

# DIFFRAC.SUITE

- User Manual

DIFFRAC.WIZARD

Original Instructions

The reproduction, transmission or use of this document or its contents is not permitted without express written authority. Offenders will be liable for damages. All rights reserved.

We have checked the contents of this manual for agreement with the hardware and software described. Since deviations cannot be precluded entirely, we cannot guarantee full agreement. However, the data in this manual are reviewed regularly and any necessary corrections are included in subsequent editions. Suggestions for improvement are welcome.

All configurations and specifications are subject to change without notice.

Order no. DOC-M88-EXX194 V5 based on software version V6. Updated: March 17, 2016.

© 2009 - 2016 Bruker AXS GmbH, Karlsruhe, Germany.

All trademarks and registered trademarks are the sole property of their respective owners.

Printed in the Federal Republic of Germany.

Bruker AXS GmbH  
Östliche Rheinbrückenstr. 49  
76187 Karlsruhe, Germany  
Tel. +49 721 50997-0  
Fax +49 721 50997-5654  
info.baxs@bruker.com  
www.bruker.com

# DIFFRAC.WIZARD

## Table of Contents

<b>DIFFRAC.WIZARD .....</b>	<b>1</b>
<b>WIZARD .....</b>	<b>1</b>
General .....	1
Screen Layout and Operation .....	1
Instrument selection.....	1
Menu overview.....	2
Creating a new experiment.....	3
Screen layout.....	3
<b>Basics of WIZARD .....</b>	<b>8</b>
Common modules.....	9
DAVINCI .....	9
Sequences .....	12
Profiles .....	16
XY positions .....	25
Options.....	32
Fixed drives.....	32
Summary.....	33
Application specific modules.....	34
XRD .....	34
High resolution XRD .....	43
Alu Bath .....	54
SAXS .....	55
Stress.....	64
Texture.....	74
TXRF.....	81
<b>Scan types overview .....</b>	<b>87</b>
Calibration .....	87
XRD.....	88
High resolution XRD .....	90
Alu Bath.....	91
SAXS.....	91
SCXRD.....	91
Stress.....	92
Texture .....	92
XRF .....	92
<b>Index .....</b>	<b>93</b>
<b>Index of Tables .....</b>	<b>94</b>
<b>Index of Figures.....</b>	<b>94</b>

(intentionally left blank)

# DIFFRAC.WIZARD

## WIZARD

### General

The WIZARD plug-in allows to prepare experiments in different fields of X-ray diffraction.

Experiments currently available are:

- XRD (with 0-D, 1-D and 2D detectors).
- High Resolution XRD (HR-XRD)
- Alu Bath
- SAXS (small angle X-ray scattering)
- Stress (with 0-D, 1-D and 2D detectors)
- Texture (with 0-D, 1-D and 2D detectors)
- TXRF

It is possible to edit more than one experiment at a time. Each experiment may correspond to another application. The experiments may be created for different instruments.

For some experiments, backward compatible types are available. These are intended to produce data files which can be handled by older evaluation software.

### Screen Layout and Operation

This chapter describes the layout and operations that are common for all applications.

#### Instrument selection

By default, the WIZARD uses the instrument to which the shell is connected. It is possible to load an instrument from the database or from a file. This allows the user to create experiments offline (i.e. without an instrument connection) or – while connected - by choosing any other instrument.



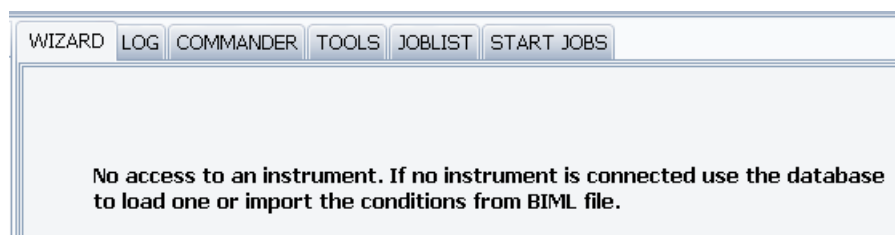
#### NOTE

If a new instrument is chosen, it will remain active for all new experiments created at a later date.

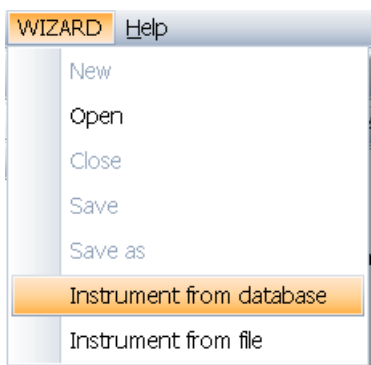
All previously created experiment will not be affected. Experiments loaded from a disk will use its own instrument.

#### Offline operation

If there is no instrument connected to the shell, the following will be displayed by WIZARD:

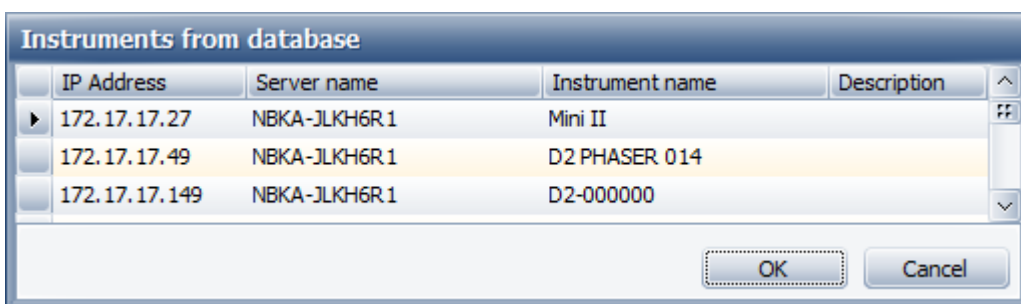


The user must load instrument conditions from the database or from a file using the WIZARD menu:



**Instrument from database**

If more than one active instrument is found in the database the following dialog opens:



Select one instrument here.

**Instrument from file**


The instrument conditions can also be loaded from the *biml file* (The biml file is a Bruker Instrument Markup Language file). This file can be saved using the Measurement Server. It is also possible to load conditions directly from a state file (a Zip file) created by the framework.

