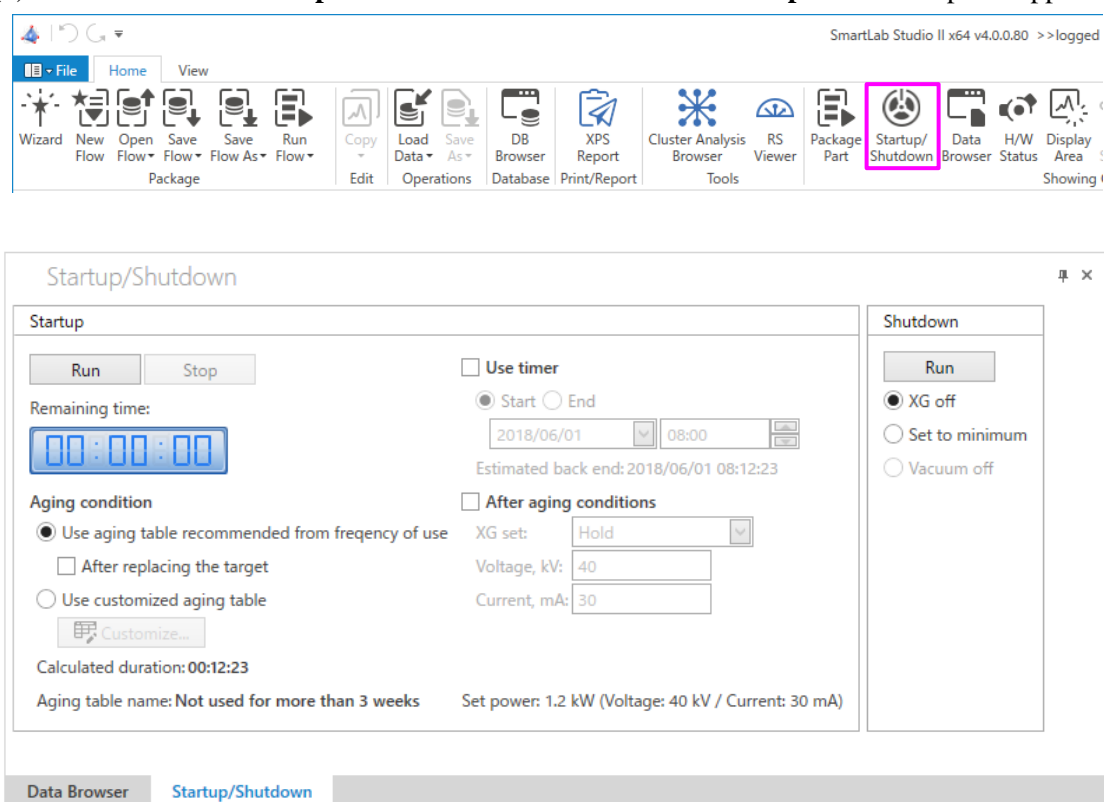
## 3 Turning on X-rays

### 3.1 Aging

Set the aging conditions of the X-ray generator. The term "aging" refers to the warming-up operation of the X-ray generator. Perform aging according to the usage frequency of X-ray generator.

#### 3.1.1 Performing aging under the recommended conditions

- (1) Click **Home – Startup/Shutdown** on the Ribbon. The **Startup/Shutdown** panel appears.

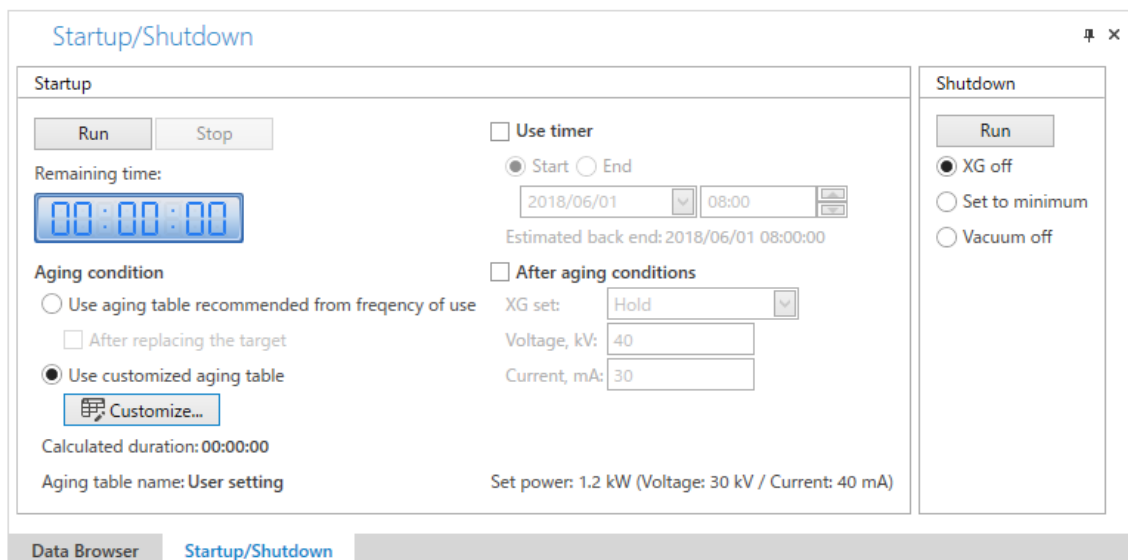


- (2) Select **Use aging table recommended from frequency of use**.

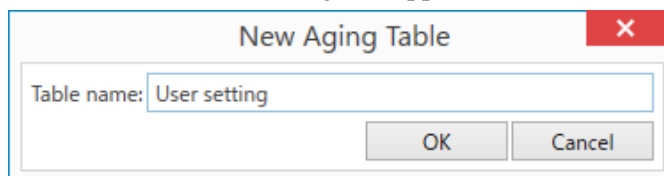
### 3.1.2 Creating an aging table

The user can create and save an aging table without using the aging table optimized for usage frequency and X-ray generator type.

- (1) Click **Home – Startup / Shutdown** on the Ribbon. The **Startup / Shutdown** panel appears.



- (2) Select **Use customized aging table** and click **Customize**. The **Edit Aging Table** dialog box appears.
- (3) Click **New**. The **New Aging Table** dialog box appears.



- (4) Enter any name in the **Table name** box. Click **OK** to close the dialog box.
- (5) Enter the value in the table below in the **Edit Aging Table** dialog box.

No.	Voltage (kV)	Current (mA)	Holding time (min.)
1	20	10	2.0
2	30	10	2.0
3	40	10	2.0
4	40	20	5.0
5	40	30	5.0

Customize - Aging Table ✕

User setting ▼ New... Delete

Total time: 00:16:24

No.	Voltage, kV	Current, mA	Holding time, min
1	20	10	2.0
2	30	10	2.0
3	40	10	2.0
4	40	20	5.0
▶ 5	40	30	5.0

Add Remove Up Down

OK Cancel

- (6) Click the **OK** button. The aging table is created and the dialog box will close.

### 3.1.3 Performing aging using a timer

The user can set the aging starting time.

- (1) Click **Home – Startup / Shutdown** on the Ribbon. The **Startup / Shutdown** panel appears.

The screenshot shows the 'Startup/Shutdown' panel with two main sections: 'Startup' and 'Shutdown'.

**Startup Section:**

- Buttons: 'Run' and 'Stop'.
- Remaining time: A digital display showing '00:00:00'.
- Aging condition:
  - ☒ Use aging table recommended from frequency of use
  - ☐ After replacing the target
  - ☐ Use customized aging table (with a 'Customize...' button)
- Calculated duration: 00:12:23
- Aging table name: Not used for more than 3 weeks
- Use timer: ☒ (with radio buttons for 'Start' and 'End', and date/time pickers set to 2018/06/01 08:00)
- Estimated back end: 2018/06/01 08:12:23
- After aging conditions: ☐ (with input fields for XG set: Hold, Voltage, kV: 40, and Current, mA: 30)
- Set power: 1.2 kW (Voltage: 40 kV / Current: 30 mA)

**Shutdown Section:**

- Buttons: 'Run'.
- Options:
  - ☒ XG off
  - ☐ Set to minimum
  - ☐ Vacuum off

At the bottom, there is a ribbon with 'Data Browser' and 'Startup/Shutdown' tabs.

- (2) Select the **Use timer** checkbox.
- (3) Select **Start** and set the date and time.
- (4) Click the **Run** button. The aging will start at the specified date and time.



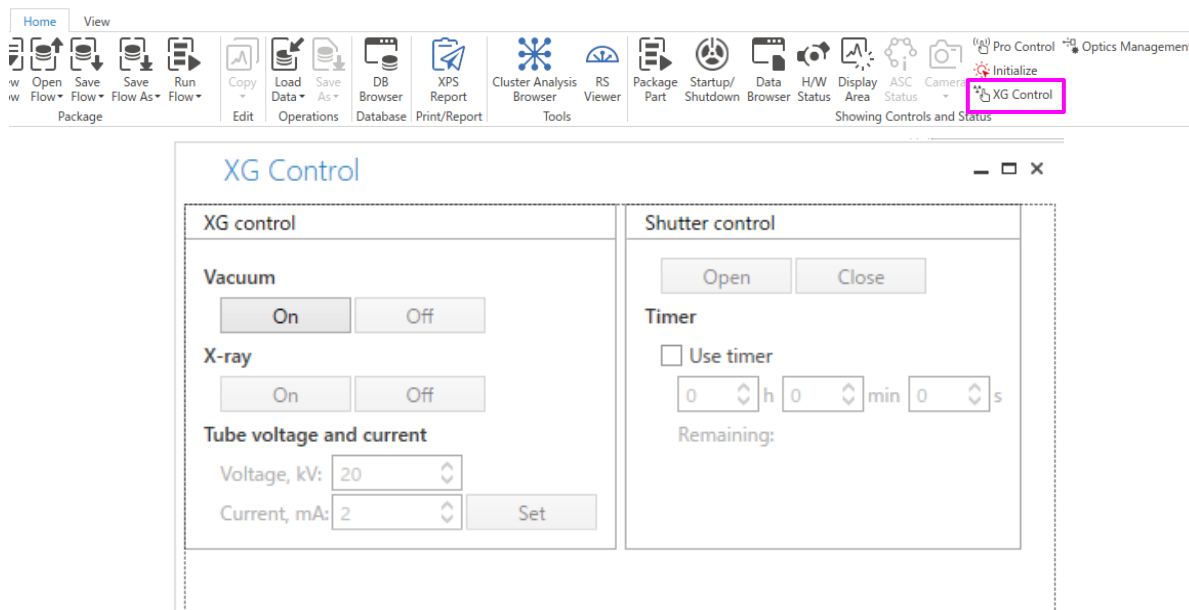
Tip: To set the aging ending time, select **End** in step (3) and set the date and time.

## 3.2 Controlling the XG manually

The following functions of the X-ray generator (XG) can be controlled manually.

- Starting/stopping vacuum control
- Turning X-ray generation ON/OFF
- Setting tube voltage and tube current

(1) Click **Home – XG Control** on the Ribbon. The **XG Control** panel appears.



(2) Click the **On** button under **Vacuum**.



- Tip:
- There is no need to click the **On** button when using the X-ray diffractometer with the sealed-off X-ray tube X-ray generator.
  - There is no need to click the **On** button when the vacuum control is already started.

(3) Click the **On** button under **X-ray**.



- Tip: There is no need to click the **On** button when the X-ray generation is already on.

(4) Under **Tube voltage and current**, enter "**40**" and "**30**" in the **Voltage** and **Current** boxes, respectively and then click the **Set** button.

(5) Click **Home - H/W Status** on the Ribbon. The **H/W Status** panel appears. Confirm that the voltage and current are displayed as set.

X-ray generator	
Vacuum	On
X-ray	On
Shutter	Close
Tube voltage	20 kV
Tube current	10 mA
IG voltage	1.64E-5 Pa

X-ray generator	
Vacuum	On
X-ray	On
Shutter	Close
Tube voltage	40 kV
Tube current	30 mA
IG voltage	1.64E-5 Pa

### 3.3 Controlling the shutter

The shutter can be opened only when the door is closed while the power of the X-ray generator and X-ray generation is on.

#### 3.3.1 Opening and closing the shutter

Open and close the shutter manually, following the procedure below.



**CAUTION:** Do not open the shutter manually for the purposes other than maintenance.  
Exposure of the detector to the high intensity X-ray may shorten its service life.

- (1) Click **Home - H/W Status** on the Ribbon. The **H/W Status** panel appears. Confirm that the **X-ray** is **On** on the **H/W Status** panel.

X-ray generator	
Vacuum	On
X-ray	On
Shutter	Close
Tube voltage	20 kV
Tube current	10 mA
IG voltage	1.64E-5 Pa

- (2) Click **Home – XG Control** on the Ribbon. The **XG Control** panel appears.

- (3) Click the **Open** button under **Shutter control** to open the shutter.
- (4) Click the **Close** button under **Shutter control** to close the shutter.



### 3.3.2 Open the shutter for 10 seconds

Open the shutter manually. The shutter closes after the set period of time.



**CAUTION:** Do not open the shutter manually for the purposes other than maintenance.  
Exposure of the detector to the high intensity X-ray may shorten its service life.

- (1) Click **Home - H/W Status** on the Ribbon. The **H/W Status** panel appears.  
Confirm that the X-ray is **On** on the **H/W Status** panel.

▲ X-ray generator	
☼ Vacuum	On
☼ X-ray	On
☼ Shutter	Close
☼ Tube voltage	20 kV
☼ Tube current	10 mA
☼ IG voltage	1.64E-5 Pa

- (2) Click **Home – XG Control** on the Ribbon. The **XG Control** panel appears.

XG Control
— □ ×

**XG control**

**Vacuum**

**X-ray**

**Tube voltage and current**

Voltage, kV:

Current, mA:

**Shutter control**

**Timer**

☒ Use timer

h
  min
  s

Remaining:

- (3) Select the **Use timer** checkbox and enter "10" in the s box.
- (4) Click the **Open** button to open the shutter.

▲ X-ray generator	
☼ Vacuum	On
☼ X-ray	On
☼ Shutter	Open
☼ Tube voltage	40 kV
☼ Tube current	30 mA
☼ IG voltage	1.58E-5 Pa

- (5) The shutter will close in 10 seconds.



## 4 Performing Measurements

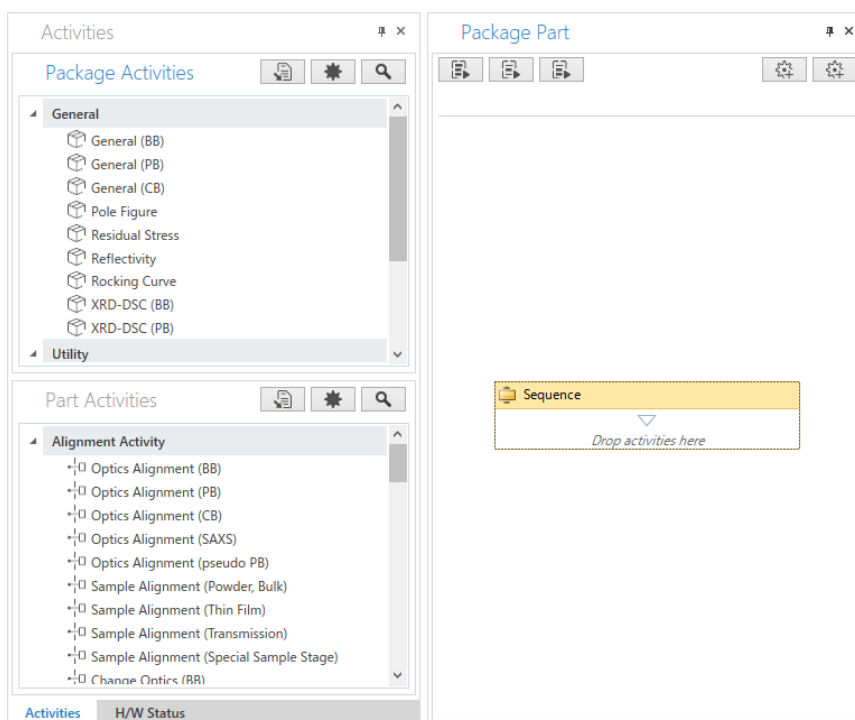
A package activity bundles optics alignment, sample alignment and data measurement process for each sample evaluation purposes. In a package activity, data collection can be done easily by setting simple conditions for the sample, changing optical devices, and mounting the sample, according to the message displayed on the screen.

A user-defined flow can also be created by registering optics alignment activities, sample alignment activities, and measurement activities included in each Package Activity.

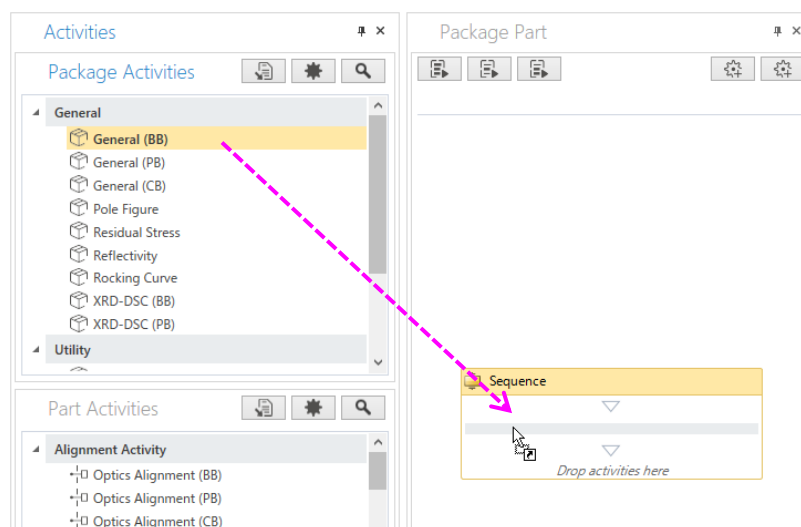
### 4.1 Using Package Activities for measurements

#### 4.1.1 Selecting a Package Activity

- (1) Click **Home – Package Part** on the Ribbon. The **Package Part** panel and the **Activities** panel appear.



- (2) Click **General – General (BB)** in **Package Activities** and drag and drop it to the **Sequence** to add it.



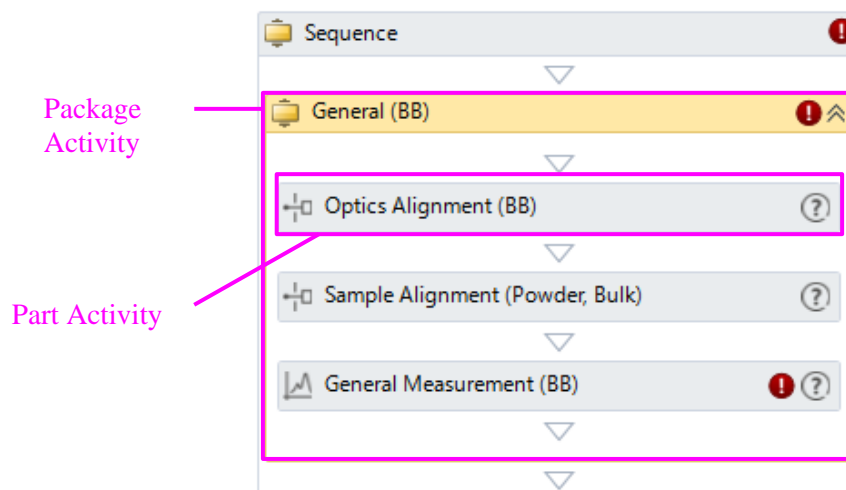
### 4.1.2 Specifying package conditions

Specify conditions of each Part Activity displayed on the **Sequence** panel.

In this manual, the **General (BB)** Package Activity is used as an example.




Tip: To display the conditions settings dialog box of the Part Activity, click the Part Activity on the **Sequence** panel.

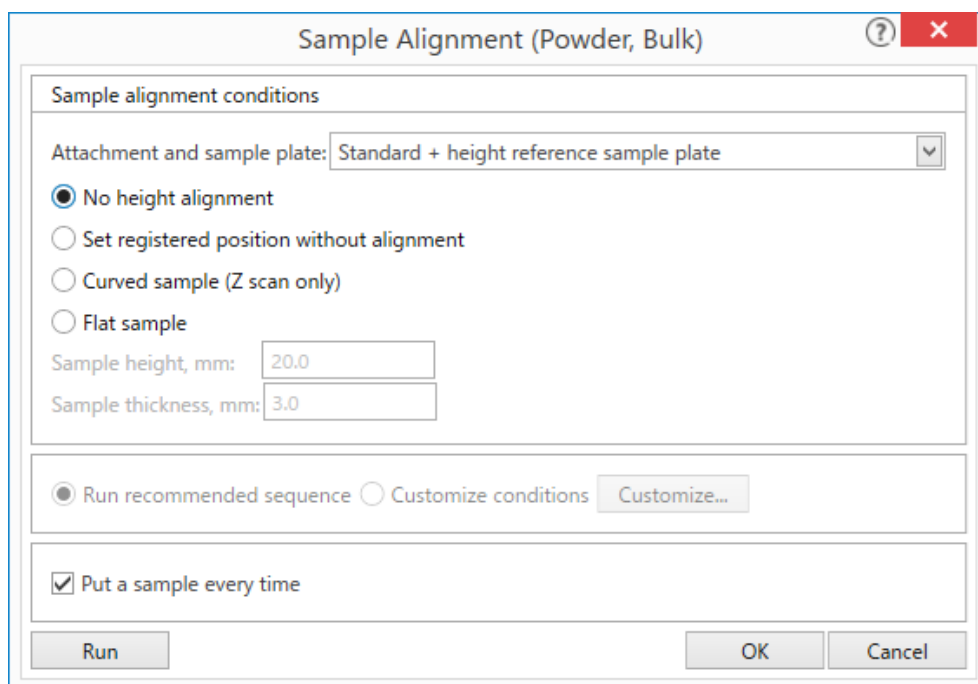


- (1) Set the conditions of the Part Activity in the **Optics Alignment (BB)** dialog box.
  1. When you change the optical components and devices to be used in the alignment, select **Customize optics** and click the **Customize** button.
  2. Select **Full** if you perform the alignment from the beginning. Select **Quick (only receiving optics)** if you perform the quick alignment based on the past alignment results.
  3. Select the name to register the alignment results from the **User settings** box, or click the **New** button and enter a new registration name.




Tip: For details on how to specify the conditions, click the  button and refer to the help topic that appears.


- (2) Set the conditions of the Part Activity in the **Sample Alignment (Powder, Bulk)** dialog box.
  1. Select the attachment and sample plate to be used in the alignment.
  2. Select one of the four alignment conditions.
  3. To customize the alignment conditions, select **Customize conditions** and click the **Customize** button.





The dialog box is titled "Sample Alignment (Powder, Bulk)" and features a help icon and a close button in the top right corner. It is divided into several sections. The first section, "Sample alignment conditions", contains a dropdown menu for "Attachment and sample plate" set to "Standard + height reference sample plate". Below this are four radio button options: "No height alignment" (selected), "Set registered position without alignment", "Curved sample (Z scan only)", and "Flat sample". Under these options are two input fields: "Sample height, mm:" with the value "20.0" and "Sample thickness, mm:" with the value "3.0". The second section contains two radio buttons: "Run recommended sequence" (selected) and "Customize conditions", with a "Customize..." button to the right of the second option. The third section has a checked checkbox labeled "Put a sample every time". At the bottom are three buttons: "Run", "OK", and "Cancel".