**Menu overview**

Menu	Toolbar	Action
New		Create a new experiment. See section Creating a new experiment on page 3
Save		Save an experiment as a <i>bsml</i> file.
Save as		Save an experiment as a <i>bsml</i> file under a new name
Open		Open an existing <i>bsml</i> file
Open from database		Open an existing <i>bsml</i> from database
Open from database (signed only)		In CFR21/Part11 only: Open an existing <i>bsml</i> from database which was already signed.
Save to database		Save an experiment to the database.
Save to database and sign		In CFR21/Part11 only: Sign it an experiment and save it to the database.
Print a report		Print a tabular view of the experiment, see Summary, p. 33

Close	Close the experiment
Instrument from database	Read the instrument definition from the database (see page 1)
Instrument from file	Read the instrument definition from a <i>biml</i> file (see page 1)
Adapt to current hardware	If connected to an experiment: adapt the fixed optics in the currently open experiment. For instance, if a soller or slit was exchanged since the creation of the experiment the WIZARD will be adapted accordingly.  Note: this will not affect motorized, chamber or tube settings.

### Creating a new experiment

Click on the menu item “New” or click on the toolbar button .

This provides a list of all experiment templates available. Please note that the list depends on the instrument connected to (for instance, SAXS is not available for a D8).

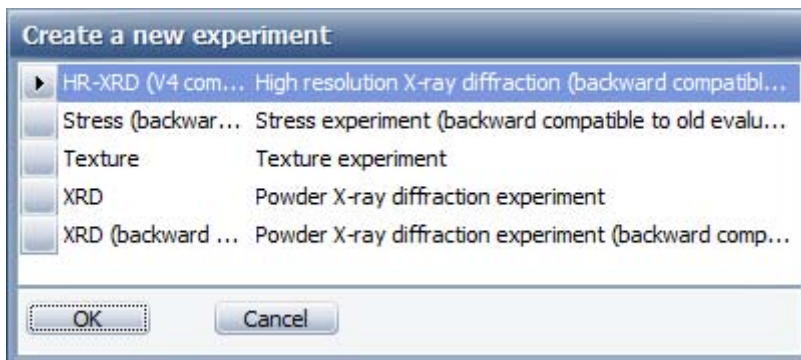


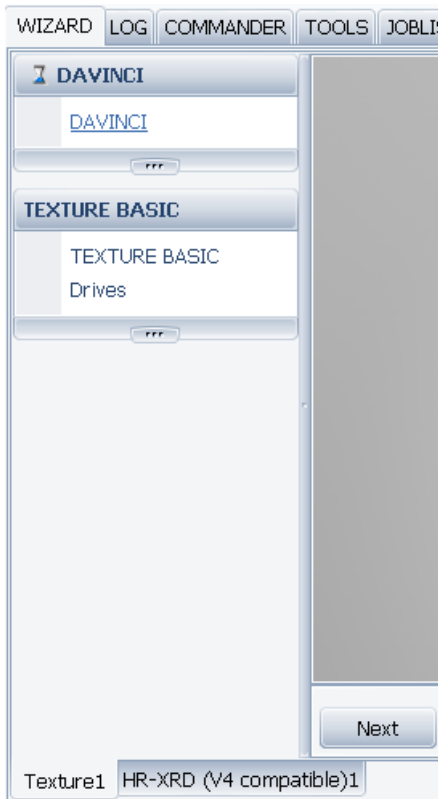
Fig. 1: Create experiment dialog

The currently available HR-XRD experiment template provides backward compatibility of the measured files with evaluation programs such as LEPTOS. If an XRD experiment is to be evaluated with old software (for instance, TOPAS) the backward compatible template should be used.

The Stress and Texture templates create experiments which can be imported by Leptos-S and MUL-TEX, respectively.

### Screen layout

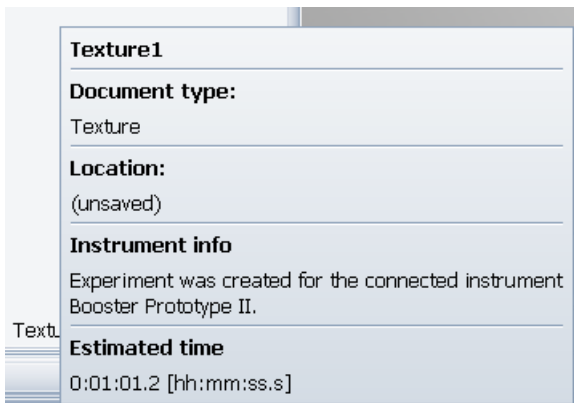
Each experiment is shown on its own tab inside the WIZARD plug-in. If two experiments are created, the layout would look similar to the layout below:



If the experiment has not yet been saved it will automatically numbered using the experiment type, for example, "Texture1".

**Experiment tooltip**

When you move the mouse cursor over the tab a tooltip appears with information about the experiment:



If saved, the name of the tab and the tooltip information will be updated accordingly:



The tooltip states the experiment template used (in the section “Document type”), the location where the file was stored (or loaded from), the instrument used to create the file and the experiment’s estimated measurement time.

**Module design**

All experiment layouts in the WIZARD plug-in follow a general design:

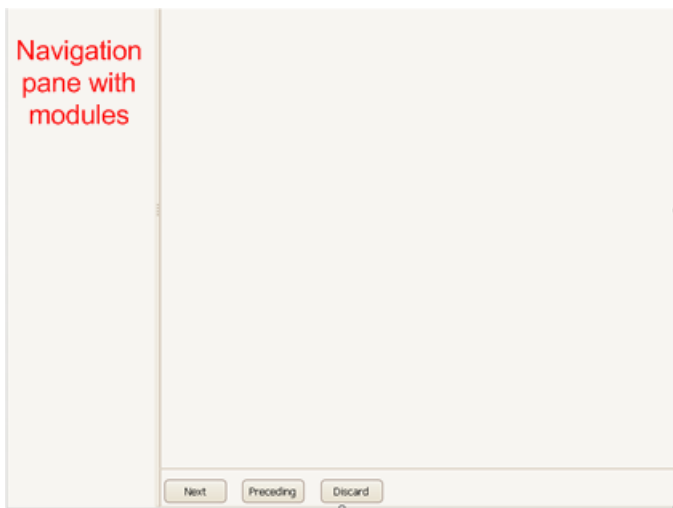
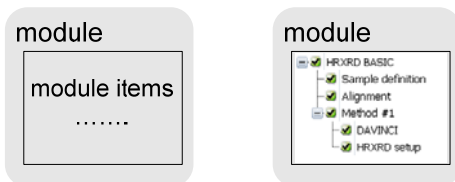


Fig. 2: WIZARD module design

To the left, a navigation pane appears. It consists of at least one module. The module may contain a varying number of module items or a tree.