Tip: For details on how to specify the conditions, click the  button and refer to the help topic that appears.

- (3) Set the conditions of the Part Activity in the **General Measurement (BB)** dialog box.
  1. If you use the manual exchange slit(s) different from the ones used in the alignment, select the **Manual exchange slit conditions** box and select the slit(s) which you are going to use.
  2. To save measurement data, select the **Save measured data** checkbox, click the  button on the right side of the **File name** box and enter a data name in it.

General Measurement (BB)  

☒ Manual exchange slit conditions ☐ K $\beta$  filter condition ☒ Detector conditions

Incident Soller slit: Soller slit 2.5 deg  
 Length-limiting slit: 10 mm  
 Receiving Soller slit: Soller slit 2.5 deg  
 Read Current Optics

K $\beta$  filter: K $\beta$  filter 1D for Cu



Detector: D/teX Ultra 250  
 Monochromator: None  
 Scan mode: 1D(scan)  
 Energy mode: Standard

Measurement conditions

	Exec.	Range	Start, °	Stop, °	Step, °	Speed, °/min	Incident Slit, °	Receiving Slit #1, mm	Receiving Slit #2, mm	Comment	Options
1	<input checked="" type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
2	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
3	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
4	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
5	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
6	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
7	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
8	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
9	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...
10	<input type="checkbox"/>	Absolute	5.0000	80.0000	0.0100	50.0	1/2	20.000	Open		Set...

☒ Save measured data

☐ Separate measured file

File name:  

Sample name:

Memo:

☐ Move to home position after the measurement completed.  
☐ Run real-time search match


Calculated scan durations: 1min 38s

Run OK Cancel

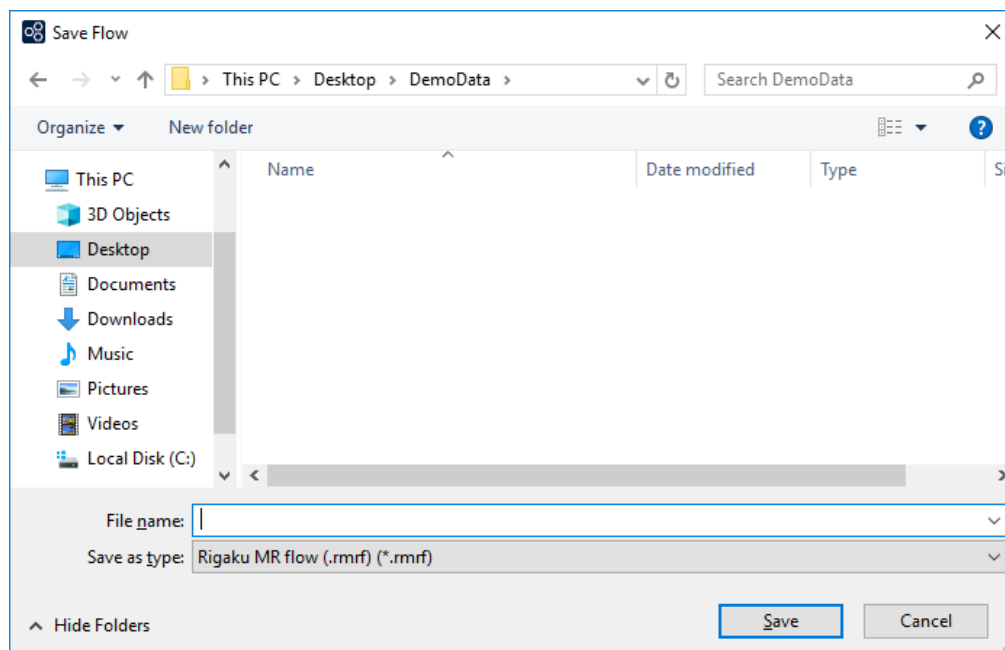


**CAUTION:** If you use the database, all measured data is saved to the database by default. To save the data to the file system, select the **Save measurement data to file system** check box in the **File – Options – XRD Measurement** on the Ribbon. Saving either to the database or to the file system cannot be set in the Part Activity conditions dialog box.



**Tip:** For details on how to specify the conditions, click the  button and refer to the help topic that appears.

- (4) Click **Home – Save flow as – File system** on the Ribbon. The **Save flow** dialog box appears. Save the package activity conditions.



### Scan mode

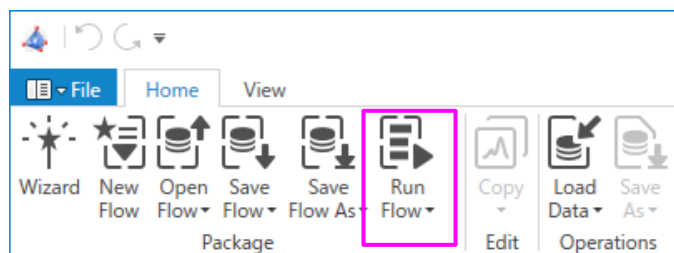
The XRD Measurement plugin contains the following eight scan modes. The options of the **Scan mode** vary based on the installed detector.

Scan mode	Description	Output data	HyPix-3000 /400	D/teX250	SC-70
2D (scan)	TDI scan	Image data Profile data	✓		
2D (Single exposure)	Detector is fixed during measurement.	Image data Profile data	✓		
2D (Multiple exposure)	Exposure and detector's movement are alternately repeated in the scan range.	Image data Profile data	✓		
1D (scan)	TDI scan	Profile data	✓	✓	
1D (Single exposure)	Detector is fixed during measurement..	Profile data	✓	✓	
1D (Multiple exposure)	Detector is fixed during exposure.	Profile data	✓	✓	
0D (continuous)	Continuous scan by 0D mode	Profile data	✓	✓	✓
0D (step)	Step scan by 0D mode	Profile data	✓	✓	✓

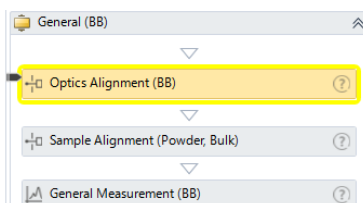
### 4.1.3 Running Package Activity

Prepare the sample and execute the Package Activity according to the procedure described below. When a message to exchange the sample appears while the Package Activity is in process, mount the sample on SmartLab.

- (1) Click **Home - Run Flow** on the Ribbon to execute the Package Activity. The optics alignment, sample alignment, and data measurement Part Activities are performed in sequence.

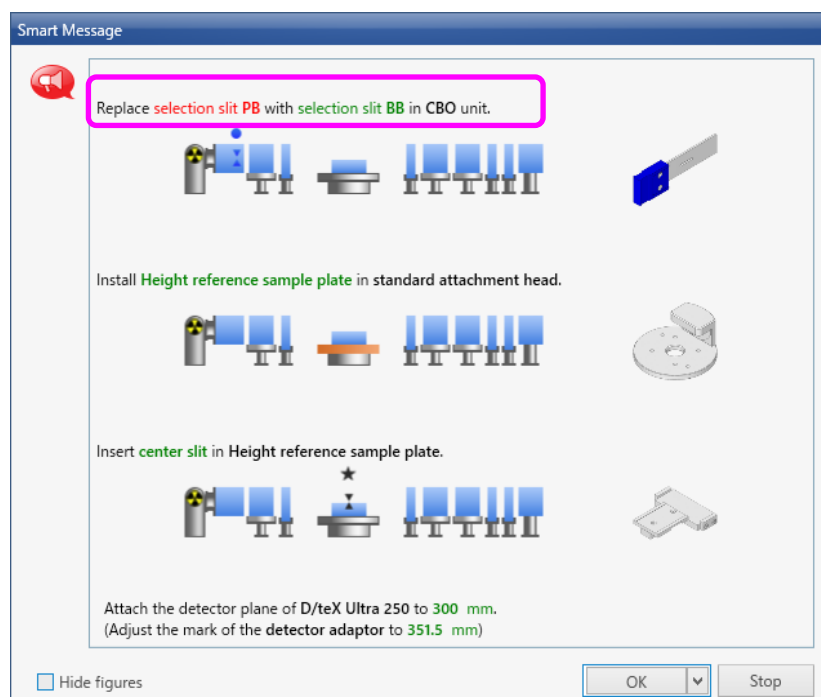


Tip: · The part activity currently running will be highlighted.



- Each part activity can also run alone. For more details, refer to the help of each Part Activity.

- (2) Follow the instruction of the displayed message and execute the Package Activity.  
If a message similar to the following message (Smart Message) appears while the measurement is in process, replace the optics, such as selection slits, according to the procedure described below.





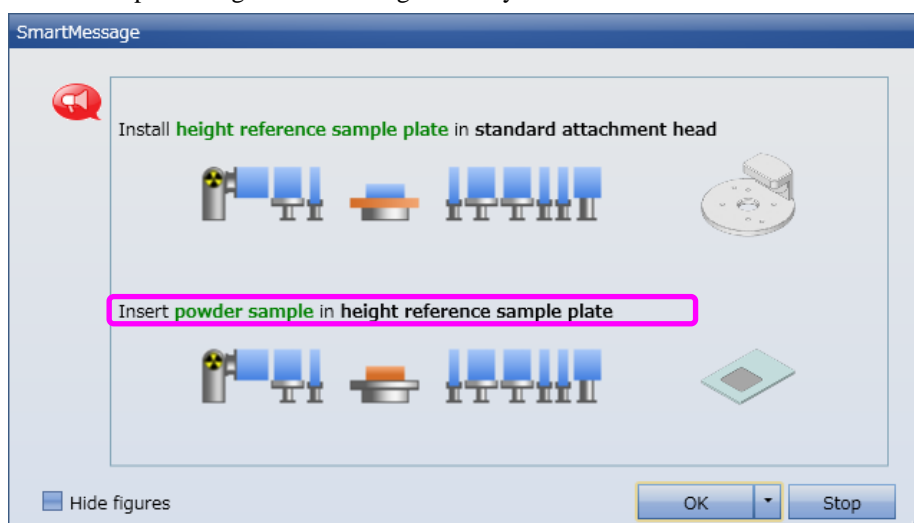
1. Open the door of the radiation enclosure after the alarm beep sound will be heard.
2. Follow the instructions in the **Smart Message** dialog box and replace the optics.
3. Close the door.
4. Click the **OK** button in the **Smart Message** dialog box.
5. The alarm beep sound will stop, and the alignment and measurement will start.



Tip: **Mounting the sample**

When the sample alignment starts, the following **Smart Message** dialog box will appear. Mount the sample according to the instruction in the **Smart Message** dialog box.

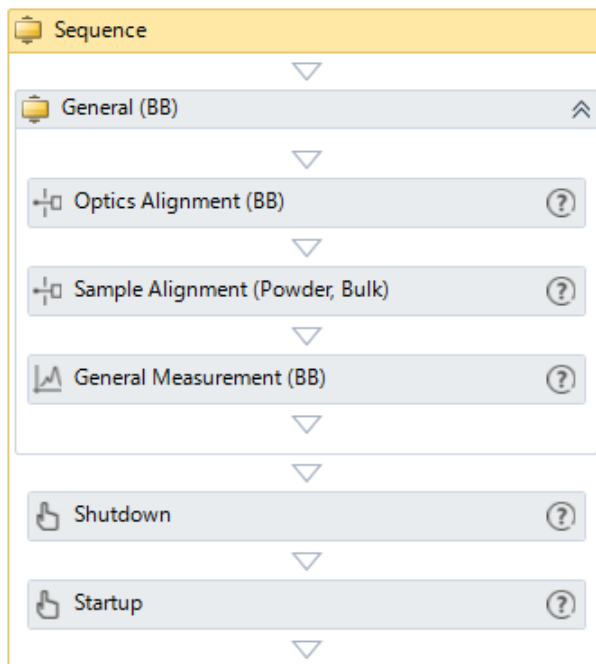
Example: Using the **BB** Package Activity



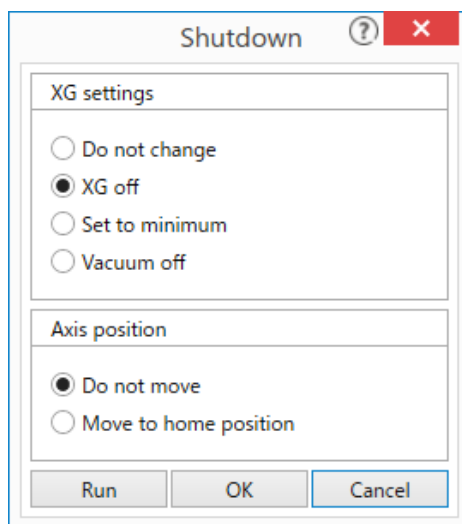
#### 4.1.4 Adding a Part Activity to the Sequence

This section describes how to add a Part Activity to the Sequence. Here, as an example, **Shutdown** and **Startup** Part Activities will be added to the **Sequence** to perform aging the next day after the Package Activity was completed and the X-ray generation was stopped.

- (1) Insert the **Shutdown** and **Startup** Part Activities to the end of the Package Activities added to the **Sequence**.



- (2) Select **XG off** under **XG settings** of the Shutdown Part Activity, and then click the **OK** button.



- (3) In Startup Part Activity, select the **Timer** checkbox and **Start** for **Target time**. Enter the date and time to start aging and then click the **OK** button.

Startup

Aging condition

☒ Use recommended aging table

☐ After replacing the target

☐ Use customized aging table

Use everyday

☐ After aging condition

☒ Timer

Target time: ☒ Start ☐ End

Date: 2018/07/01

Time: 08:00

Estimated back end: 2018/07/01 13:00

Run OK Cancel

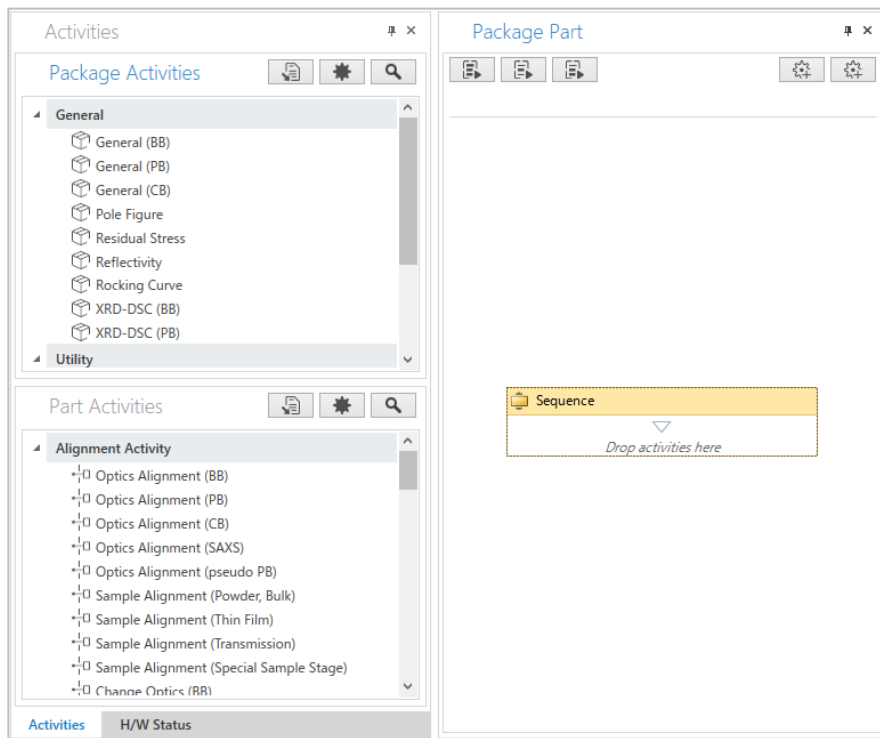
- (4) Click **Home – Run Flow** on the Ribbon.


## 4.2 Creating a flow

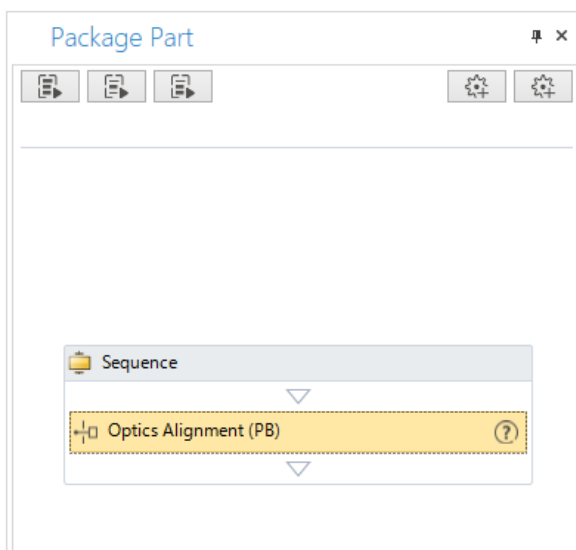
### 4.2.1 Adding Part Activities to a flow


Add the **Optics Alignment (PB)** and the **D/teX Adjustment** Part Activities to the **Sequence**.

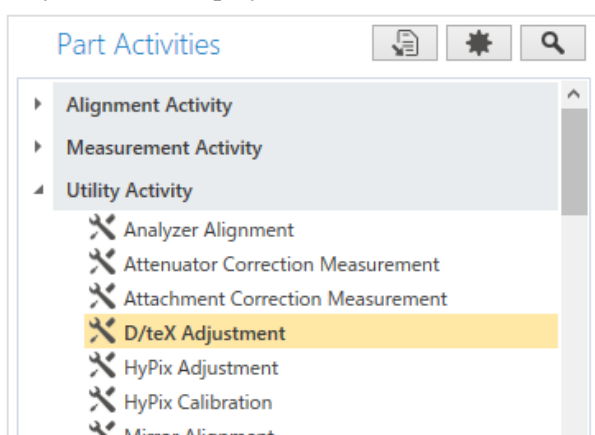
- (1) Click **Home – Package Part** on the Ribbon. The **Activities** panel and **Package Part** appear.



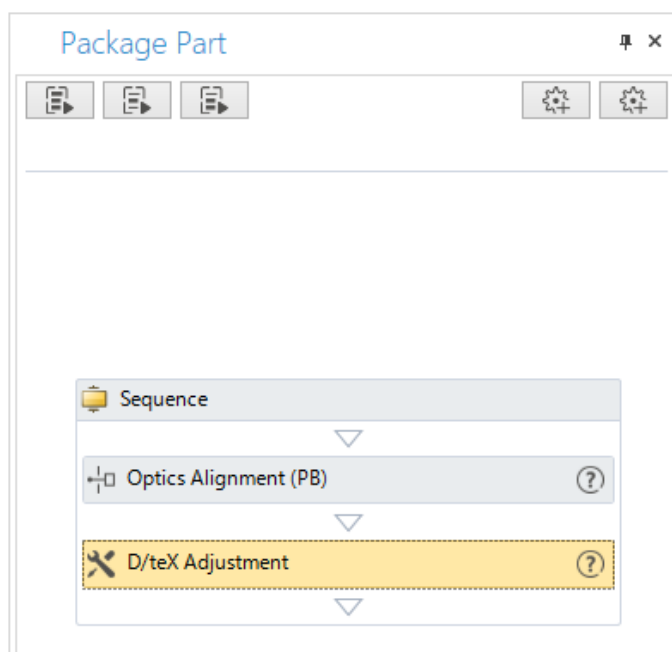
- (2) If the Alignment Activity list is not displayed in **Part Activities**, click  to display it.
- (3) Select **Optics Alignment (PB)** in the Alignment Activity list and drag and drop it to the **Sequence** to add it.



- (4) If the Utility Activity list is not displayed in **Part Activities**, click  to display it.

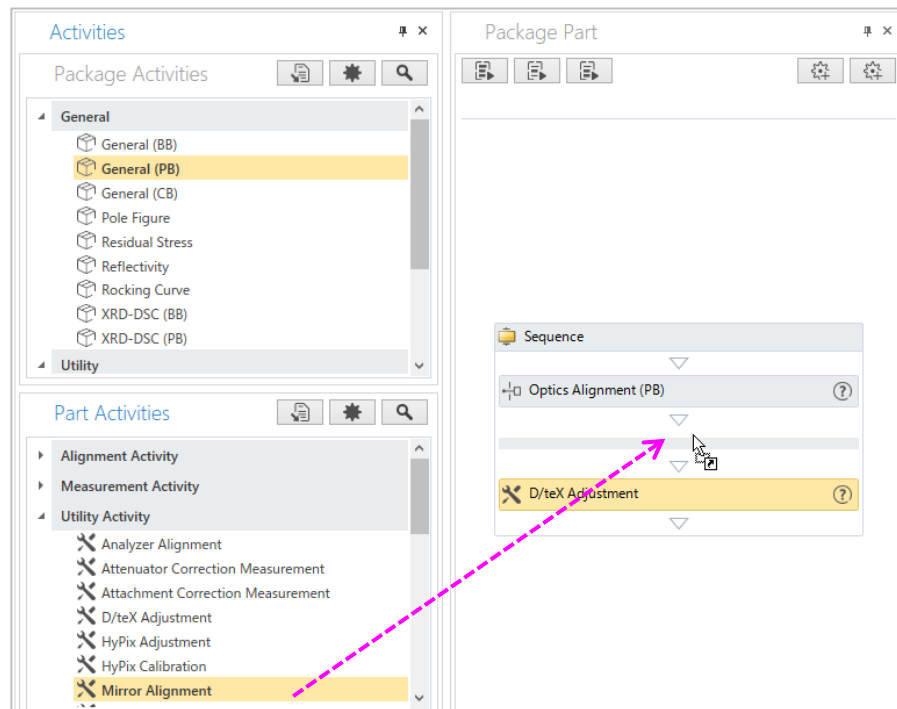


- (5) Select **D/teX Adjustment** from the Utility Activity list and drag and drop it to the **Sequence** to add it.

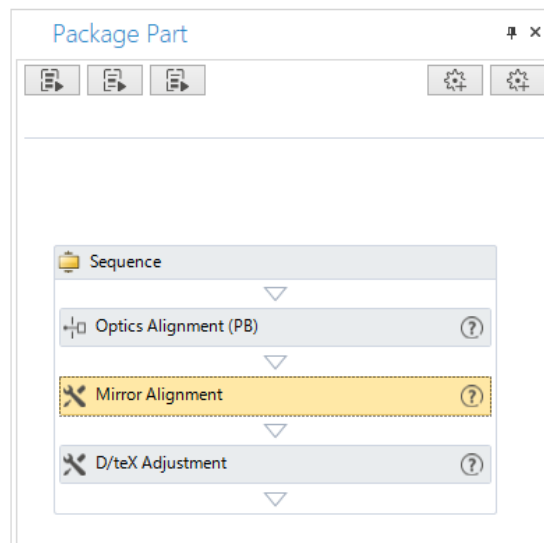


**Adding Mirror Alignment Part Activity before the Optics Alignment (PB) Part Activity**

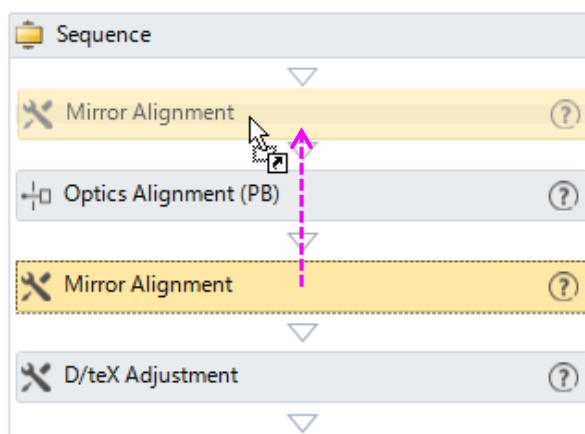
- (1) Select **Mirror Alignment** in **Part Activities** and drag and drop it under the **Optics Alignment (PB)** Part Activity in the **Sequence**.



- (2) The **Mirror Alignment** Part Activity will be added to the **Sequence**.



- (3) Drag and drop the **Mirror Alignment** Part Activity above the **Optics Alignment (PB)** Part Activity.




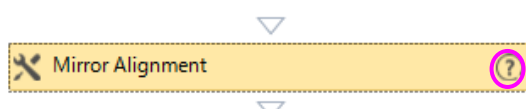
### 4.2.2 Setting conditions of the added Part Activity

The alignment conditions or measurement conditions of the Part Activity added to the flow are set in the conditions settings dialog box of the Part Activity.



Tip: To display the conditions settings dialog box of the Part Activity, click the Part Activity on the **Sequence** panel.


For details on how to specify the conditions of each Part Activity, refer to Help of the Part Activity, which is displayed by clicking the  (Help) button on each Part Activity title bar in the **Sequence**.

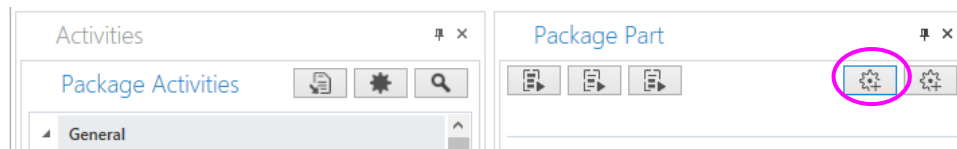


### 4.2.3 Saving flows and conditions

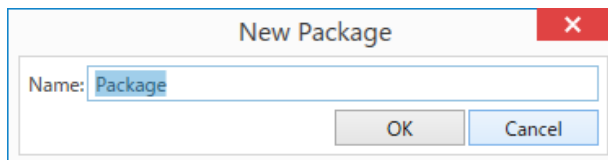
Created flows and Part Activity conditions in the flows can be saved by any of the following procedures.

#### Saving to the Package Activities list

- (1) Click  (Add user definition) on **Package Part**. The **New Package** dialog box appears.



- (2) Enter a name for the flow in the **Name** box and click the **OK** button.  
The flow is saved under **Administrator** in **Package Activities**.



- (3) Select the saved flow and drag and drop it to the **Sequence** to add it.

#### Saving as file

- (1) Click **Home – Save flow as – File system** on the Ribbon. The **Save flow** dialog box appears. Save the flow.
- (2) Click **Home – Open flow – File system** on the Ribbon. The **Open flow** dialog box appears. Select the saved flow. The saved flow will appear in the **Package Part**.

#### Saving to DB

- (1) Click **Home – Save flow as – Database** on the Ribbon. The **XRD Measurement - Save flow** dialog box appears. Save the flow.
- (2) Click **Home – Open flow – Database** on the Ribbon. The **XRD Measurement - Open flow** dialog box appears. Select the saved flow. The saved flow will appear in the **Package Part**.

### 4.2.4 Running flows

The procedure to run flows is similar to that of running Package Activities.

For details on how to run package Activities, see [4.1.3 Running Package Activity](#).



## 4.3 Performing measurements manually

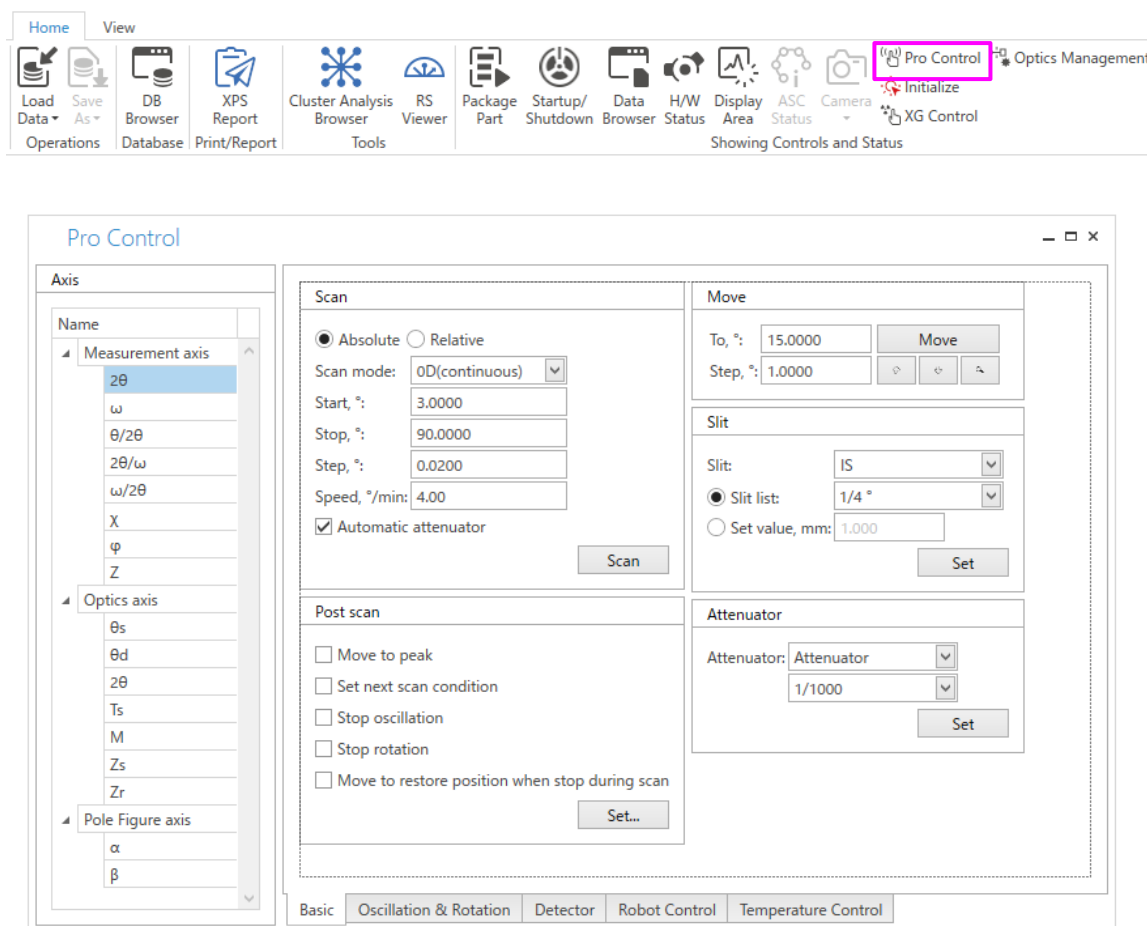
Moving the axis, making setting of the attenuator and slit, and scanning can be manually controlled by the user without using Package Activities. To perform scanning manually, X-ray generation needs to be turned on beforehand.

### [3.2 Controlling the XG manually](#)

#### 4.3.1 Displaying the Pro Control panel

The conditions for axis movement, attenuator, slit and scanning are set in the **Pro Control** panel.

- (1) Click **Home – Pro Control** on the Ribbon. The **Pro control** panel appears.

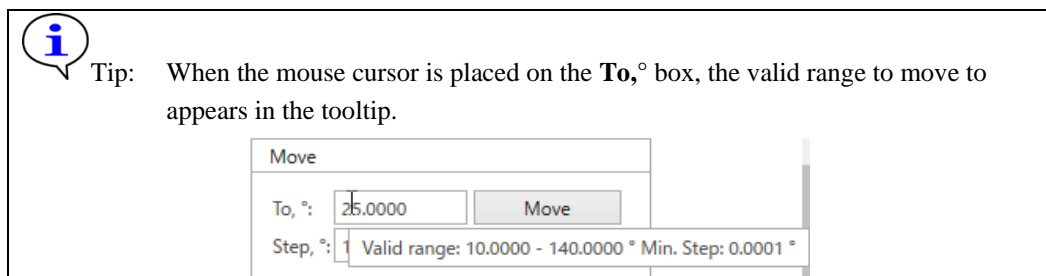


- (2) Click the **Basic** tab.

### 4.3.2 Executing axis movement and scanning

#### Moving $2\theta$ axis to $15^\circ$

- (1) Select  **$2\theta$**  from the axis list of **Measurement axis** in the **Axis** pane.
- (2) Enter "**15.0000**" in the **To, °** box for axis movement condition.



- (3) Click the **Move** button to move the  $2\theta$  axis.
- (4) When the axis starts to move, the **Hardware Control** dialog box appears. The  $2\theta$  axis will move to the position specified in the **To, °** box ( $=15^\circ$ ).

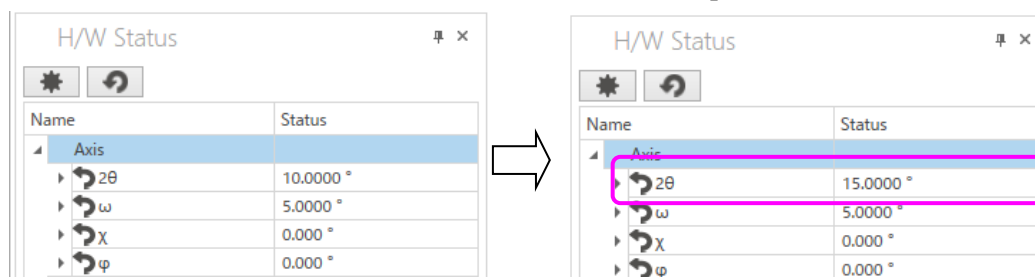
To pause the axis movement, click the **Pause** button. To end the axis movement, click the **Stop** button.

When the axis movement is completed, the **Hardware Control** dialog box closes.



#### 4.3.3 Stopping scan

- (5) The axis movement can be confirmed in the **H/W Status** panel.



#### Executing $2\theta/\omega$ scan in the range of $0.1000$ to $8.0000^\circ$

- (1) Select  **$2\theta/\omega$**  from the axis list of **Measurement axis** in the **Axis** pane.
- (2) Select **Absolute** as **Scan**.
- (3) Select **0D (continuous)** in the **Scan mode** box.
- (4) Enter "**0.1000**" and "**8.0000**" in the **Start, °** and **Stop, °** boxes respectively.
- (5) Enter the step width in the **Step, °** box.
- (6) Enter the scan speed in the **Speed, °/min** box.
- (7) When setting the parameters of **Slit**, take the following steps:
  1. Select a slit in the **Slit** box.
  2. Either select **Slit list** and select a slit width from the box, or select **Set value, mm** and enter a slit width in the box, and then click the **Set** button.

- (8) When setting the parameters of **Attenuator**, select an attenuator from the **Attenuator** box and click the **Set** button. When executing an automatic attenuator scan, select the **Automatic attenuator** checkbox.
- (9) Click the **Scan** button to start the scan.
- (10) When the scan starts, the **Hardware Control** dialog box appears.  
To end the scan, click the **Stop** button.  
When the scan is completed, the **Hardware Control** dialog box closes.

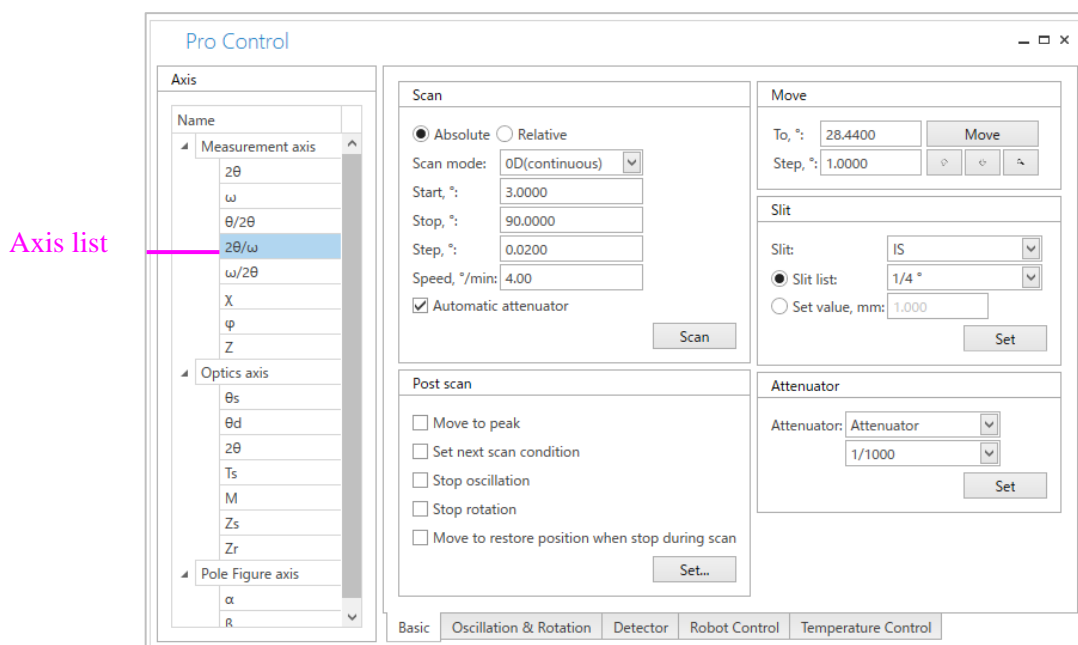


### 4.3.3 Stopping scan

The profile of the scanned data appears in the **Display Area** panel.

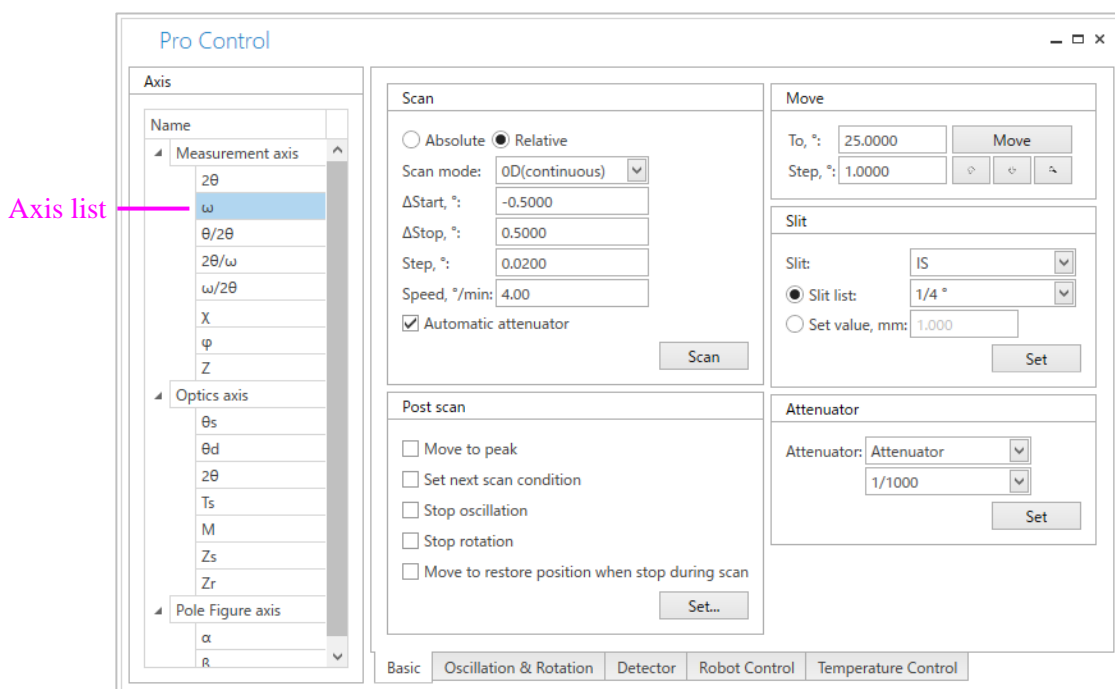
### Executing a rocking curve scan of Si (111) in the range of $\pm 0.5^\circ$

- (1) Select  $2\theta/\omega$  from the axis list of **Measurement axis** in the **Axis** pane.
- (2) Enter the diffraction angle of Si (111) "**28.44**" (when wavelength is  $\text{CuK}\alpha$ ) in the **To, °** box.



- (3) Click the **Move** button. The  $2\theta/\omega$  axis moves to  $28.44^\circ$ .

- (4) Select  $\omega$  from the axis list.



- (5) Select **Relative** as **Scan**.
- (6) Select **0D (continuous)** in the **Scan mode** box.
- (7) Enter "**-0.5000**" and "**0.5000**" in **ΔStart,°** and **ΔStop,°** boxes, respectively.
- (8) Enter the step width in the **Step,°** box.
- (9) Enter the scan speed in the **Speed,°/min** box.
- (10) When setting the parameters of **Slit**, take the following steps:
1. Select a slit name in the **Slit** box.
  2. Either select **Slit list** and select a slit width from the box, or select **Set value, mm** and enter a slit width in the box, and then click the **Set** button.
- (11) To set the parameters of **Attenuator**, select an attenuator from the **Attenuator** box and click the **Set** button. To execute an automatic attenuator scan, select the **Automatic attenuator** checkbox.
- (12) Click the **Scan** button to start the scan.
- (13) When the scan starts, the **Hardware Control** dialog box appears.  
To end the scan, click the **Stop** button.  
When the scan is completed, the **Hardware Control** dialog box closes.

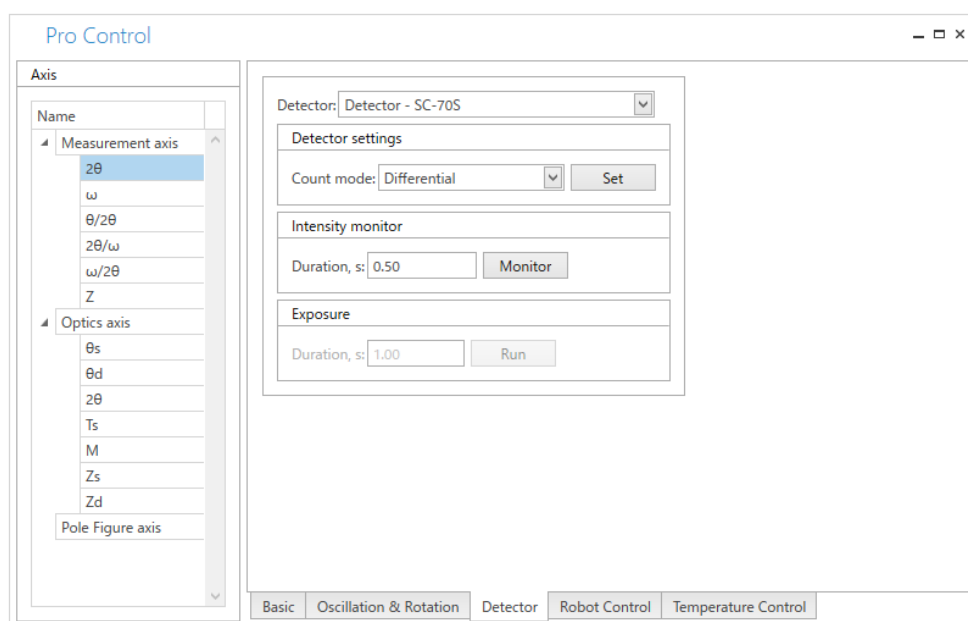


#### 4.3.3 Stopping scan

The profile of the scanned data appears in the **Display Area** panel.

**Setting the  $\omega$  axis to 25° and monitoring the intensity**

- (1) Select  $\omega$  from the axis list of **Measurement axis** in the **Axis** pane.
- (2) Click the **Basic** tab and enter "25.0000" in the **To, °** box.
- (3) Click the **Move** button to move the axis.  
When the axis starts to move, the **Hardware Control** dialog box appears. The  $\omega$  axis will move to the position specified in the **To, °** box (=25°).
- (4) When setting the parameters of **Slit**, take the following steps:
  1. Select a slit name in the **Slit** box.
  2. Either select **Slit list** and select a slit width from the box, or select **Set value, mm** and enter a slit width in the box, and then click the **Set** button.
- (5) When setting the parameters of **Attenuator**, select an attenuator from the **Attenuator** box and click the **Set** button.
- (6) Click the **Detector** tab. Select either **Integral** or **Differential** in **Count mode**, and then click the **Set** button.
- (7) Enter the count time in the **Duration, s** box of **Intensity monitor**



Tip: Normally, it is recommended to set the count time to about 0.3 to 0.5 seconds.

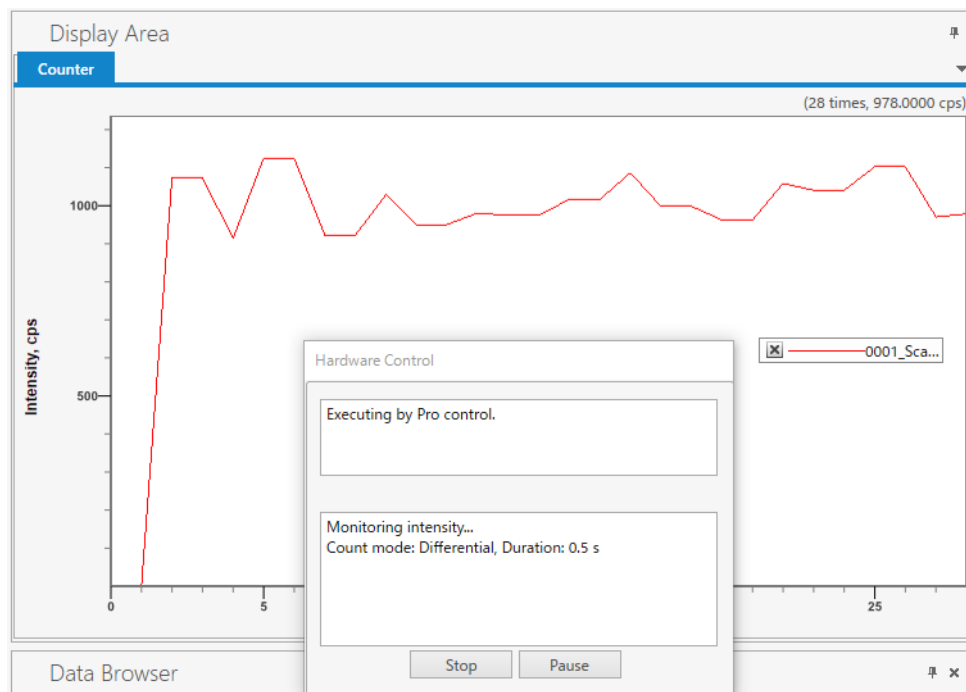
- (8) Click the **Monitor** button to start the intensity monitor.