Each item in a module is connected to an associated display at the right (usually a form to enter data or a graphical editor). The bottom right buttons allows the user to move to the next or preceding display or to discard all changes.



Fig. 3: WIZARD module design

### Module items and navigation

As stated above, a module may consist of one or more items. If the user moves the mouse over an item, it will be underlined and the mouse cursor changes to a hand, as in a Web browser or link. When it is clicked on, the associated display to the right displays the item content.

The Next and Preceding buttons at the lower right allow the user to navigate between different items inside one module and between various other modules.

The module can be collapsed with a click on the collapse button (Note: The button appearance and position changes according to the skin chosen for the whole shell):



### Module status

The status of a module is indicated by an icon:



content is valid



module is currently edited



content is invalid

### Modules in different experiment templates

The number of modules and the module content differ between the experiment templates:

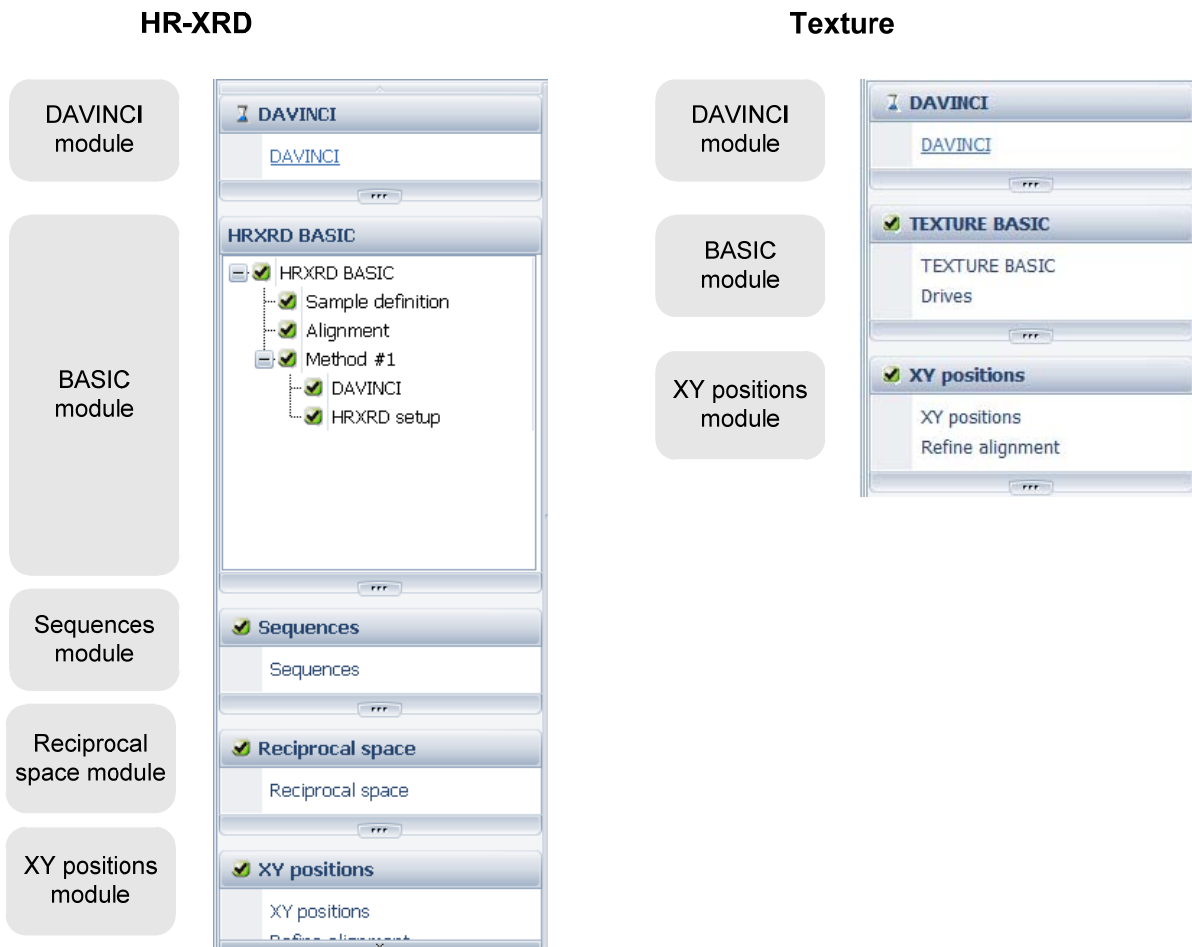


Fig. 4: Module design for HR-XRD and Texture

The DAVINCI module located at the top of the navigation bar and one basic module are common to all experiment templates. More complex experiment types (like HR-XRD) can provide many more modules.

## Basics of WIZARD

The following terms are used for the WIZARD plug-in:

### Experiment

An **experiment** describes a complete measurement to be executed as a job. An experiment is created by WIZARD from an experiment template that is application specific, for example, an HR-XRD template. An experiment is stored to the hard disk as a *bsml file* and can be measured using the START JOBS plug-in. Normally, the experiment consists of at least one base method.

### Base method

A **base method** contains exactly one scan and can move one or more drives. It can also contain a still scan without any drive movements. A base method also describes the settings of all hardware components which are not changed during the scan. The following are examples of these settings: all drives that are not moved, generator settings (like voltage and current), detector settings (like high voltage), to name just a few.

Depending on the application, it is possible to define one or more methods. These methods are independent of each other. For example, one method could describe an HR-XRD Omega-2Theta scan using a scintillation detector and the second method could describe a PSD still scan using a LYNX-EYE detector:

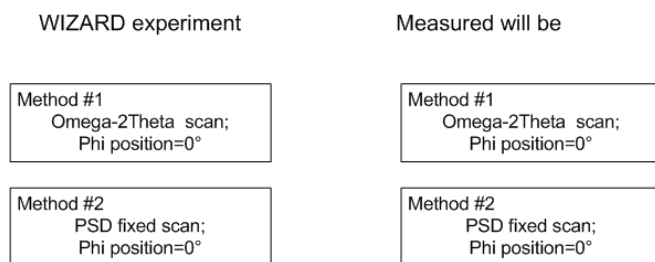


Fig. 5: WIZARD created experiment without a sequence

Because these method(s) build the basic seed for more complex measurements (please see below) they are named **base methods**.

### Sequences

The method(s) which have previously been defined can be repeated using one or more sequences. A sequence will modify one (or more) parameters of the base method(s).

We take the experiment with the two base methods from above as an example and create a sequence that modifies the Phi drive position. The aim is to measure each method at Phi = -10°, 20° and 70°.

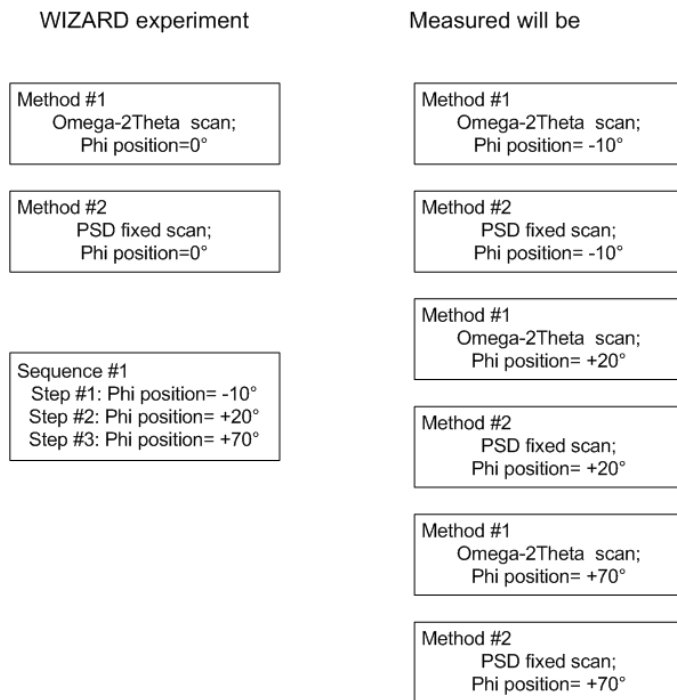


Fig. 6: WIZARD created experiment with one sequence

There will be six resulting measurements, as displayed above.

Two different types of sequences are available:

A regular sequence, which defines a parameter varying between a start and a stop value.

A step list sequence, which defines any number of steps. The parameter's value at each single step can be any value. The example above is an example of a step list sequence.

It is possible to have more than one sequence. How sequences are created is described in the section Sequences on page 12.

## Common modules

In this chapter all modules which are not specific to certain applications are described.

### DAVINCI



Fig. 7: DAVINCI module

All experiments provide a DAVINCI module on the top. In the default mode, all mounted components and their selected subcomponents of the instrument conditions are displayed. (The DAVINCI module allows changing any component to carry out the measurement.)

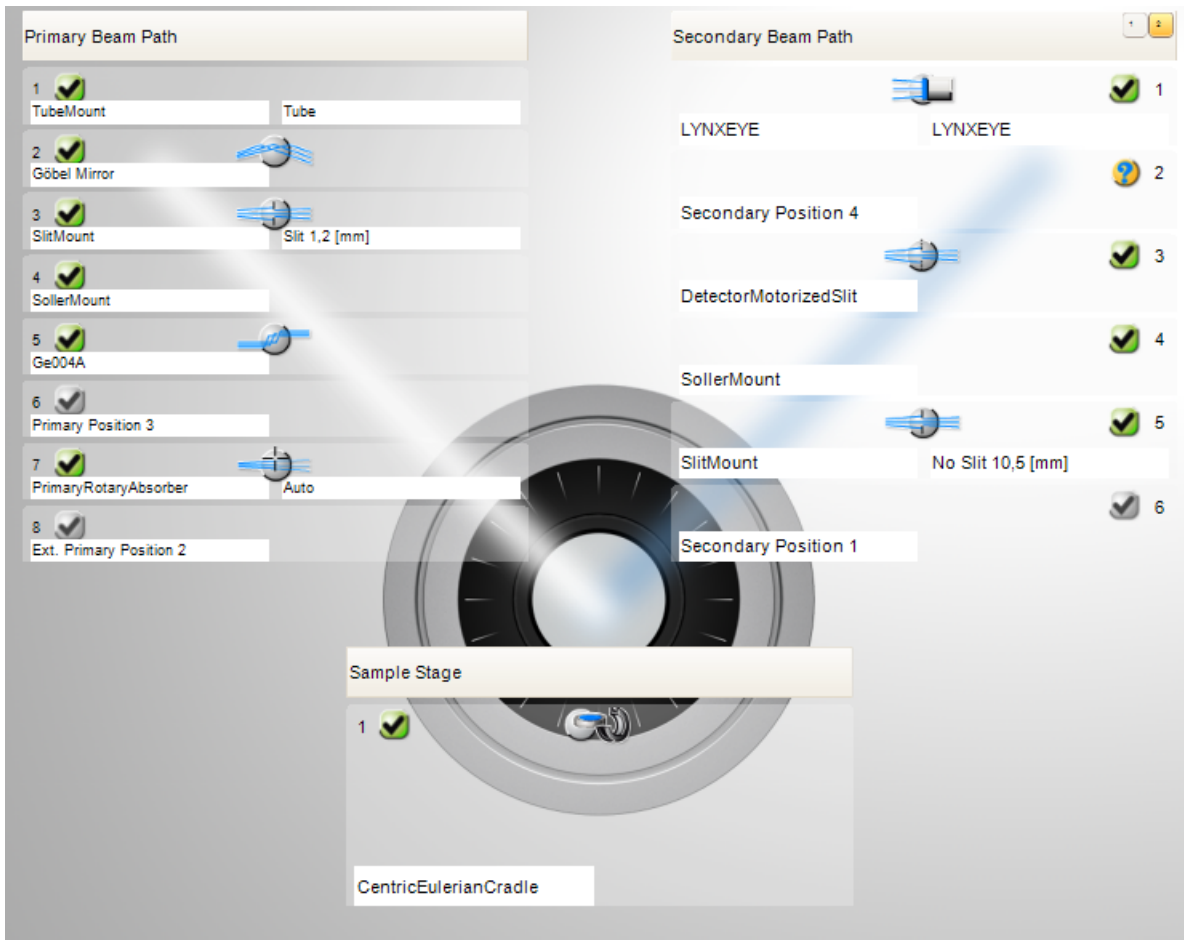


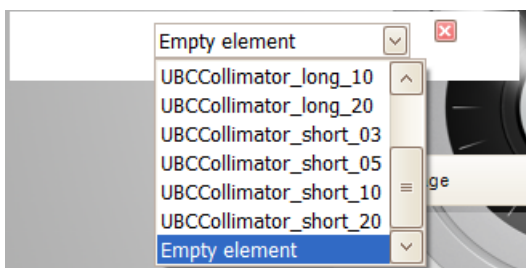
Fig. 8: DAVINCI display

**Virtually mounting components**

In the example displayed above, the Primary position 2 - which is empty in the figure above – can be changed to contain another allowed component. This means that the new component will be *virtually mounted*, i.e. it will be mounted in the WIZARD but not on the real instrument:



In the virtual goniometer, click on the last item to change the Primary position 2 from an empty element to an UBC collimator:



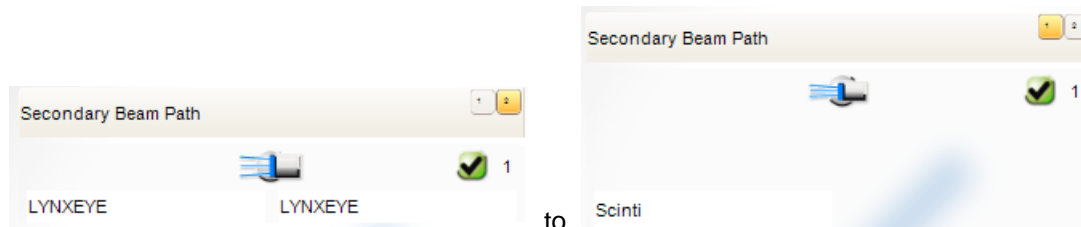
For instance, to:



If the user carries out the experiment, the UBC collimator must be mounted. Otherwise, the measurement will not begin.

It is possible to virtually un-mount a component. For example, the detector can also be changed by virtually mounting another detector in the same way.

The instrument shown above in figure 8 has a double secondary track. A second detector. can be switched by activating the corresponding track (click on the track number 1 or 2 at the upper right after "Secondary Beam Path"):



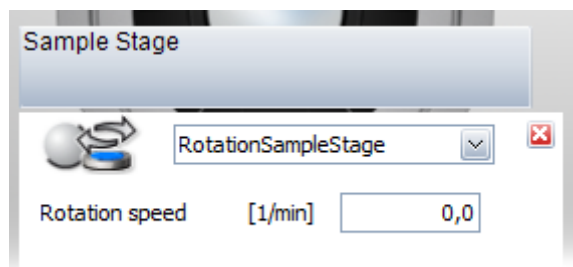
#### NOTE

If the instrumental conditions stored with the experiment do not match the current conditions when the *bsml* file is started in a job, the validation undertaken by the START JOB plug-in will fail.

Some experiment templates, such as HR-XRD allow changes in method specific DAVINCI displays i.e. for each single base method. The mount state of components cannot be changed, since this would require user interaction between measurements. However, the experiment templates allow switching all motorized components and settings (such as the slit size of a motorized slit or detector settings) and activating single tracks in a multi-track system.

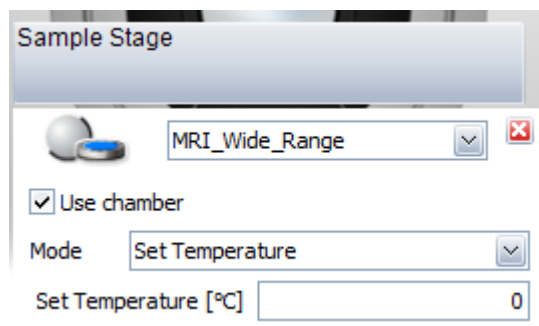
#### **Rotation and Non-ambient settings**

If the stage provides a rotation you can click on the stage to open a small dialog:



The rotation may be a variable one (as in the example shown) or a synchronous one.

If a non-ambient stage is connected temperature and other parameters can be set. For instance:



The available modes (here: Set Temperature) depend on the controller used. To ignore the chamber you have to uncheck the Use chamber field.

### Confirmation

The settings in the DAVINCI module affect the entire experiment and all base methods. When changing these settings a warning is displayed:



### NOTES

Changes in the DAVINCI module affect the entire experiment. Certain modifications, such as changing the detector slit width, will not alter a defined scan. However, choosing another detector will reset all scans to an appropriate scan type.

Therefore, the user should first decide on the principal decisions such as choosing the detector or mounting optics and then decide on the detailed experimental design.

### Sequences

A **sequence** is a variation of one or more parameters in an existing method either as a step list sequence or a regular sequence (see definitions on page 9).



Fig. 9: Sequences module

As an example, two methods are shown. In both methods it should be measured at different Phi positions (see section Basics of WIZARD on page 8).