- (9) When the intensity monitor starts, the **Hardware Control** dialog box appears. To pause the intensity monitor, click the **Pause** button. To end the intensity monitor, click the **Stop** button.

When the scan is completed, the **Hardware Control** dialog box closes.



#### 4.3.3 Stopping scan



The profile during the intensity monitor appears in the **Display Area** panel.



Tip: Any axis can be moved during intensity monitor.

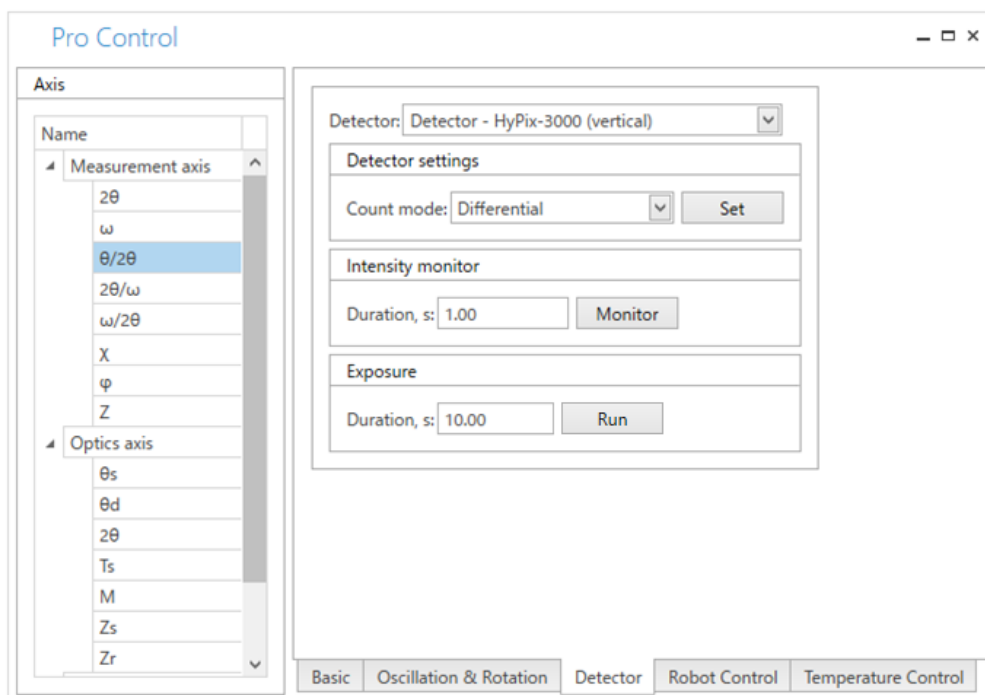
#### Setting the $\theta/2\theta$ axis to $25^\circ$ and performing the exposure



Tip: The exposure is available only for the HyPix detector.

- (1) Select  **$\theta/2\theta$**  from the axis list of **Measurement axis** in the **Axis** pane.
- (2) Click the **Basic** tab and enter "**25.0000**" in the **To, °** box.
- (3) Click the **Move** button to move the axis.  
When the axis starts to move, the **Hardware Control** dialog box appears. The  $\theta/2\theta$  axis will move to the position specified in the **To, °** box ( $=25^\circ$ ).
- (4) When setting the parameters of **Slit**, take the following steps:
  1. Select a slit name in the **Slit** box.
  2. Select **Slit** list and select a slit width from the box, or select **Set value, mm** and enter a slit width in the box, and then click the **Set** button.
- (5) When setting the parameters of **Attenuator**, select an attenuator from the **Attenuator** box and click the **Set** button.
- (6) Click the **Detector** tab. Select either **Integral** or **Differential** in **Count mode**, and then click the **Set** button.

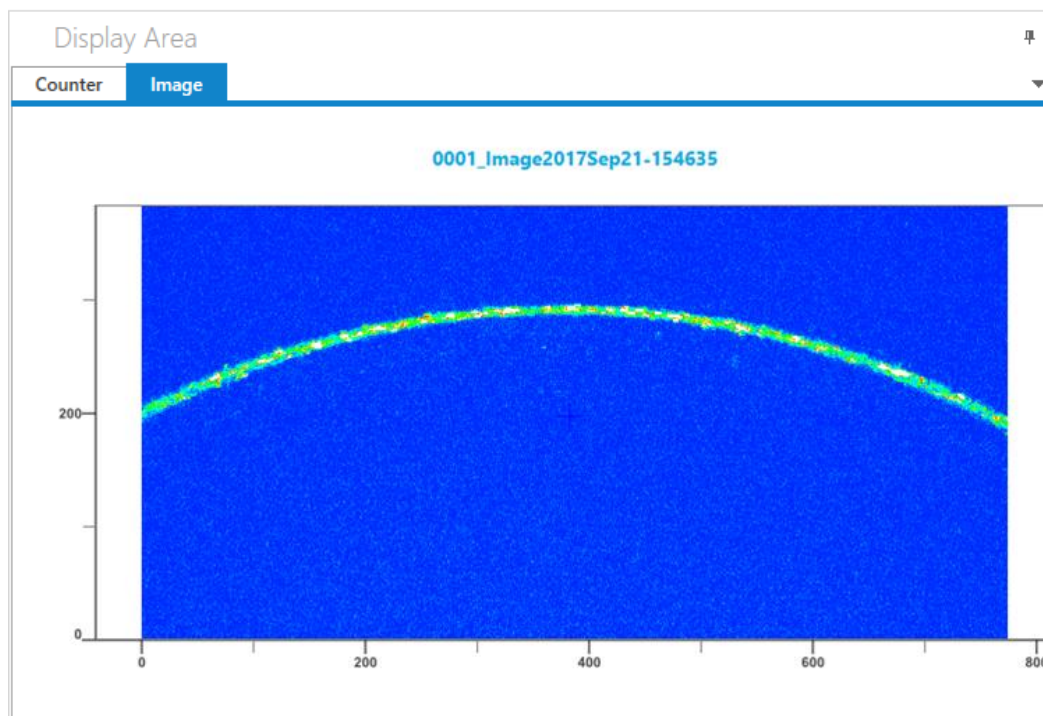
- (7) Enter duration in the **Duration** box of **Exposure**.



- (8) Click the **Run** button to start exposure.
- (9) The measured image is displayed in the Display Area after the exposure is finished.



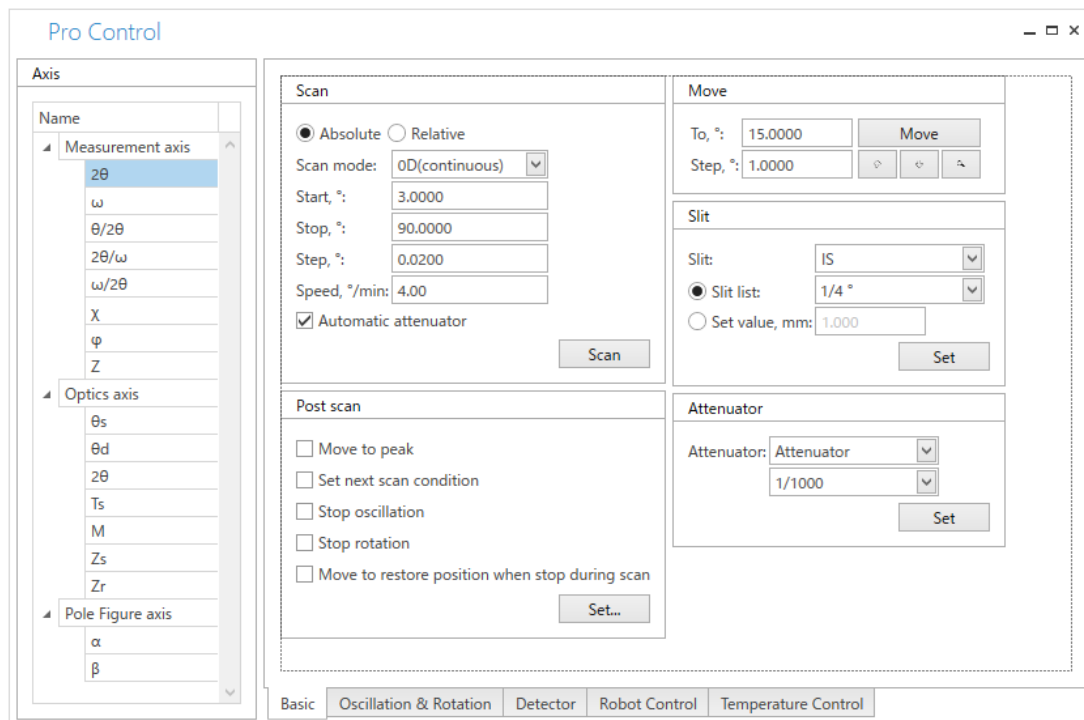
#### 4.3.3 Stopping scan



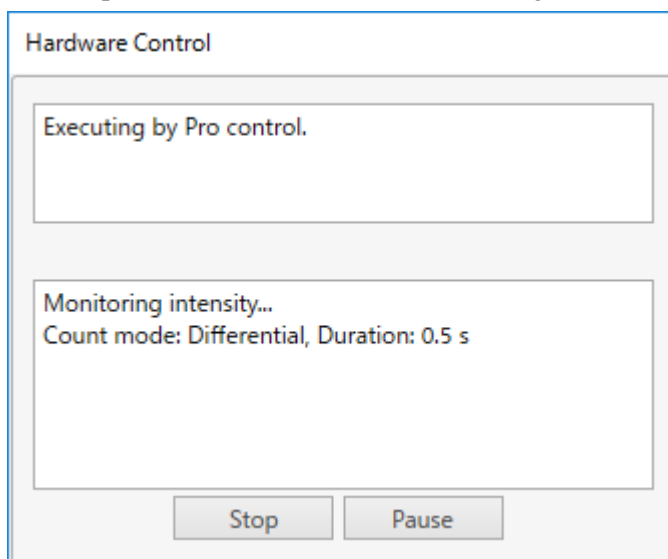
### 4.3.3 Stopping scan

To stop or pause an action such as axis movement, use the **Hardware Control** dialog box..

- (1) Click **Home – Pro Control** on the Ribbon. The **Pro Control** panel appears.



- (2) Select the axis to scan and set the scan condition.
- (3) Click the **Scan** button to start the scan.
- (4) When the scan starts, the **Hardware Control** dialog box appears.  
To stop the scan, click the **Stop** button.  
When the scan is completed, the **Hardware Control** dialog box closes.



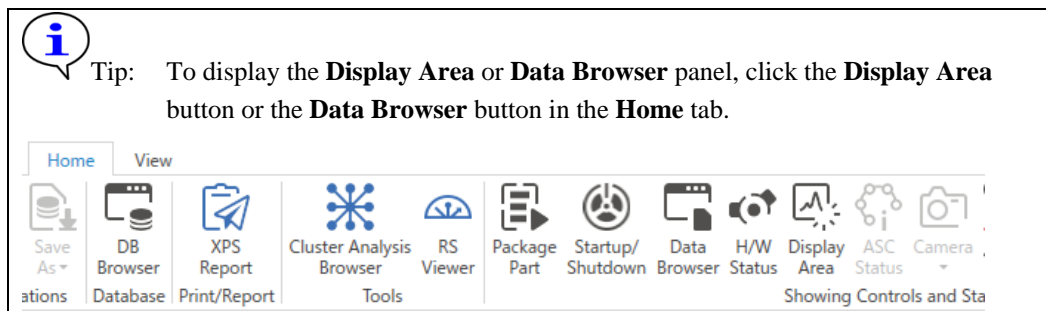


## 4.4 Displaying and saving profiles

When a measurement is executed in the **XRD Measurement** plugin, a profile appears in the **Display Area** panel. The **Display Area** panel allows zooming in/out of profile, changing the scale, making display settings, etc. and the **Data Browser** panel allows saving profile data, peak search etc.

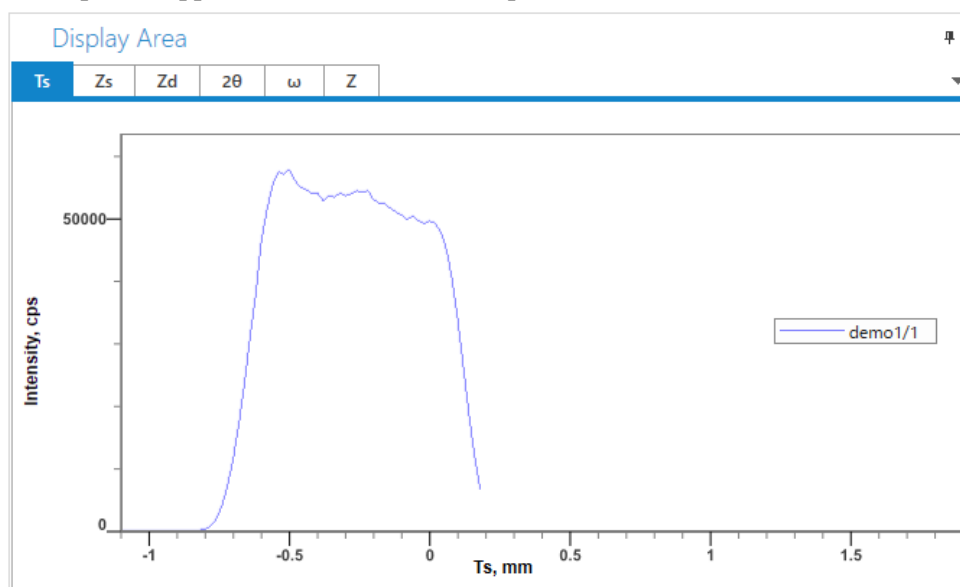
The XRD Measurement plugin loads and saves measurement data.

This chapter describes the procedure to load measurement data and save profile.



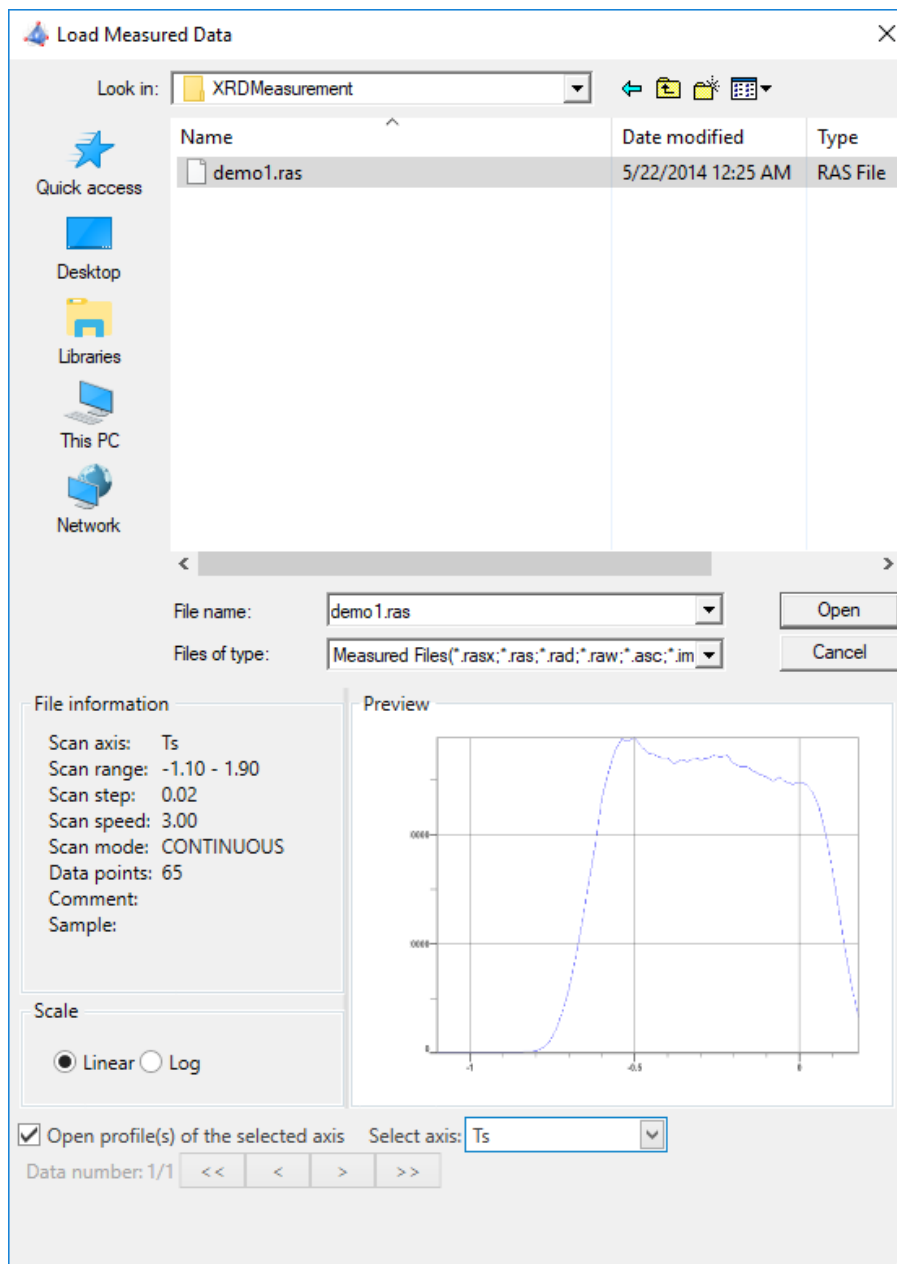
### 4.4.1 Loading and overlaying measurement data

- (1) Load measurement data by either of the steps below:
  1. Click **Home – Load data – File system** on the Ribbon. The **Load Measurement Data** dialog box appears.
  2. Click **Home – Load data – Database** on the Ribbon. The **XRD Measurement - Load Measured Data** dialog box appears.
- (2) Select the measurement data and click the **Open** button.
- (3) A new profile appears in the **Display Area** panel.



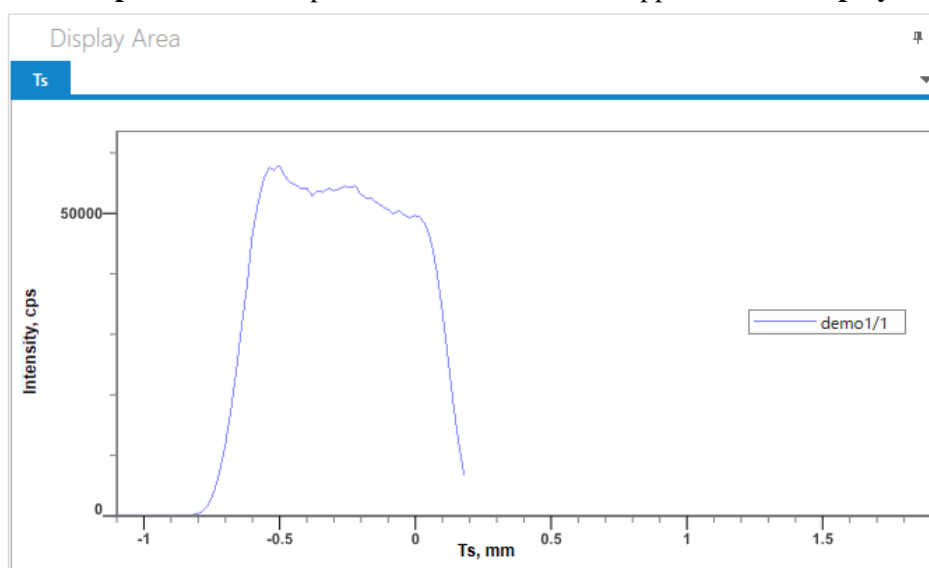
**Loading measurement data of a single axis from a file containing data of multiple axes**

- (1) Click **Home – Load data – File system** on the Ribbon. The **Load Measured Data** dialog box appears.



- (2) Select the measurement data and select the **Open profile(s) of the selected axis** checkbox.
- (3) Select the axis to load in the **Select axis** box.

- (4) Click the **Open** button. The profile of the selected axis appears in the **Display Area** panel.



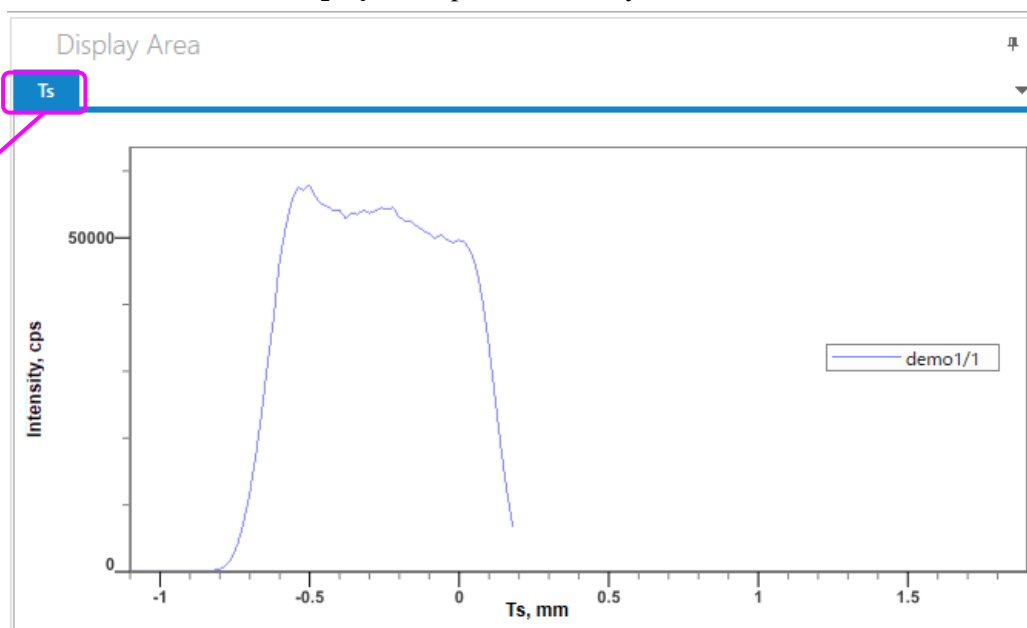
### Overlaying data on the Display Area panel



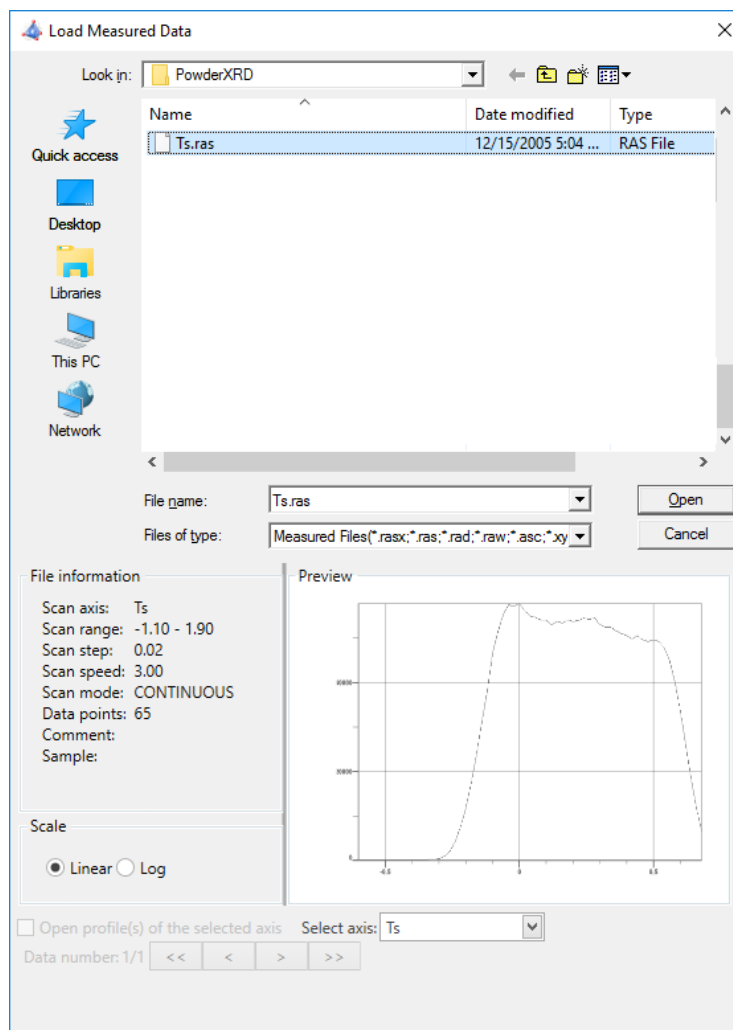
Tip: If the axis of loaded data is the same, the data can be overlaid.

- (1) Select the axis tab of **Display Area** panel to overlay data.

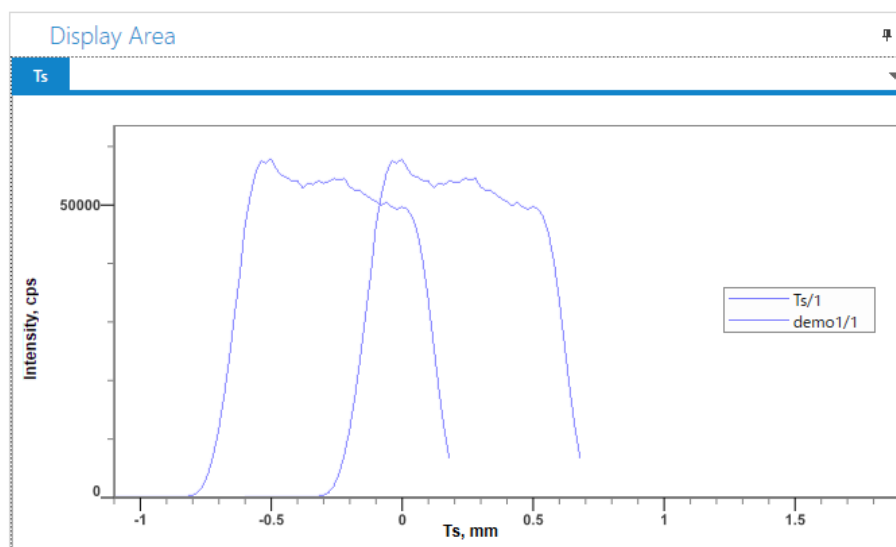
Axis tab



- (2) Click **Home – Load data – File system** on the Ribbon. The **Load Measured Data** dialog box appears.



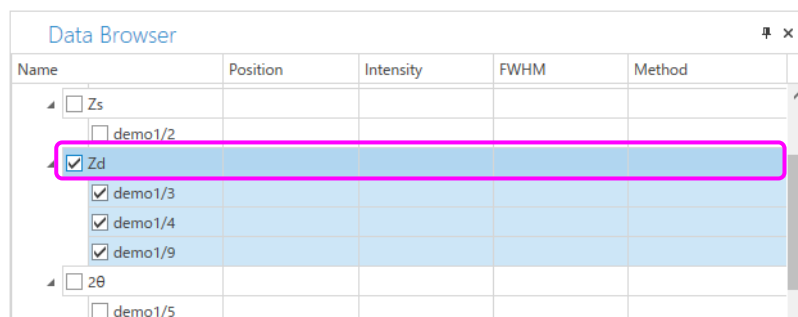
- (3) Select the measurement data in **File Name** and click the **Open** button. The loaded data will be overlaid in the **Display Area** panel.



### 4.4.2 Saving profiles

#### Saving all profiles included in a single axis

- (1) Select the axis which includes the profiles to save in the **Data Browser** panel.



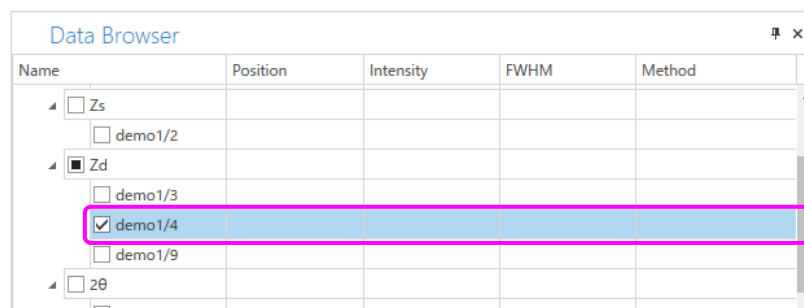
- (2) Click **Home – Save as – File system** on the Ribbon. The **Save As** dialog box appears.
- (3) Enter the file name in the **File Name** box, and click **Save**.

#### Saving only selected profiles

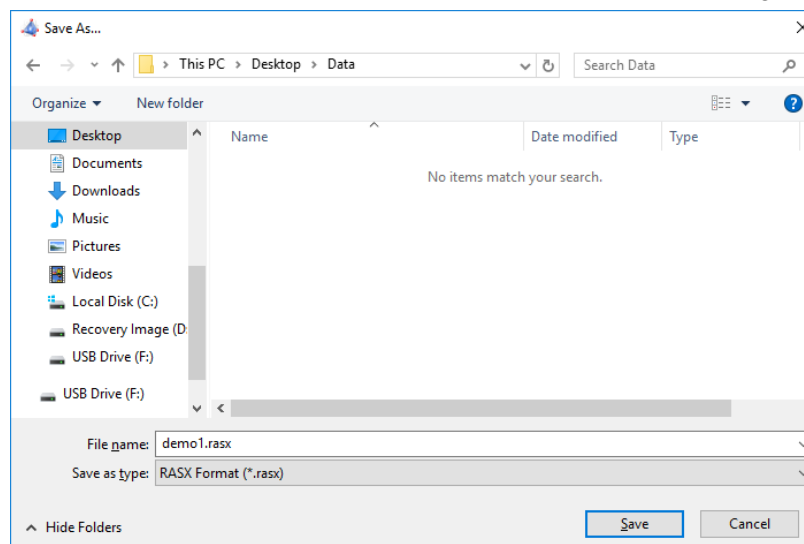


**CAUTION:** The actions below will delete profiles other than the selected profile. If there are several profiles to save, save all profiles of the selected axis before executing the action below.

- (1) Select the profile to save in the **Data Browser** panel.




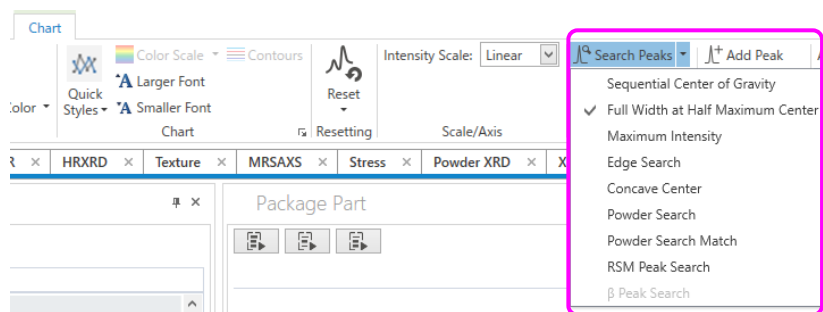
- (2) Click **Home – Save as – File system** on the Ribbon. The **Save As** dialog box appears.



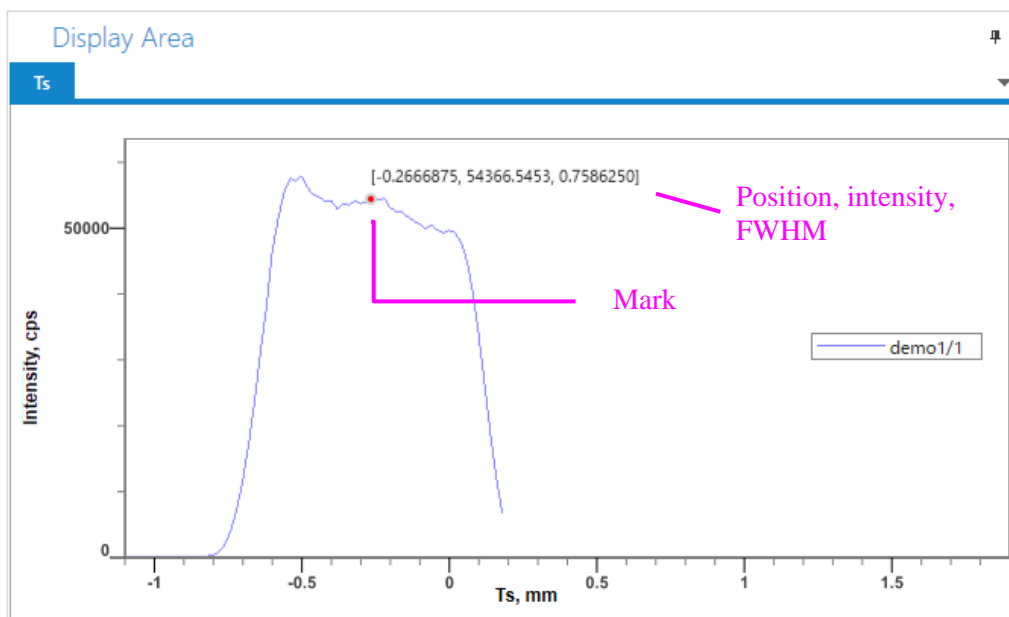
- (3) Enter the file name in the **File Name** box, and click the **Save** button.

### 4.4.3 Performing peak search

- (1) Select a tab in the **Display Area** panel in which the profile to execute peak search is displayed.
- (2) Click the  on the right side of **Search peaks** in the **Chart** tab on the Ribbon. The peak search method list appears.



- (3) Click one of the methods displayed on the list (such as **Full Width at Half Maximum Center**) to execute peak search. A "•" mark appears at the peak top position. The peak position, intensity, and full width at half maximum are displayed on the mark in numerical values.



## 5 Performing Alignments

The performance of the instrument may be impaired after events such as a change of the focus position due to X-ray tube replacement or changes of the detector characteristics.

In such cases, the performance of the instrument can be maintained by running the corresponding Alignment Part or Package Activities, or **Maintenance Package Activity**.

Events that require alignment	Content of the alignment	Corresponding Alignment Part or Package Activities
After replacement of X-ray tube or filament	Multilayer mirror alignment	<b>Mirror Alignment Part Activity</b>
After maintenance of X-ray generator		
Profiles show height differences when measured with automatic attenuator	Remeasurement of the attenuation coefficient	<b>Attenuator Correction Measurement Package Activity</b>
Changes of the detector characteristics due to aging deterioration	Detector realignment	<b>D/teX Adjustment Package Activity</b> or <b>HyPix Adjustment Package Activity</b>
The position of the diffraction peaks differs from the theoretical values	Alignment of the Z axis position during Optics alignment	<b>Attachment Correction Measurement Part Activity</b>

### 5.1 Running the Maintenance Package Activity

Alignments of the detector (D/teX Ultra), multilayer mirror, attenuator, or the mounting position of attachments can be performed by running the Maintenance Package Activity.

- (1) Click **Home – Package Part** on the Ribbon. The **Package Parts** panel and the **Activities** panel appear.
- (2) Click **Utility – Maintenance** in **Package Activities** and drag and drop it to the **Sequence** to add it.
- (3) Edit the conditions of Parts in the **Sequence** as necessary.
- (4) Click **Home – Run Flow** on the Ribbon to run the **Maintenance Package Activity**.



Tip: For details on how to run package activities, see [4.1.3 Running Package Activity](#).

For details on the different Parts in the **Maintenance Package Activity**, refer to the help of the specific Part.



[4.2.2 Setting conditions of the added Part Activity](#)



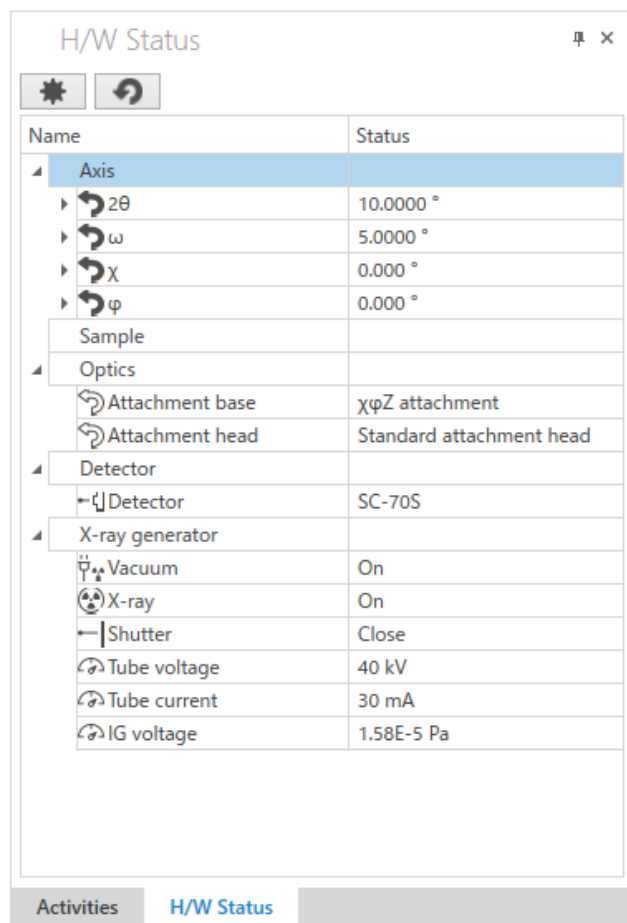


## 6 Other Functions


### 6.1 Checking the current instrument status

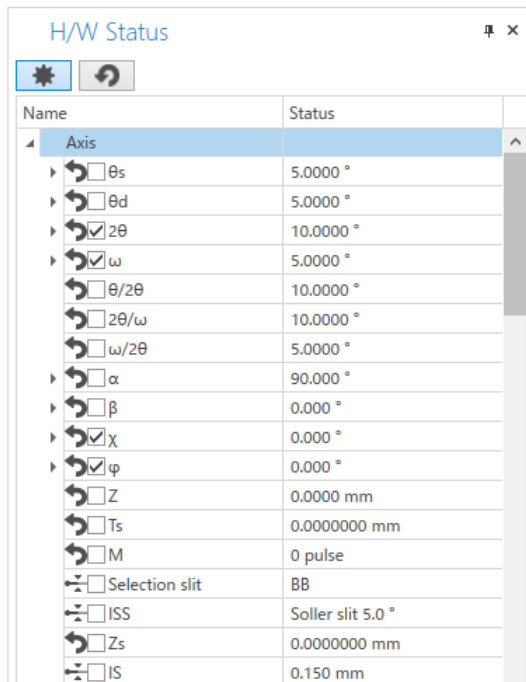
#### 6.1.1 H/W Status panel

Click **Home – H/W Status** on the Ribbon. The **H/W Status** panel appears.

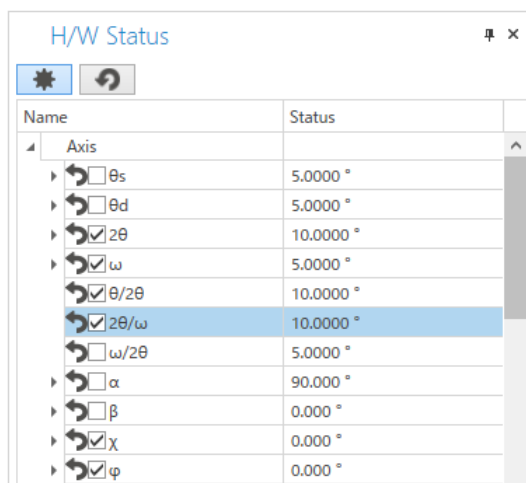



**Displaying only the selected axis**

- (1) Click the  (Customize) button in the **H/W Status** panel.











- (2) A checkbox appears in front of the name of each axis. Select the checkbox of the axis to display.




- (3) Click the  (Customize) button. Only the axis selected in step (2) appears.

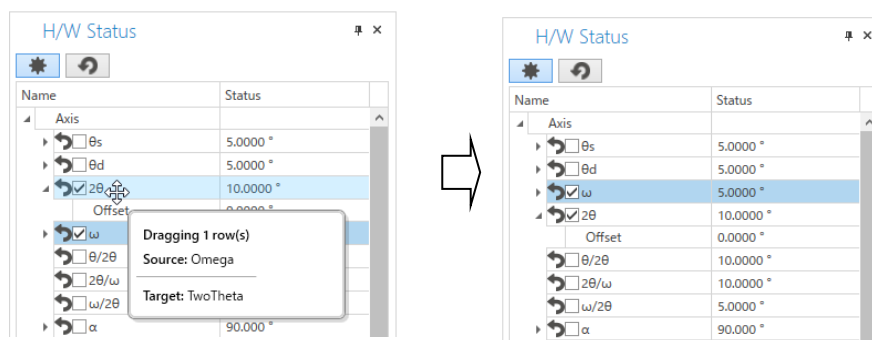
H/W Status ⌵ ×


 

Name	Status
Axis	
▶  $2\theta$	10.0000 °
▶  $\omega$	5.0000 °
▶  $\theta/2\theta$	10.0000 °
▶  $2\theta/\omega$	10.0000 °
▶  $\chi$	0.000 °
▶  $\varphi$	0.000 °
Sample	
Optics	
▶ Attachment base	$\chi\varphi Z$ attachment
▶ Attachment head	Standard attachment head

### Changing the order of axes to display (when displaying $2\theta$ axis below $\omega$ axis)

- (1) Click the  (Customize) button in the H/W Status panel.

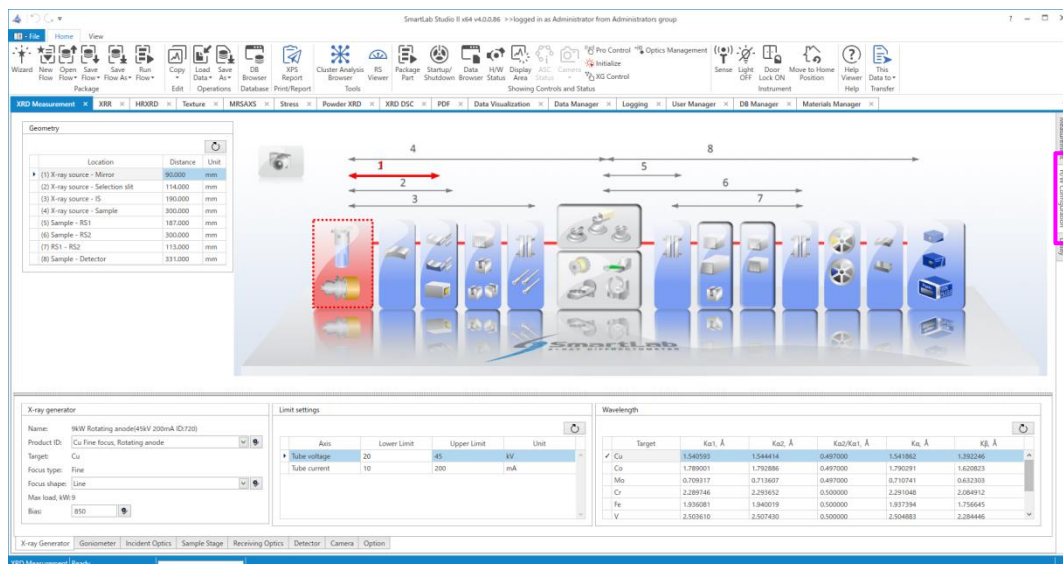


- (2) Drag and drop the icon of  $2\theta$  axis over the icon of  $\omega$  axis.
- (3) The order of axes to display is changed.
- (4) Click the  (Customize) button to end the settings of customization.

### 6.1.2 Hardware Configuration panel

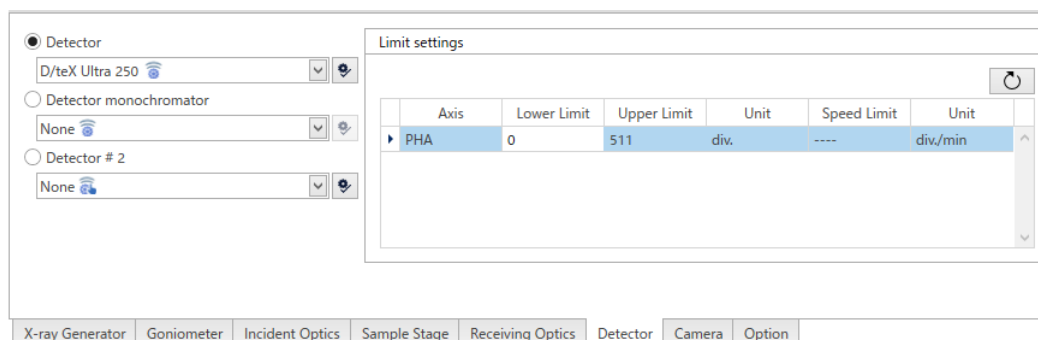
The Hardware Configuration panel is used to change and confirm the hardware configuration of SmartLab. Normally, these settings do not need to be made.

This section describes how to change X-ray tube type, detector energy mode and detection area.

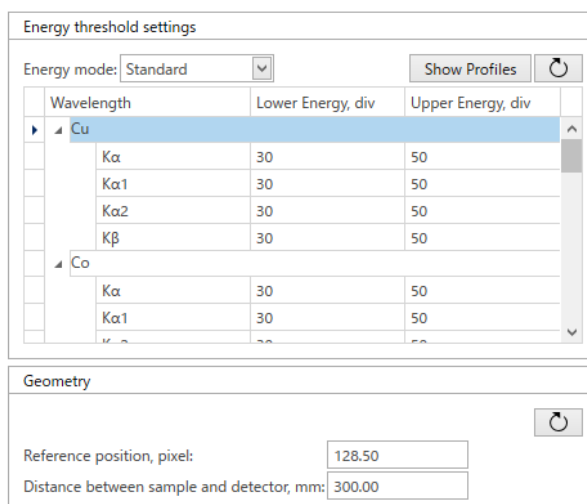


#### Changing the energy mode of the detector

- (1) Click the **H/W Configuration** tab. The Hardware Configuration panel appears.
- (2) Click the **Detector** tab.



- (3) Select the detector to be used from the **Detector** box. The current energy mode for the selected detector is shown on **Energy threshold settings**.



- (4) To change the energy mode for measurements, select a different energy mode from the **Energy mode** box.

### Changing the Detection area for converting to profile data

When using a 2D detector for acquisition of 1D profiles (intensity versus scan axis), set the Detection area of the detector in the horizontal direction.