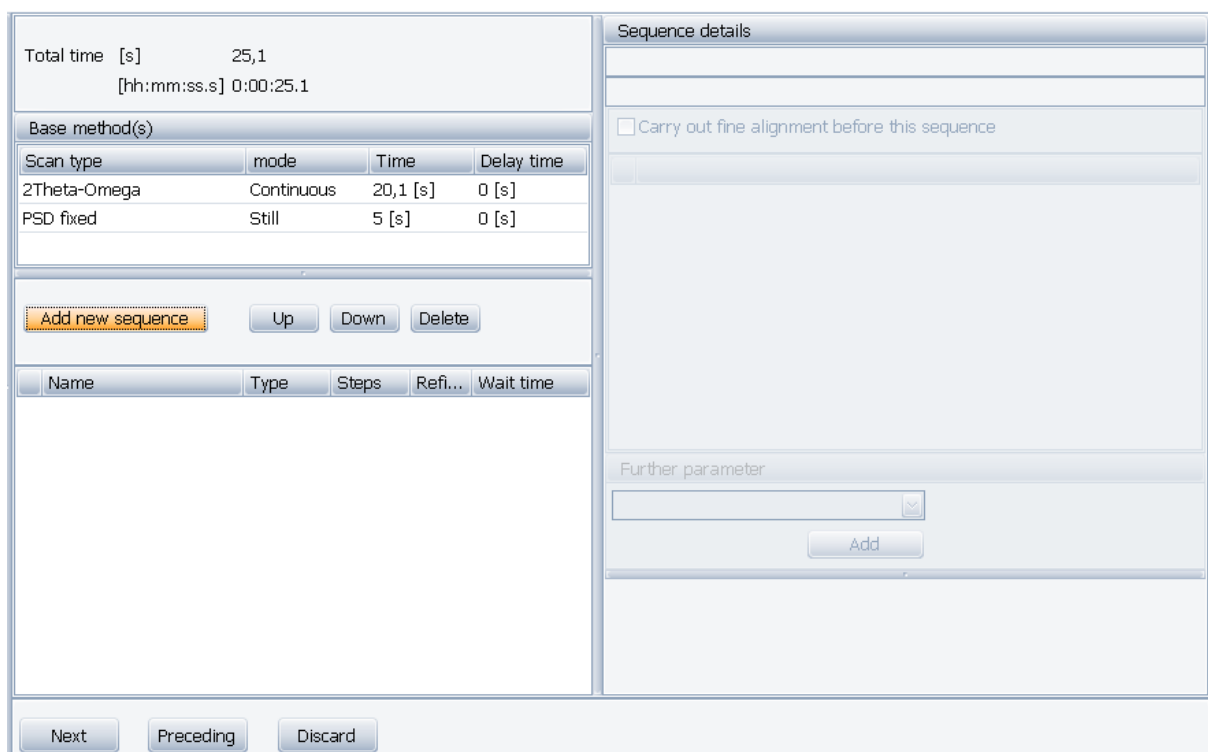



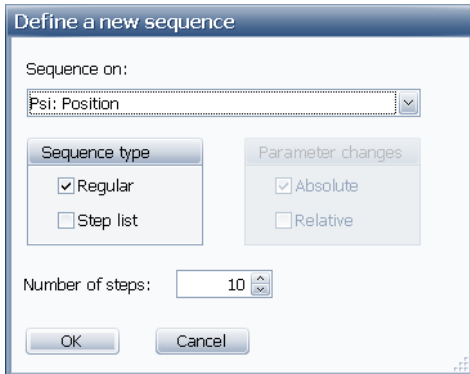
Fig. 10: Sequences display

The total time is shown at the upper left of the sequence display, followed by a list of base methods. In this example a 2Theta-Omega scan and a PSD fixed scan is shown.

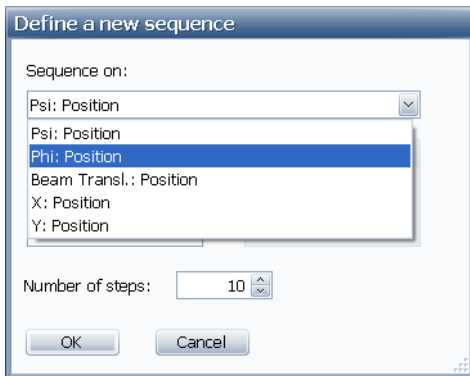
**Step list sequence**

To add a new sequence press the button  :

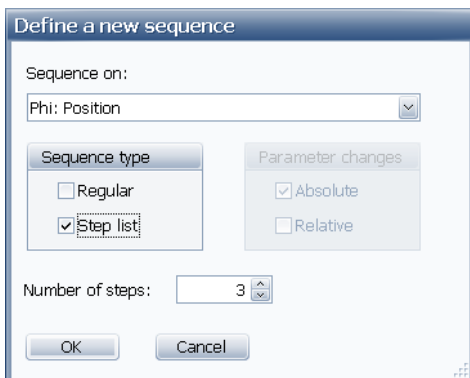
A dialog window will open:



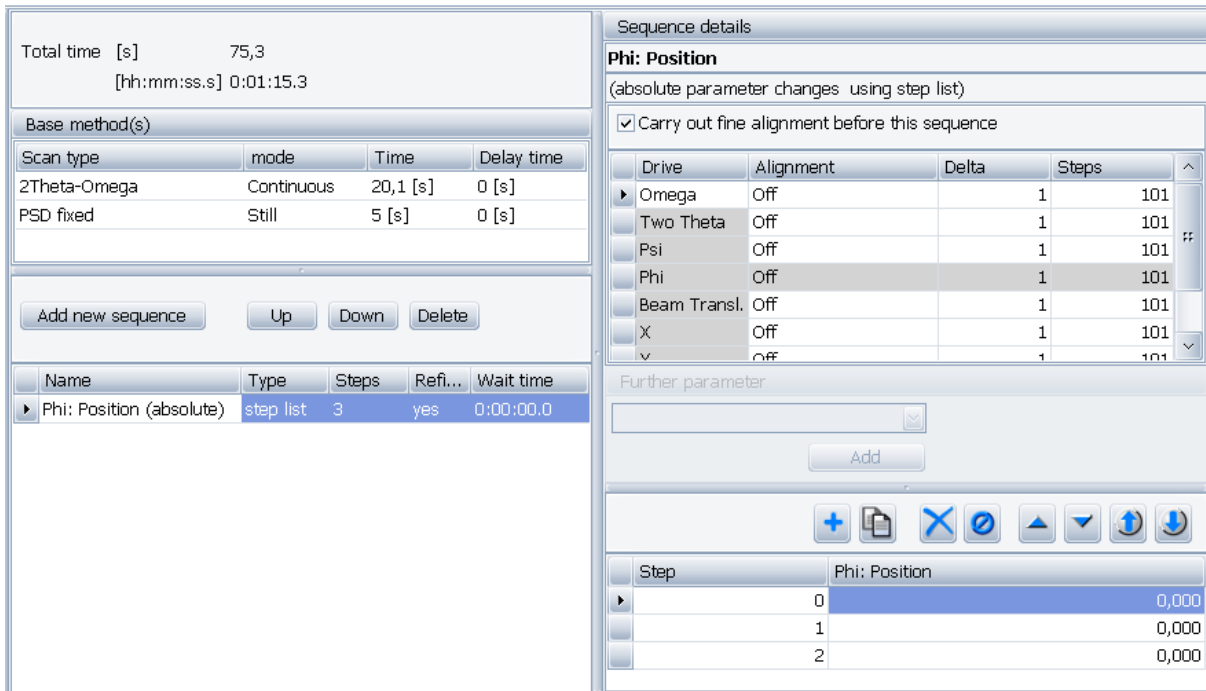
Choose "Phi: Position" from the drop-down list of available sequences.