- (1) Click the **H/W Configuration** tab. The Hardware Configuration panel appears.  
 (2) Click the **Detector** tab.

Axis	Lower Limit	Upper Limit	Unit	Speed Limit	Unit
PHA	0	511	div.	----	div./min

Navigation tabs: X-ray Generator | Goniometer | Incident Optics | Sample Stage | Receiving Optics | **Detector** | Camera | Option

- (3) Select the 2D detector to be used from the **Detector** box. In the **Geometry – Detection area for profile data** box, the detection area of the detector for acquisition of 1D profiles is displayed.

**Energy threshold settings**

Energy mode: Standard

Target	Lower Energy, keV	Upper Energy, keV
✓ Cu	6.0keV	12.0keV

**Geometry**

Reference position X, pixel: 382.50 Y, pixel: 197.50

Detection area for profile data X, mm: 20.0

Distance between sample and detector, mm: 200.00

Integrated mode: ☒ Line ☐ Arc

- (4) Enter the width of the detection area in the horizontal direction in the **Detection area for profile data** box.

## 6.2 Initializing axes

This function initializes the axes of goniometer and attachments.

### 6.2.1 Initializing each category

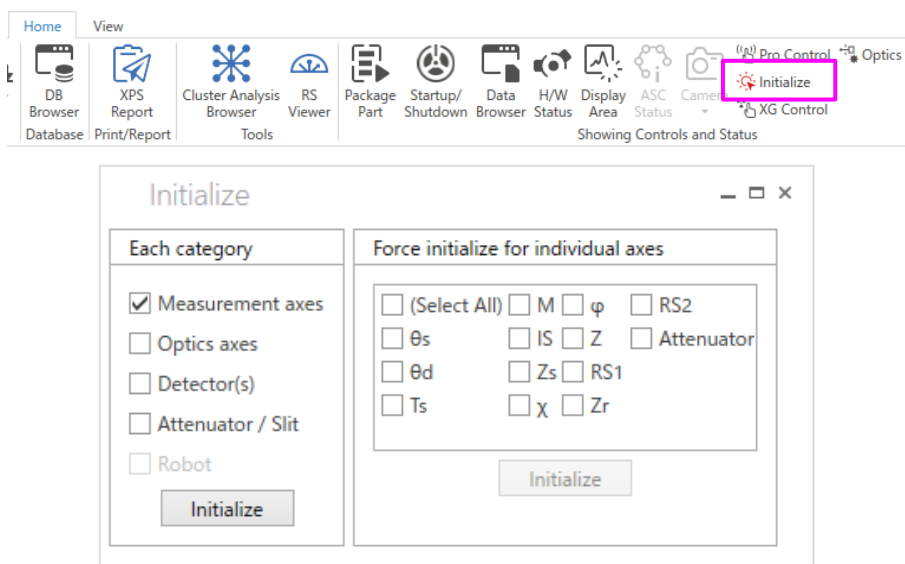
When the **Initialize** button in the **Initialize** panel – **Each category** is clicked, initialization will be performed for the axes which have not been initialized. For the axes which have already been initialized, initialization will not be performed and the current position will be loaded.



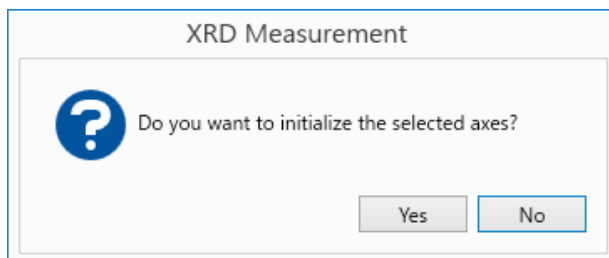
Tip: To forcefully initialize an axis regardless of whether the initialization is completed or not, see [6.2.2 Initializing only selected axes](#).

Here, how to initialize measurement axes is explained as an example.

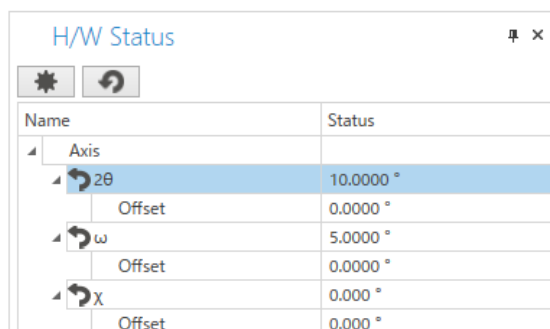
- (1) Click **Home** – **Initialize** on the Ribbon. The **Initialize** panel appears.



- (2) Select the **Measurement axes** checkbox and click the **Initialize** button.
- (3) A confirmation message for the initialization appears. Click the **Yes** button.



- (4) After the initialization of the measurement axes is completed, the current position and the offset value set last time will appear in **H/W Status** panel.



Name	Status
Axis	
2θ	10.0000 °
Offset	0.0000 °
ω	5.0000 °
Offset	0.0000 °
χ	0.000 °
Offset	0.000 °

### 6.2.2 Initializing only selected axes

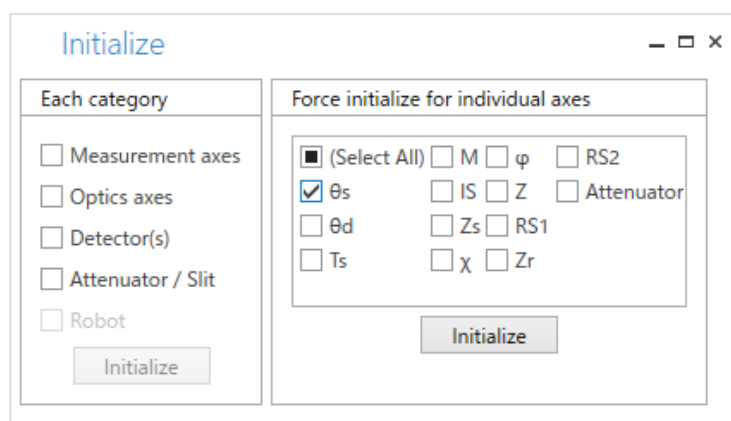
Initialize axes one by one at a time.



**CAUTION:** Unlike initializing each category in the **Initialize** panel, this initialization will be forcibly performed for axes whose initialization are already completed as well.

This subsection describes how to initialize the  $\theta_s$  axis as an example.

- (1) Click **Home – Initialize** on the Ribbon. The **Initialize** panel appears.



**Each category**

☐ Measurement axes

☐ Optics axes

☐ Detector(s)

☐ Attenuator / Slit

☐ Robot

**Initialize**

**Force initialize for individual axes**

☒ (Select All) ☐ M ☐ φ ☐ RS2

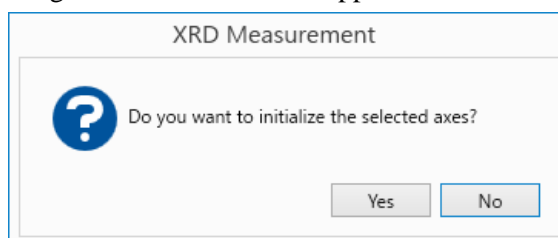
☒  $\theta_s$  ☐ IS ☐ Z ☐ Attenuator

☐  $\theta_d$  ☐ Zs ☐ RS1


☐ Ts ☐ χ ☐ Zr

**Initialize**

- (2) Select  $\theta_s$  in **Force initialize for individual axes** list and click **Initialize**.
- (3) A confirmation message for the initialization appears. Click the **Yes** button.



XRD Measurement



Do you want to initialize the selected axes?

**Yes** **No**

- (4) The  $\theta_s$  axis is initialized.

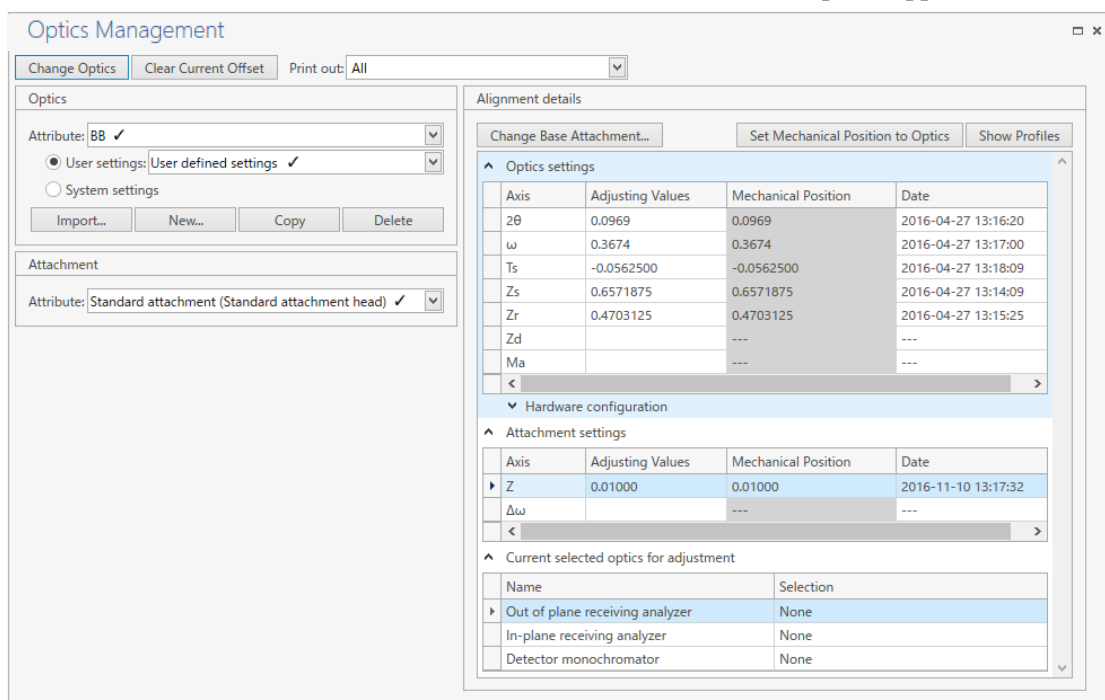
## 6.3 Managing optics alignment results

In a measurement using X-rays, the origin point of the optics needs to be determined first by optics alignment.

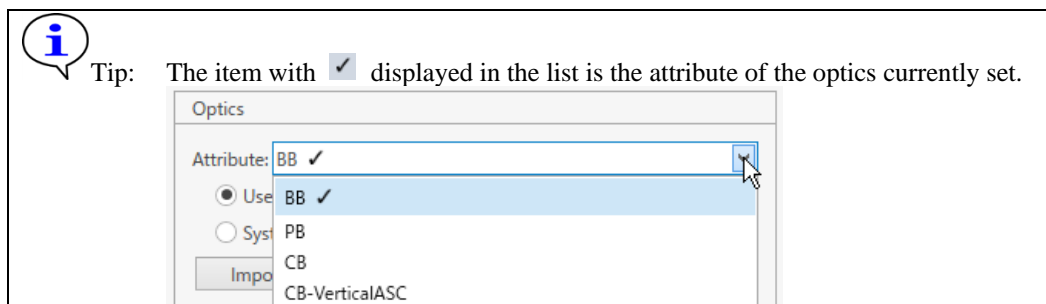
The difference between mechanical origin point and optics origin point is called “offset”. Depending on the optics used, the type and numbers of axis to determine the origin point of the optics differ. In the optics management database, the offset and axis position to determine the origin point of the optics are saved for each optical element and each combination of attachments.

### 6.3.1 Checking optics adjusting values

- (1) Click **Home – Optics Management**. The **Optics Management** panel appears.



- (2) From the **Attribute** box under **Optics**, select the name of the attribute you want to check the axial adjusting values.



- (3) To check the adjusting values set by individual users, select the **User settings** button and the name of optics from the box, which was created to register user's adjusting values. To check common adjusting values for all users, select the **System settings** option button.
- (4) The adjusting values appear in **Optics settings** of **Alignment details**.
- (5) From the **Attribute** box in **Attachment**, select the name of the attribute you want to check the axial adjusting values.





Tip: The item with ☒ displayed in the list corresponds to the attachment currently mounted.

- (6) The adjusting values appear in the **Attachment settings** of **Alignment details**.

### 6.3.2 Registering or deleting optics

#### Additionally registering the optics name "Rigaku" to Optics Attribute "BB"

- (1) Click **Home – Optics Management** on the Ribbon. The **Optics Management** panel appears.
- (2) Select **BB** in the **Attribute** box under **Optics**.
- (3) Select **User settings** and click the **New** button.

**Optics Management**

Change Optics Clear Current Offset Print out: All

**Optics**

Attribute: BB ✓

● User settings: User defined settings ✓

○ System settings

Import... New... Copy Delete

**Attachment**

Attribute: Standard attachment (Standard attachment head) ✓

**Alignment details**

Change Base Attachment... Set Mechanical Position to Optics Show Profiles

**Optics settings**

Axis	Adjusting Values	Mechanical Position	Date
2θ	0.0969	0.0969	2016-04-27 13:16:20
ω	0.3674	0.3674	2016-04-27 13:17:00
Ts	-0.0562500	-0.0562500	2016-04-27 13:18:09
Zs	0.6571875	0.6571875	2016-04-27 13:14:09
Zr	0.4703125	0.4703125	2016-04-27 13:15:25
Zd	---	---	---
Ma	---	---	---

**Hardware configuration**

**Attachment settings**

Axis	Adjusting Values	Mechanical Position	Date
Z	0.01000	0.01000	2016-11-10 13:17:32
Δω	---	---	---

**Current selected optics for adjustment**

Name	Selection
Out of plane receiving analyzer	None
In-plane receiving analyzer	None
Detector monochromator	None

- (4) Select **User settings** and enter **"Rigaku"** in the box as the name of optics.

**Optics**

Attribute: BB ✓

● User settings: Rigaku

○ System settings

Import... New... Copy Delete

- (5) A confirmation message for the change appears. Click the **Yes** button.

**XRD Measurement**

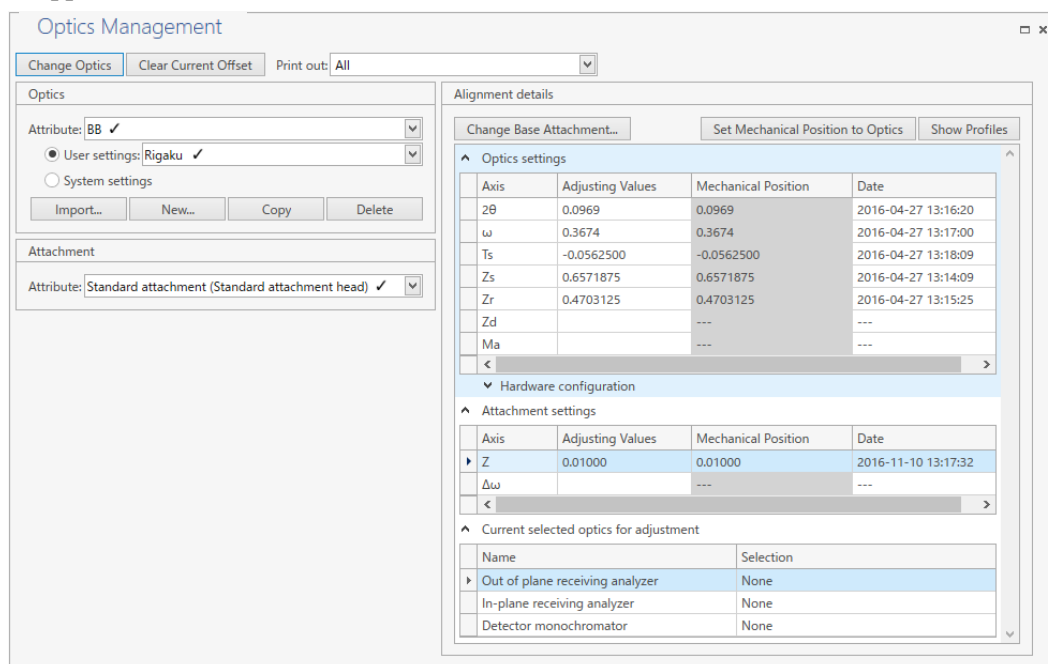
Do you want to rename the optics user settings "User defined settings" to "Rigaku"?

Yes No

- (6) Click **Set Mechanical Position to Optics** under **Alignment details** to save the position of adjusted mechanical origin point, or enter the offset or adjusting value in the **Adjusting values** cells.
- (7) Now the optics information and adjusting values of the optics named "**Rigaku**" are saved in the optics attribute "**BB**".

### Deleting the additionally registered optics name "Rigaku"

- (1) Click **Home – Optics Management** on the Ribbon. The **Optics Management** panel appears.



- (2) From the **Attribute** box under **Optics**, Select the name of the optics to delete.
- (3) Select **User settings** and select the optics name "**Rigaku**" from the box, which was created to register the adjusting values.
- (4) Click the **Delete** button.
- (5) A confirmation message for the deleting appears. Confirm the selected content and click the **Yes** button to delete the optics name.

### 6.3.3 Switching the optics

- (1) Click **Home – Optics Management** on the Ribbon. The **Optics Management** panel appears.

- (2) Select the optics to switch from the **Attribute** box under **Optics**.
- (3) To switch to the adjusting value set by individual users, select the **User settings** option button and the name of optics from the box, which was created to register the user's adjusting value. To switch to common adjusting values for all users, select the **System settings** option button.



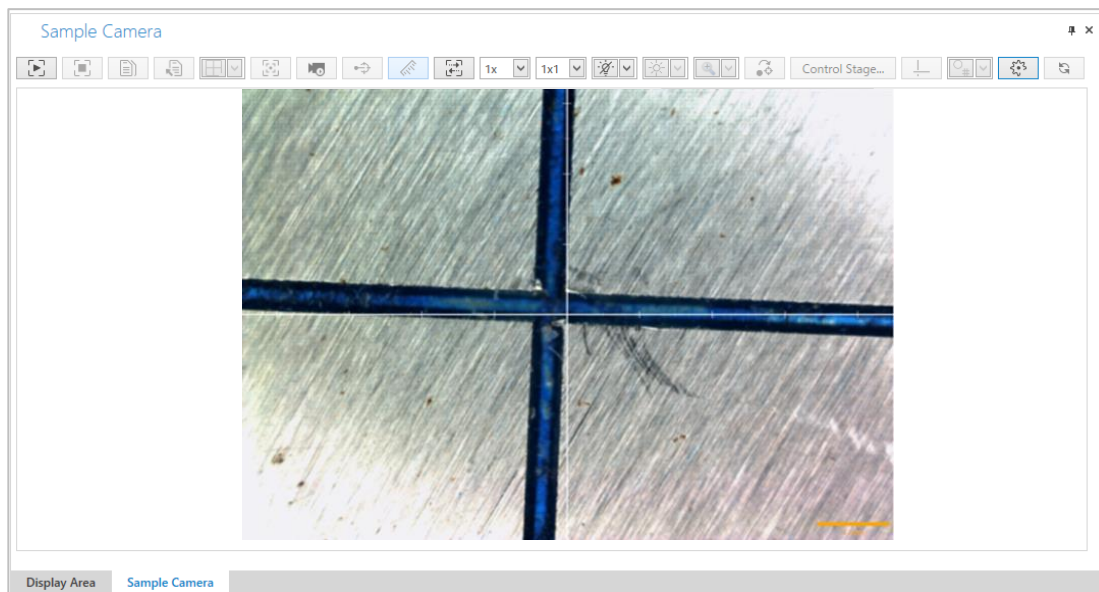
**CAUTION:** The attribute that corresponds to the currently mounted hardware configuration will automatically be set in **Attachment**.



- (4) Click the **Change Optics** button.
- (5) The message to confirm the switching appears. Confirm the selected content and click the **Yes** button to switch the optics.

## 6.4 Observing a sample













Observe a sample using the sample observation camera.








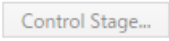






- (1) Click **Camera - Sample Camera** in the **Home** tab to display the **Sample Camera** panel.



- (2) To start capturing with the sample camera, click the  (Start capture) button.
- (3) To stop capturing with the sample camera, click the  (Stop capture) button.

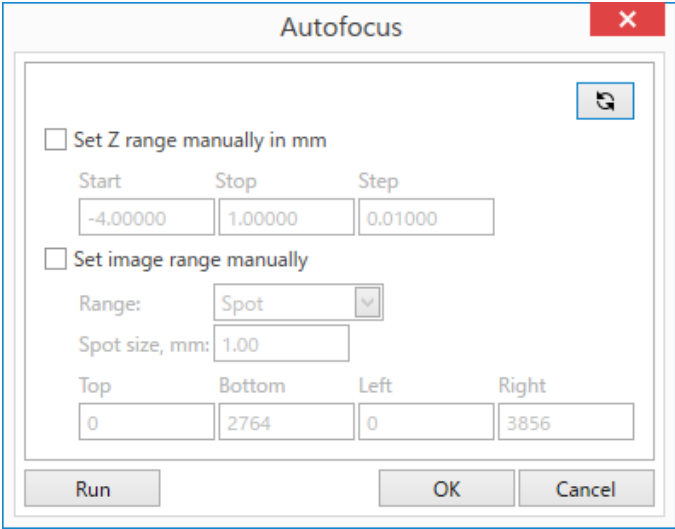
The description of the **Sample Camera** panel is as follows:

		
	(Start capture)	Starts image capturing with the sample camera.
	(Stop capture)	Stops image capturing with the sample camera.
	(Image copy)	Copies the images stores in a selected tab to the clipboard.
	(Export image)	Exports the images stored in a selected tab.
	(Grid)	Select a grid type from <b>Cross</b> , <b>Mesh</b> , or <b>None</b> .
	(Auto focus)	Opens the <b>Autofocus</b> dialog box to set conditions. Perform the autofocus to the selected measurement points.   <a href="#">Autofocus dialog box</a>
	(Start monitoring)	Start monitoring the contrast value within the autofocus range of the image being captured. This value is used to adjust the sample height when using a sample stage with no motorized Z axis.
	(Beam)	Shows or hides the sample irradiation area. The X-ray incident angle and direct beam radius can be edited in the <b>Image Viewer Settings</b> dialog box.   <a href="#">Image Viewer Settings dialog box</a>
	(Scale)	Shows or hides the scale.

	(Move to capture position)	Moves the sample camera to the capture position.
	(Lens ratio)	Select the lens magnification of the sample observation camera. The lens magnification selected here must be the same as that of the actual sample observation camera. Confirm it before capturing images or taking snapshot images.
	(Binning)	Select the binning rate of captured images from <b>1x1</b> , <b>2x2</b> , or <b>4x4</b> .
	(LED light ON / LED light OFF)	Turns on or off the sample camera's LED.
	(Brightness)	Adjusts the brightness of the sample observation camera.
	(Digital Zoom)	Changes the digital zoom magnification of captured images.
	(Move to position)	Moves the stage to a clicked position on a captured image.
		Opens the <b>Control Stage</b> dialog box.  <a href="#">Control Stage dialog box</a>
	(Show coordinate)	Shows or hides the coordinate.
	(Number style)	Select a display format of measurement points that are displayed when the Loop (Mapping) Part Activity is performed: <b>Highlight</b> , <b>Standard</b> , <b>Highlight with point</b> , <b>Standard with point</b> or <b>Hide</b> .
	(Image viewer settings)	Opens the <b>Image Viewer Settings</b> dialog box.  <a href="#">Image Viewer Settings dialog box</a>
	(Reset)	Resets the measurement points list that is displayed after the Loop (Mapping) Part Activity ended.

**Autofocus dialog box**

Perform the Z axis adjustment based on the sample observation camera’s contrast.



**Set Z range manually in mm** Enables setting the Z axis adjustment range for the autofocus. Enter values in the **Start**, **Stop**, and **Step** boxes.

**Set image range manually** Enables setting the image range for the autofocus. When the check box is cleared, the entire image will be displayed.

**Range** Select **Manual** or **Spot**.

Manual	Enter the values in the <b>Top</b> , <b>Bottom</b> , <b>Left</b> and <b>Right</b> boxes to specify the range.
Spot	Enter the desired distance from the center of the image in the <b>Spot size</b> box.

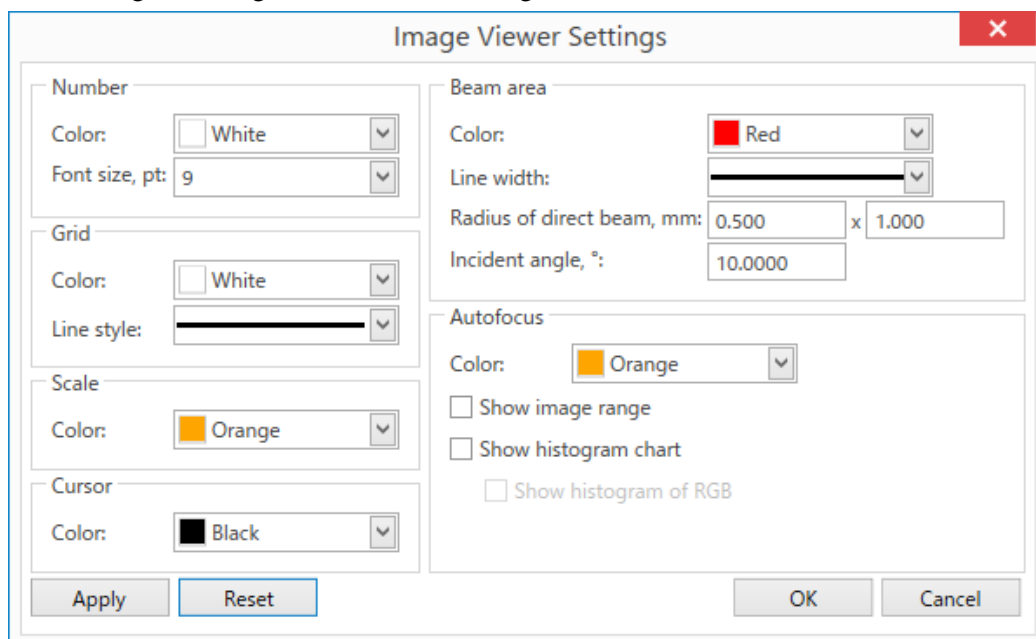
**Run** Runs the Z axis adjustment under the set conditions.

**OK** Sets the conditions and closes the dialog box.

**Cancel** Closes the dialog box without setting the conditions.

**Image Viewer Settings dialog box**

Perform the settings for Image Viewer in this dialog box.

**Number**

Set the font color and font size of the number.

**Grid**

Set the color and line type of the grid.

**Scale**

Set the color of the scale.

**Cursor**

Set the color of the cursor.

**Beam area**

Set the color and line width of the beam area. Set the rectangular irradiation field based on the direct beam radius and incident angle.

**Autofocus**

Set the color of the autofocus range and whether to show or hide the histogram chart.

**Apply**

Applies the entered conditions to the Image Viewer.

**Reset**

Resets the conditions to the initial values.

**OK**

Sets the conditions and closes the dialog box.

**Cancel**

Closes the dialog box without setting the conditions.

**Control Stage dialog box**

Perform the measurement point settings in this dialog box.

	Current	Move to		Step
X, mm	0.0000	0.0000	Move	0.0200
Y, mm	0.0000	0.0000	Move	0.0200
Z, mm	1.01000	0.00000	Move	0.02000
φ		0	Move	0

Move method: ☒ Step ☐ Continuous

X-Y: [Left Arrow] [Up Arrow] [Right Arrow]  
 [Left Arrow] [Add Icon] [Right Arrow]  
 [Left Arrow] [Down Arrow] [Right Arrow]

Z: [Up Arrow]  
 [Add Icon]  
 [Down Arrow]

φ: [Left Arrow] [Add Icon] [Right Arrow]

Close

**Current**

Displays the current position of each axis of the sample stage.

**Move to**

Enter the destination of each axis of the sample stage. Click the **Move** button to move the corresponding axis to the position entered in the box.

**Step**

Enter the step width for moving the corresponding axis when **Step** is selected at **Move method**.

**Move method**

Select **Step** or **Continuous**. If **Step** is selected here, the corresponding axis of the stage will move the step width per click in the clicked arrow's direction. If **Continuous** is selected here, the corresponding axis of the stage will keep moving in the clicked arrow's direction while clicking it.

**X-Y**

Moves the X or Y axis in the clicked arrow's direction.

**Z**

Moves the Z axis in the clicked arrow's direction.

**φ**

Moves the φ axis in the clicked arrow's direction.

**Close**

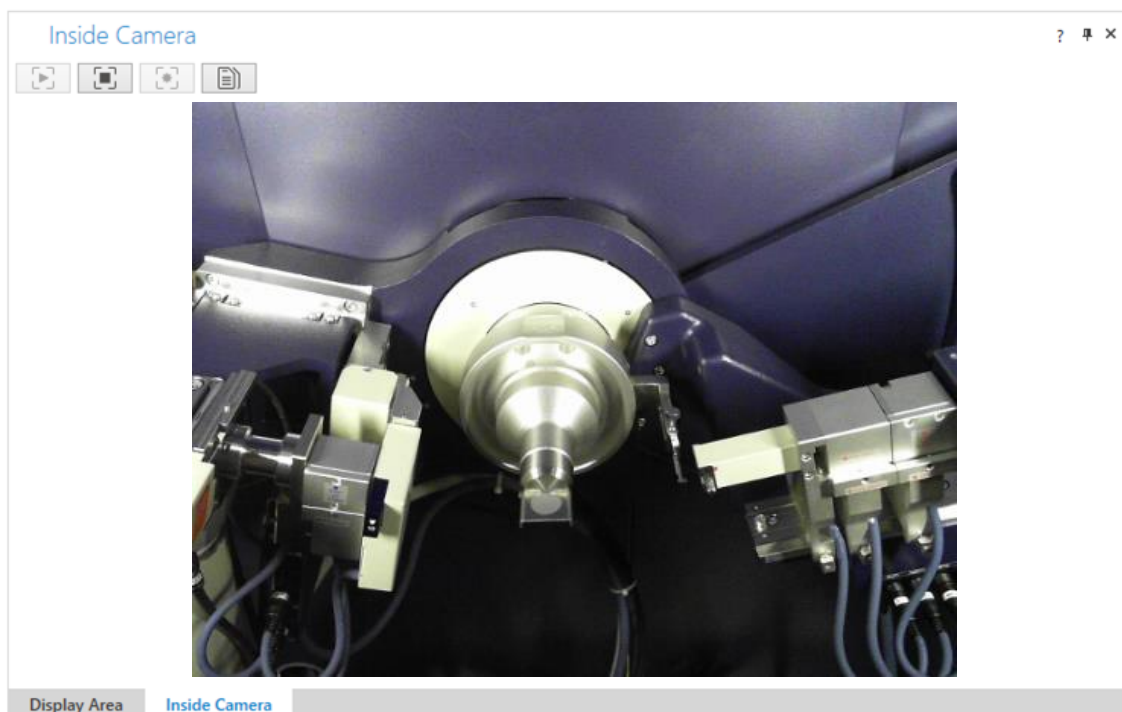
Closes the **Control Stage** dialog box.





## 6.5 Capturing images of the inside









The images of the inside of the instrument can be acquired using the inside camera.

- (1) Click **Camera - Inside Camera** in the **Home** tab to display the **Inside Camera** panel.



- (2) To start capturing with the inside camera, click the  (Start capture) button.
- (3) To stop capturing with the inside camera, click the  (Stop capture) button.

The description of the **Inside Camera** panel is as follows:

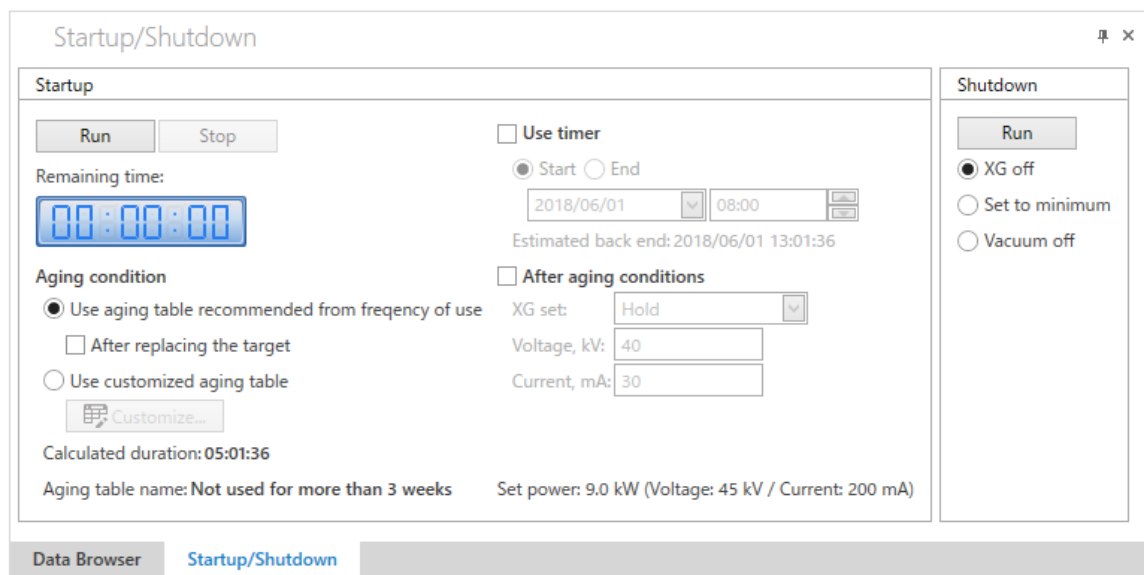
				
 (Start capture)	Starts image capturing with the inside camera.			
 (Stop capture)	Stops image capturing with the inside camera.			
 (Settings)	Opens a dialog box for the inside camera settings.			
 (Image copy)	Copies the images stores in a selected tab to the clipboard.			



## 7 Turning off X-ray generation

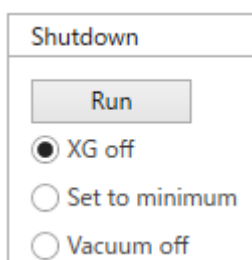
After all measurements are completed, turn off the X-ray generation according to the procedure described below.

- (1) Click **Home – Startup/Shutdown** on the Ribbon to display the **Startup / Shutdown** panel.



The screenshot shows the 'Startup/Shutdown' panel with two main sections: 'Startup' and 'Shutdown'. The 'Startup' section includes a 'Run' button, a 'Stop' button, a 'Remaining time' digital display showing '00:00:00', and a 'Use timer' checkbox. Below the timer is a date and time selector set to '2018/06/01' and '08:00', with an 'Estimated back end' of '2018/06/01 13:01:36'. The 'Aging condition' section has three radio buttons: 'Use aging table recommended from frequency of use' (selected), 'After replacing the target', and 'Use customized aging table'. There is also a 'Customize...' button. The 'After aging conditions' section has a checkbox and three input fields: 'XG set' (set to 'Hold'), 'Voltage, kV' (set to '40'), and 'Current, mA' (set to '30'). At the bottom, it shows 'Calculated duration: 05:01:36', 'Aging table name: Not used for more than 3 weeks', and 'Set power: 9.0 kW (Voltage: 45 kV / Current: 200 mA)'. The 'Shutdown' section on the right has a 'Run' button and three radio buttons: 'XG off' (selected), 'Set to minimum', and 'Vacuum off'. The panel has a title bar with a maximize and close button. At the bottom, there are tabs for 'Data Browser' and 'Startup/Shutdown'.

- (2) Select **XG off** under **Shutdown**. Click the **Run** button.



This is a close-up of the 'Shutdown' section of the panel. It features a 'Run' button at the top, followed by three radio buttons: 'XG off' (which is selected), 'Set to minimum', and 'Vacuum off'.

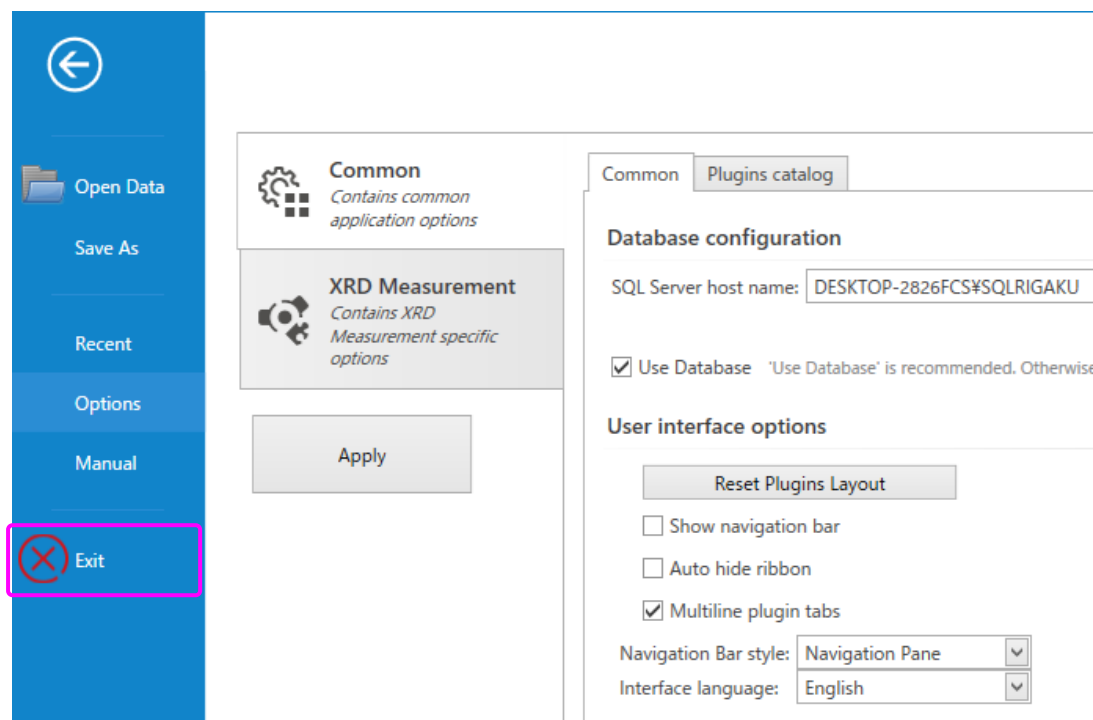
- (3) The X-ray generation will be turned off within a few minutes after clicking the **Run** button.



## 8 Exiting SmartLab Studio II

After turning off the X-ray generator, shut down SmartLab Studio II according to the procedure described below.

- (1) To shut down the SmartLab Studio II program, Click **File — Exit** on the Ribbon or click the “x” button in the main window.



- (2) Turn off the power of the SmartLab control PC and the SmartLab main unit.



**CAUTION:** For details on how to turn off the system, refer to the Quick start guide.

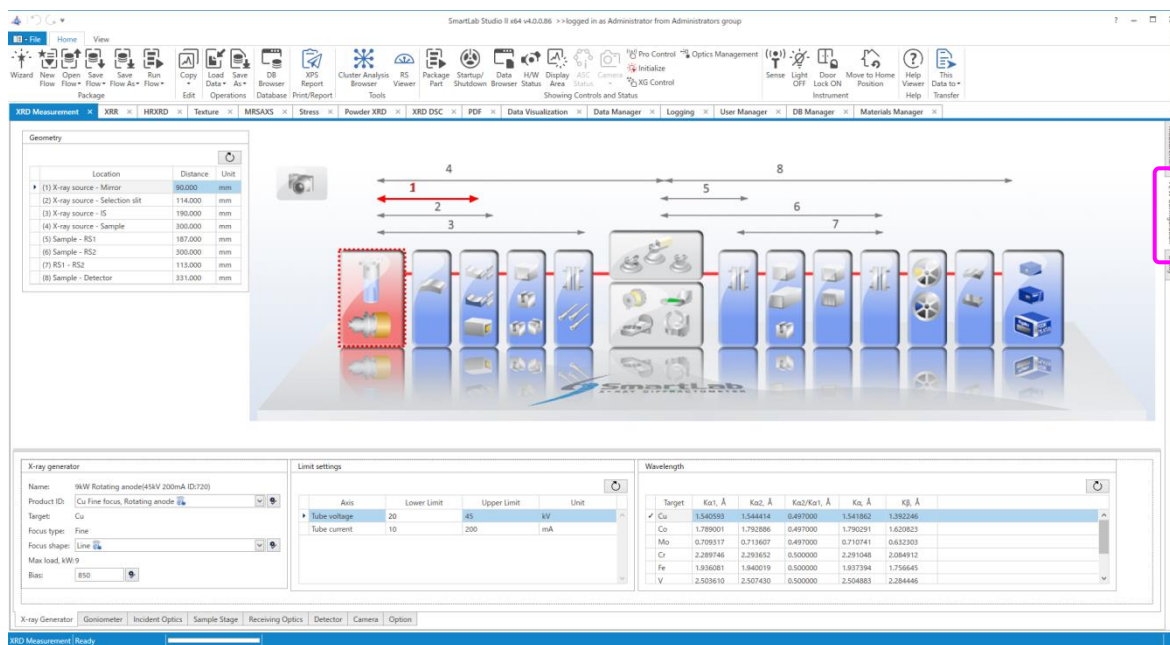


## 9 Administrator Menus


### 9.1 Hardware Configuration panel

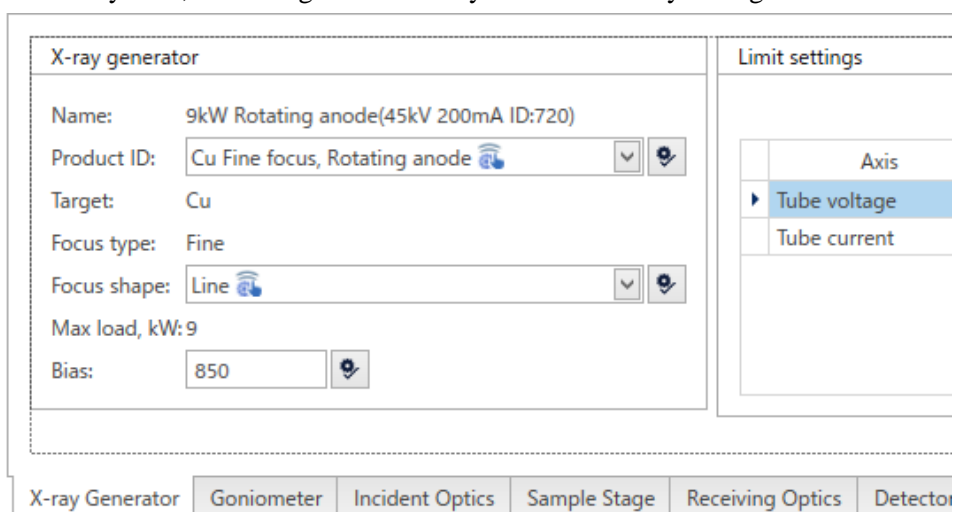
Detailed instrument configuration and limit settings for the SmartLab system can be changed and confirmed in the **Hardware Configuration** panel.



- (1) Click the **H/W Configuration** tab. The **Hardware Configuration** panel appears.

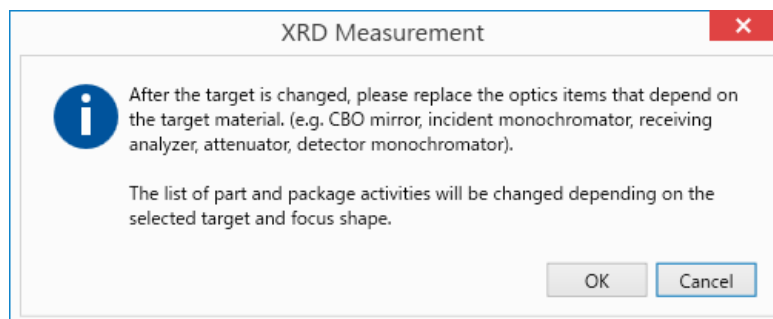


#### 9.1.1 Changing the X-ray tube

- (1) Click the **X-ray generator** tab on the **Hardware Configuration** panel. The **X-ray generator** panel appears. In the **Product ID** box, an  icon is shown next to the name of the X-ray tube, indicating that the X-ray tube is currently configured.



- (2) Click  next to the **Product ID** box, select the X-ray tube name, and click the  (Apply) button. A message appears indicating that the optics items that depend on the target material need to be replaced.
- (3) Replace the optics items that depend on the target material according to the following message.



- (4) Click the **OK** button.

### 9.1.2 Checking the settings of X-ray generator

- (1) Click the **X-ray generator** tab on the **Hardware Configuration** panel. The **X-ray generator** panel appears.
- (2) Check the values of **Lower Limit** and **Upper Limit** for tube voltage and tube current on **Limit settings**.

	Axis	Lower Limit	Upper Limit	Unit	
▶	Tube voltage	20	45	kV	^
	Tube current	10	200	mA	

- (3) Check the wavelengths set for the different target elements on **Wavelength**.

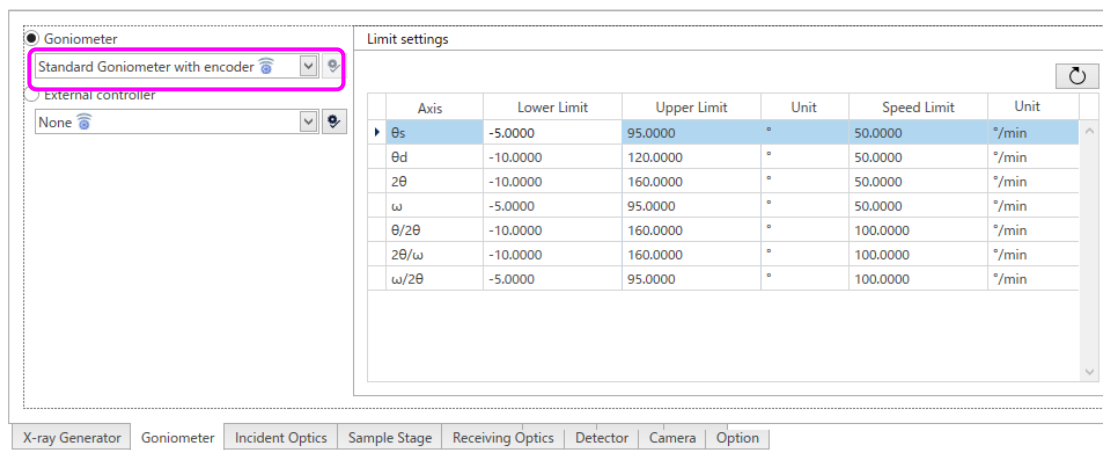
	Target	K $\alpha$ 1, Å	K $\alpha$ 2, Å	K $\alpha$ 2/K $\alpha$ 1, Å	K $\alpha$ , Å	K $\beta$ , Å
✓	Cu	1.540593	1.544414	0.497000	1.541862	1.392246
	Co	1.789001	1.792886	0.497000	1.790291	1.620823
	Mo	0.709317	0.713607	0.497000	0.710741	0.632303
	Cr	2.289746	2.293652	0.500000	2.291048	2.084912
	Fe	1.936081	1.940019	0.500000	1.937394	1.756645
	V	2.503610	2.507430	0.500000	2.504883	2.284446



### 9.1.3 Checking the limit settings of units

Check the **Lower Limit**, **Upper Limit** values etc. set on the axes of each unit (goniometer, incident optics, sample stage, and receiving optics).