Choose a step list sequence with 3 steps:

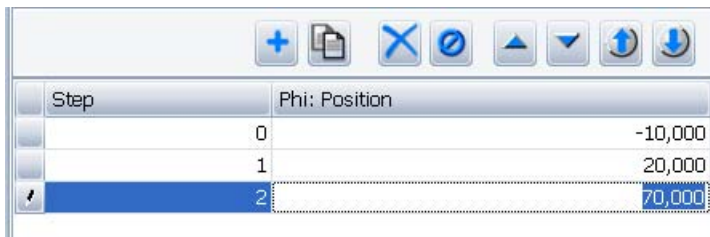


The appearance of the sequence display changes:



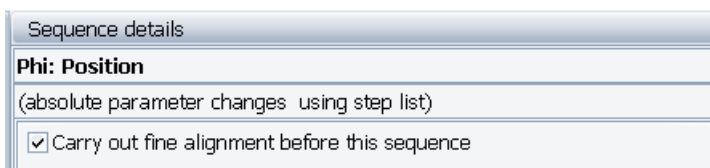
The total estimated time is updated at the top left. The sequence list contains summary information about the new Phi sequence at the lower left.

In the sequence details the Phi position values can be changed at the lower right:



An alignment can be defined in the sequence details in the upper right.

This function can be switched off by un-checking the check box:



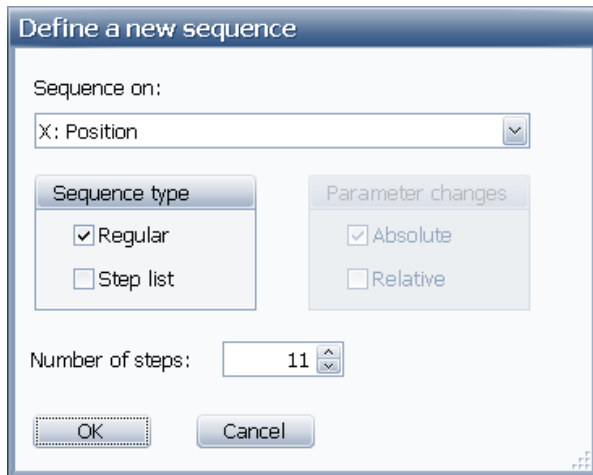
**NOTE**

How the alignment for a sequence is used depends on the measurement script.

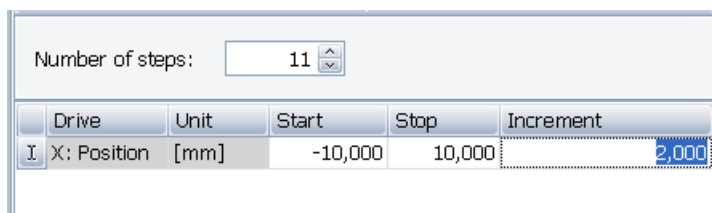
**Regular sequence**

In the following example a further sequence has been added. But now we choose a **regular sequence**. This indicates that the user is specifying a start, stop and increment.

Click on the button . Then, enter:

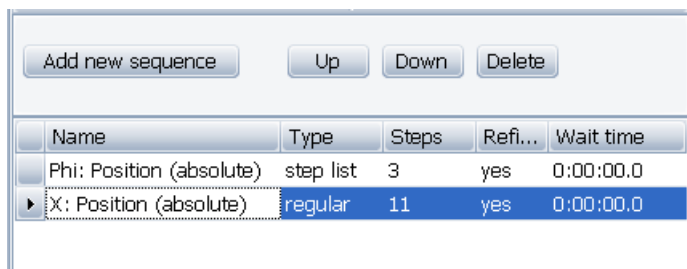


Enter the X start, stop and increment in the sequence details at the lower right.



### Changing the sequence order

To change the order of the sequence, use the sequence list. Mark the sequence and press the Up or Down button.



### Other sequence variations

Until now, only sequences with a varied parameter (in this example: a drive position) have been defined absolutely.

It is possible to define sequences for relative changes depending on the application.

Special sequences may vary. Even scan axes themselves may vary.

## Profiles

A profile is a special type of sequence and is set-up using the **Profile** module: This module provides three module items: the settings (to define the profile), a table editor and a graphical editor:

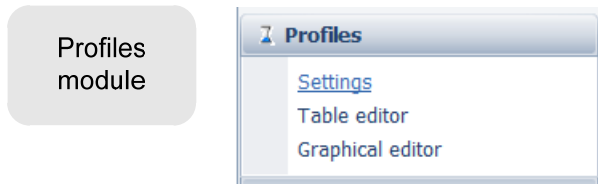


Fig. 11: Profiles module

## Introduction to profiles

For the further discussion it is useful to define several terms:

A segment is a change of one (or more) physical parameters (for instance: of a temperature) over a time interval.

A segment item is a part of a segment. It is either a delay or a measurement.

These terms may be best understood by the example shown in the following figure. It shows one parameter which varies between  $y_0$  and  $y_1$  over the time (for instance between two temperatures). Three segments are positioned on the time axis. Segment #1 is just a constant (i.e. the parameter does not vary between time  $t_0$  and  $t_1$ ), segment #2 is an increase from the parameter value  $y_0$  to  $y_1$  (for instance a heating). Segment #3 is again a constant one.

While segment# 1 provides no segment items, segment #2 consists of three items: a delay (that is: a wait time) and two measurements using different methods. Segment #3 consists of a delay and a further measurement.