- (1) Click one of the **Goniometer**, **Incident Optics**, **Sample stage**, or **Receiving optics** tab on the **Hardware Configuration** panel to display the corresponding panel.

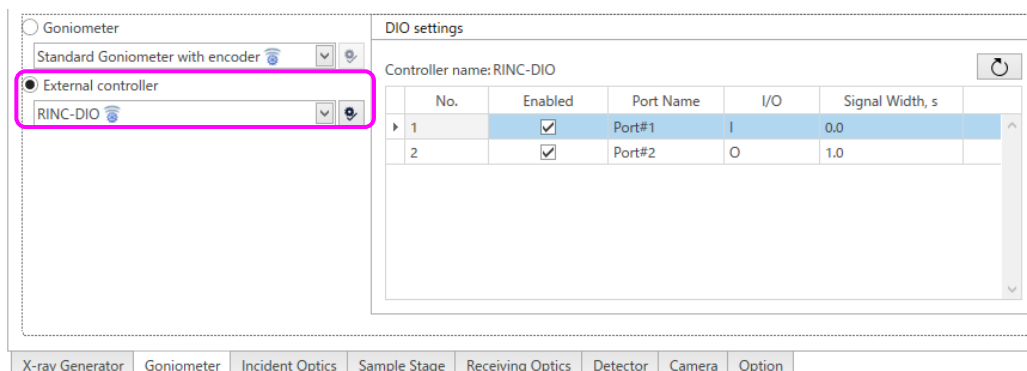


- (2) Select the unit to check from the unit box (here, from the **Goniometer** box). The **Lower Limit**, **Upper Limit** values etc. are displayed on **Limit settings**.

### 9.1.4 Confirming the external controller settings

Combination of External Trigger/IO Part Activity or Loop Part Activity with a measurement Part Activity enables the measurement synchronized with the external controller.

- (1) Click the **Goniometer** tab on the **Hardware Configuration** panel to display the **Goniometer** panel.



### 9.1.5 Checking the results of detector adjustment

Check the result of a detector adjustment performed with the Package Activity for detector adjustment.

- (1) Click the **Detector** tab on the **Hardware Configuration** panel. The **Detector** panel appears.

The screenshot shows the 'Hardware Configuration' panel with the 'Detector' tab selected. The 'Detector' section has three radio buttons: 'Detector' (selected), 'Detector monochromator', and 'Detector # 2'. Below each radio button is a dropdown menu. The 'Detector' dropdown shows 'D/teX Ultra 250'. The 'Detector monochromator' dropdown shows 'None'. The 'Detector # 2' dropdown shows 'None'. To the right is the 'Limit settings' section, which contains a table with columns: Axis, Lower Limit, Upper Limit, Unit, Speed Limit, and Unit. The table has one row: PHA, 0, 511, div., ----, div./min. At the bottom of the panel is a tab bar with 'X-ray Generator', 'Goniometer', 'Incident Optics', 'Sample Stage', 'Receiving Optics', 'Detector' (selected), 'Camera', and 'Option'.

Axis	Lower Limit	Upper Limit	Unit	Speed Limit	Unit
PHA	0	511	div.	----	div./min

- (2) In the **Detector** panel, select the **Detector** option button and the name of the detector to check the result from the box. The set values will be displayed.

The screenshot shows the 'Energy threshold settings' and 'Geometry' sections. The 'Energy mode' is set to 'Standard'. The 'Energy threshold settings' section contains a table with columns: Wavelength, Lower Energy, div, and Upper Energy, div. The table has two main sections: Cu and Co. The Cu section has four rows: Kα, Kα1, Kα2, and Kβ. The Co section has two rows: Kα and Kα1. The 'Geometry' section has two input fields: 'Reference position, pixel' (128.50) and 'Distance between sample and detector, mm' (300.00).

Wavelength	Lower Energy, div	Upper Energy, div
▲ Cu		
Kα	30	50
Kα1	30	50
Kα2	30	50
Kβ	30	50
▲ Co		
Kα	30	50
Kα1	30	50

Note: The displayed items vary depending on the detector type.

### 9.1.6 Checking the settings of the sample camera

- (1) Click the **Camera** tab on the **Hardware Configuration** panel. The **Camera** panel appears.

The screenshot shows the 'Camera' tab selected in the 'Hardware Configuration' panel. The panel is divided into two main sections: 'Sample camera' on the left and 'Camera settings' on the right. The 'Sample camera' section has a dropdown menu showing 'Above type' with a camera icon and a refresh button. The 'Camera settings' section includes a refresh button, 'Camera type: SENTEC', 'Width, pixel: 640', 'Height, pixel: 480', 'Lens ratio: 0.6x' with a dropdown and camera icon, and two input fields for 'Pixels size of X, μm' and 'Pixels size of Y, μm', both set to 12.33. At the bottom, a horizontal tab bar contains the following tabs: X-ray Generator, Goniometer, Incident Optics, Sample Stage, Receiving Optics, Detector, Camera (selected), and Option.

Sample camera	
Above type	

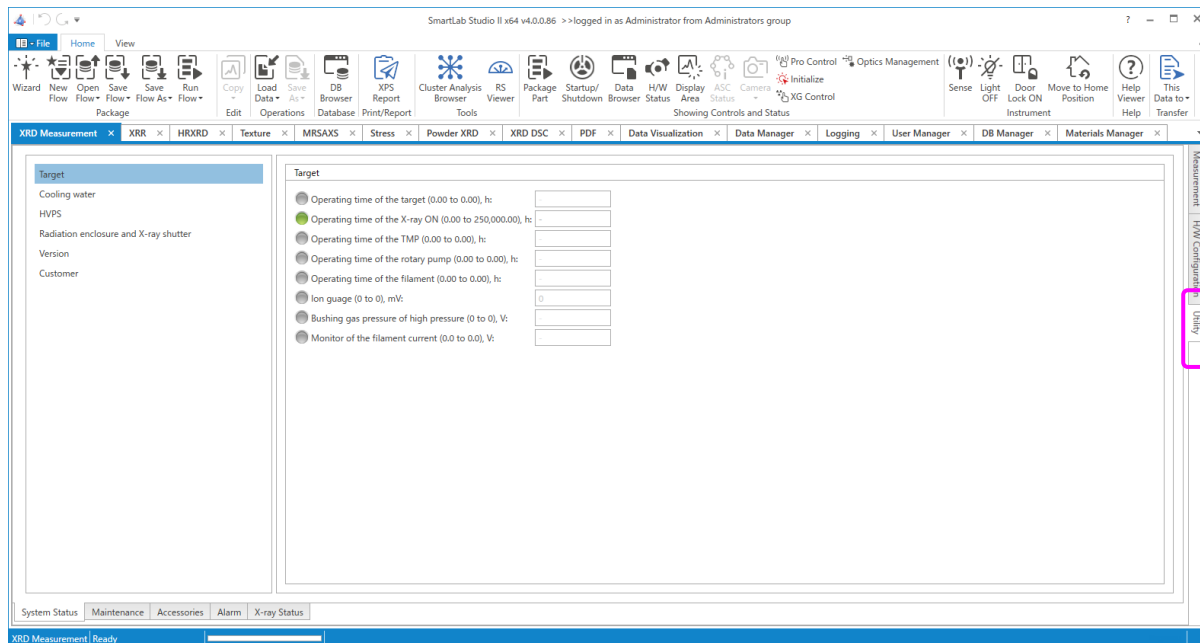
Camera settings	
Camera type:	SENTEC
Width, pixel:	640
Height, pixel:	480
Lens ratio:	0.6x
Pixels size of X, μm:	12.33
Pixels size of Y, μm:	12.33

X-ray Generator	Goniometer	Incident Optics	Sample Stage	Receiving Optics	Detector	Camera	Option
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## 9.2 Utility panel

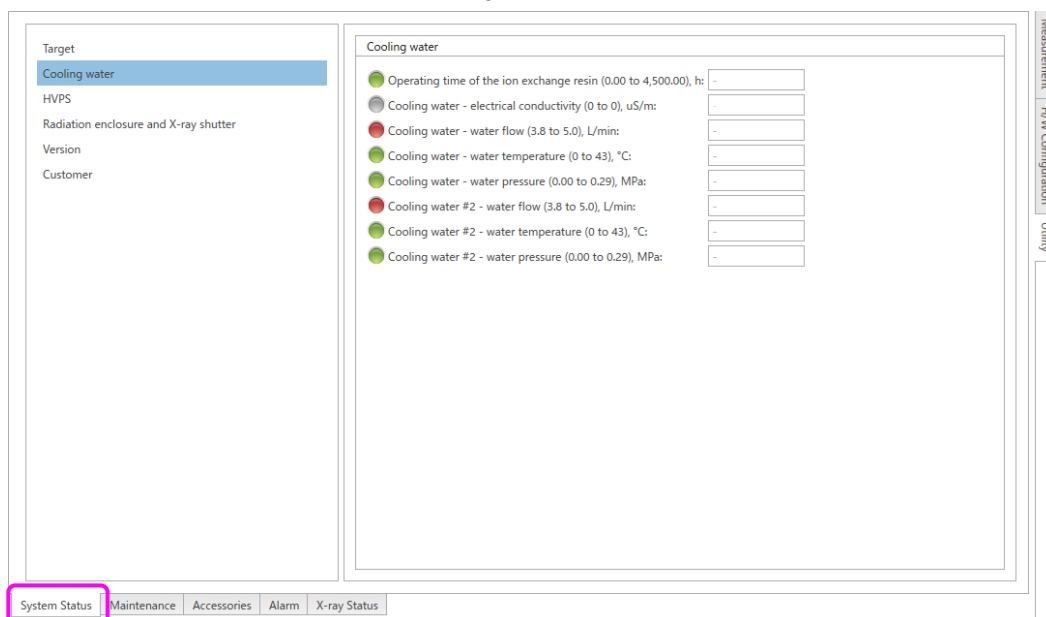
The **Utility** panel allows displaying detailed information on SmartLab, managing service parts, and viewing alarms, accessories, and the usage history of the X-ray generator.

- (1) Click the **Utility** tab. The **Utility** panel appears.



### 9.2.1 Viewing the detailed instrument status

- (1) Click the **System Status** tab on the **Utility** panel. The **System Status** panel appears.
- (2) The color of the circles displayed on the left of each item indicates its current status. Green indicates normal operation, red indicates abnormalities, and gray indicates items that are not included in the hardware configuration.



### 9.2.2 Registering the X-ray tube exchange history

- (1) Click the **Maintenance** tab on the **Utility** panel. The **Maintenance** panel appears.
- (2) Click the **Target Manager** tab.

No.	Product ID	Target Name	Use Start Date	Use End Date
1	Cu Fine focus, Rotating anode	Cu Fine focus, Rotating anode-1		

Target Exchange **Target Manager**

System Status Maintenance Accessories Alarm X-ray Status

- (3) Click the **Add** button. The **Edit Target Information** dialog box appears.

**Edit Target Information** [X]

Target name: Cu Fine focus, Rotating anode-2

Product ID: Cu Fine focus, Rotating anode ▼

OK Cancel

- (4) Enter the name of the newly installed X-ray tube (any desired name) in the **Target name** box, then click ▼ next to the **Product ID** box and select the product ID.
- (5) Click the **OK** button to close the **Edit Target Information** dialog box.

- (6) Click the **Target Exchange** tab.

Exchange Cu Fine focus, Rotating anode-2 Delete Save As...

Target

No.	Date of Exchange	Product ID	Target Name	Operator	Op
1	2017-11-20 13:17:19	Cu Fine focus, Rotating anode	Cu Fine focus, Rotating anode-1	Administrator	Exc

X-ray tube selection box

Target Exchange Target Manager

System Status Maintenance Accessories Alarm X-ray Status

- (7) Select the newly installed X-ray tube (the part name entered in step (4)) from the X-ray tube selection box, and then click the **Exchange** button. A confirmation message appears.

XRD Measurement

Do you want to exchange the selected item?

Yes No

- (8) Click the **Yes** button. The newly installed X-ray tube will be registered in the part exchange history.

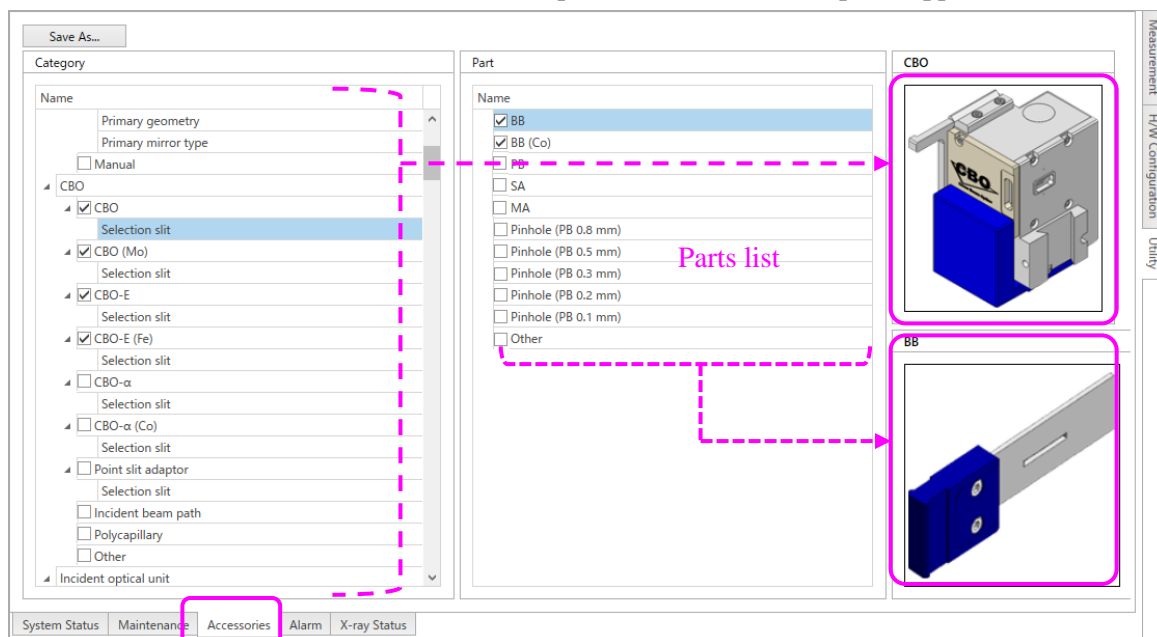
Exchange Cu Fine focus, Rotating anode-2 Delete Save As...

Target

No.	Date of Exchange	Product ID	Target Name	Operator	Operation	Accu
1	2017-11-20 13:17:19	Cu Fine focus, Rotating anode	Cu Fine focus, Rotating anode-1	Administrator	Exchange	0.00
2	2017-11-21 14:47:18	Cu Fine focus, Rotating anode	Cu Fine focus, Rotating anode-2	Administrator	Exchange	0.00

### 9.2.3 Viewing the accessories

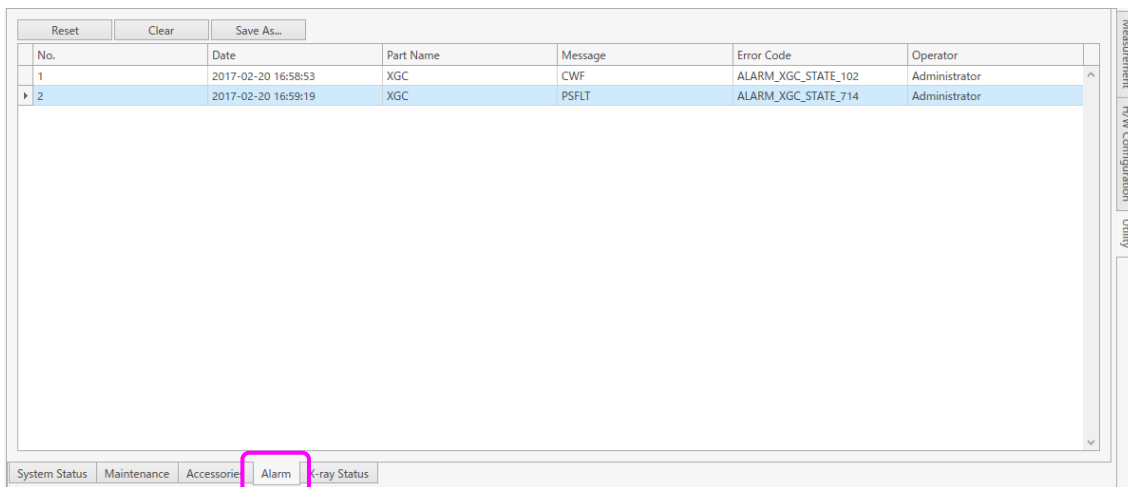
- (1) Click the **Accessories** tab in the **Utility** panel. The **Accessories** panel appears.



- (2) Select the name of the unit to view in **Category**. The list of the parts constituting the unit and their figures will be displayed. The unit names with check marks in the **Name** of parts list indicate purchased accessories.

### 9.2.4 Viewing the alarm history

- (1) Click the **Alarm** tab on the **Utility** panel. The **Alarm** panel appears.

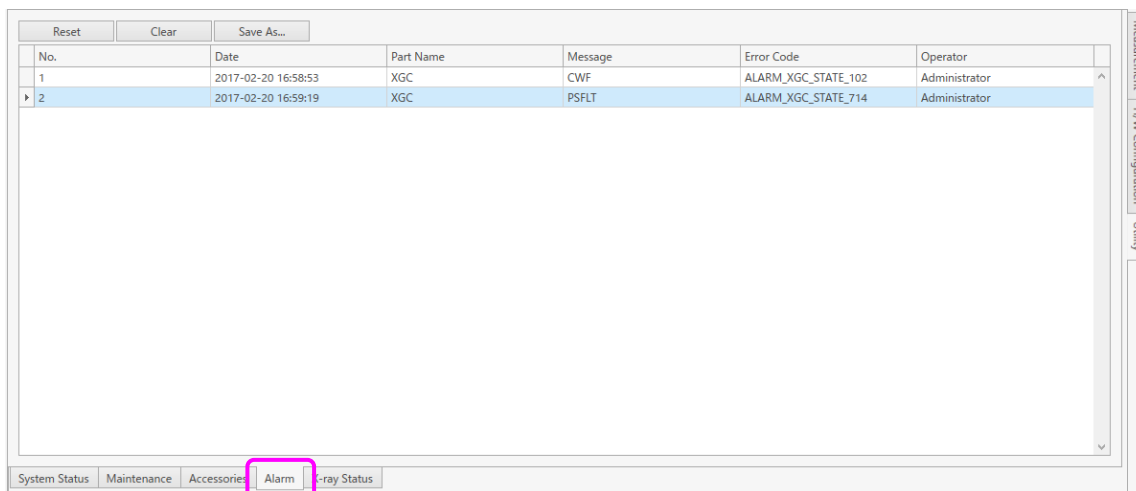




### 9.2.5 Resetting alarms

If an instrument alarm has occurred, e.g., from the water chiller, confirm the cause of the alarm, the alarm needs to be reset.

- (1) Click the **Alarm** tab on the **Utility** panel. The **Alarm** panel appears.



- (2) Click the **Reset** button on the **Alarm** panel.
- (3) A confirmation message appears. Click the **Yes** button to reset the alarm.



### 9.2.6 Viewing the usage history of the X-ray generator

The usage history of the X-ray generator can be viewed as described below.

- (1) Click the **X-ray status** tab on the **Utility** panel. In the **X-ray status** panel that appears, the usage history of the X-ray generator is displayed.

Clear		Save As...							Measurement H/W Configuration Utility
No.	Date	Part Name	Operator	State	Voltage, kV	Current, mA	Accumulated Time, h		
1	2016-11-25 17:30:39	Cu_Fine_Sealed	Administrator	X-ray On	20	10	0		
2	2016-11-28 08:43:33	Cu_Fine_Sealed	Administrator	X-ray Off	-	-	63		
3	2016-12-06 15:04:25	Cu_Fine_Sealed	Administrator	X-ray On	20	10	198		
4	2016-12-07 08:39:48	Cu_Fine_Sealed	Administrator	X-ray Off	-	-	18		
5	2016-12-07 11:34:18	Cu_Fine_Sealed	Administrator	X-ray On	20	10	3		
6	2016-12-08 08:56:01	Cu_Fine_Sealed	Administrator	X-ray Off	-	-	21		
7	2017-02-09 13:21:48	Cu_Fine_Sealed	Administrator	X-ray On	20	10	1516		
8	2017-02-09 13:23:33	Cu_Fine_Sealed	Administrator	X-ray On	25	10	0		
9	2017-02-09 13:23:34	Cu_Fine_Sealed	Administrator	X-ray On	30	10	0		
10	2017-02-09 13:23:36	Cu_Fine_Sealed	Administrator	X-ray On	35	10	0		
11	2017-02-09 13:23:37	Cu_Fine_Sealed	Administrator	X-ray On	40	10	0		
12	2017-02-09 13:23:38	Cu_Fine_Sealed	Administrator	X-ray On	40	15	0		
13	2017-02-09 13:23:40	Cu_Fine_Sealed	Administrator	X-ray On	40	20	0		
14	2017-02-09 13:23:41	Cu_Fine_Sealed	Administrator	X-ray On	40	25	0		
15	2017-02-09 13:23:42	Cu_Fine_Sealed	Administrator	X-ray On	40	30	0		
16	2017-02-09 13:31:35	Cu_Fine_Sealed	Administrator	X-ray On	40	25	0		
17	2017-02-09 13:31:36	Cu_Fine_Sealed	Administrator	X-ray On	40	20	0		
18	2017-02-09 13:31:37	Cu_Fine_Sealed	Administrator	X-ray On	40	15	0		
19	2017-02-09 13:31:39	Cu_Fine_Sealed	Administrator	X-ray On	40	10	0		
20	2017-02-09 13:31:40	Cu_Fine_Sealed	Administrator	X-ray On	35	10	0		
System Status Maintenance Accessories Alarm <b>X-ray Status</b>									

## Rigaku Corporation

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