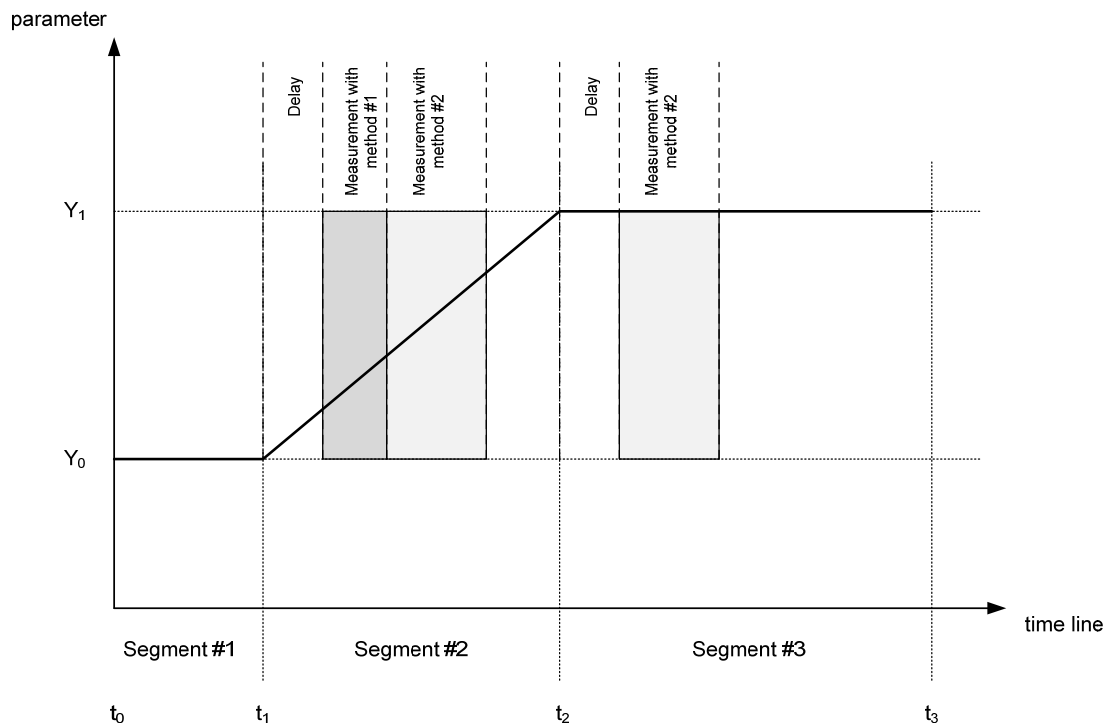


Fig. 12: Example of a profile with three segments

How would such a profile get executed?

The measurement library will first achieve the point  $(t_0, y_0)$  independent what the current chamber state is. To achieve this, a special still scan is carried out (without a goniometer movement). Such a scan may not be displayed by the evaluation software.

At time  $t_1$ , the parameter will be varied with a constant gradient to  $y_1$ . The two different measurement methods will get measured after the delay. The delay after the second measurement is created automatically by the measurement library.

At time  $t_2$ , a further a non-ambient still scan is carried out, followed by a delay and a third measurement.



#### NOTE

The measurement library assures that both start and end parameters in the profile are reached. I.e. if you would add a decline of the parameter to  $y_0$ , the measurement will stop only after  $y_0$  has been reached (if not aborted before).

### Settings

In the Settings, the profile is chosen (currently, it is only possible to define one profile). The form shows an overview on existing profiles in its upper part and the currently selected profile definition at the bottom.

**Overview**

Overview current profile(s)

Total time [s] 2501  
[hh:mm:ss.s] 0:41:41.0

Up Down Delete

Name	Segments	Refine	Total time

**Profile definition**

Define a new profile

Available for profiling are:

Constant Humidity Add

Available parameters

Name	Unit	Minimum	Maximum	Default	Default change
▶ Set Temp...	[°C]	20.0	80.0	20.0	10.0
▶ Set Temp...	[°C/min]	-5.0	5.0	0.1	
▶ Set Humidity	[%]	5.0	95.0	5.0	0.0

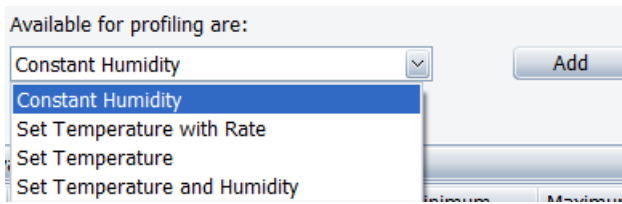
Next Preceding Discard

Fig. 13: Profiles settings

### Available modes

The available profile definitions – or: modes - depends on the hardware and are defined by the firmware in the instrument.

The profile modes are shown in a combo box.



Each mode provides one or more parameters which are shown in the table below. The parameters have default values and default change values. These defaults will be used when new segments are created.

### A special case of a Non-ambient chamber : the CHC

A CHC non-ambient chamber provides four modes :

#### **Constant Humidity**

Available parameters					
Name	Unit	Minimum	Maximum	Default	Default change
▶ Set Temperature	[°C]	20.0	80.0	20.0	10.0
Set Temperature (change)	[°C/min]	-5.0	5.0	0.1	
Set Humidity	[%]	5.0	95.0	5.0	0.0

This mode allows to specify parameters for temperature and humidity. However, the humidity can be chosen for the first segment only. For all following segments it is kept constant.

#### **Set Temperature with Rate**

Available parameters					
Name	Unit	Minimum	Maximum	Default	Default change
▶ Set Temperature	[°C]	20.0	300.0	20.0	10.0
Set Temperature (change)	[°C/min]	-30.0	30.0	30.0	

This is the so-called “dry mode”, i.e. the humidity is not used. The heating or cooling are carried out by the specified rate.

#### **Set Temperature**

Available parameters					
Name	Unit	Minimum	Maximum	Default	Default change
▶ Set Temperature	[°C]	20.0	300.0	20.0	10.0

This is the so-called “dry mode”, i.e. the humidity is not used. The heating or cooling is always done at the maximum possible speed.

#### **Set Temperature and Humidity**

Available parameters					
Name	Unit	Minimum	Maximum	Default	Default change
▶ Set Temperature	[°C]	20.0	80.0	20.0	10.0
Set Humidity	[%]	5.0	95.0	5.0	10.0

The heating or cooling and the humidity are reached at the maximum possible speed.

### A step by step example



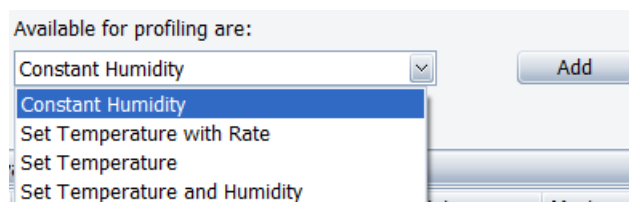
#### NOTE

In the example below, we assume a CHC temperature/humidity chamber using the “constant humidity” mode. The profile types available and their parameters will differ from those provided if you have other hardware components.

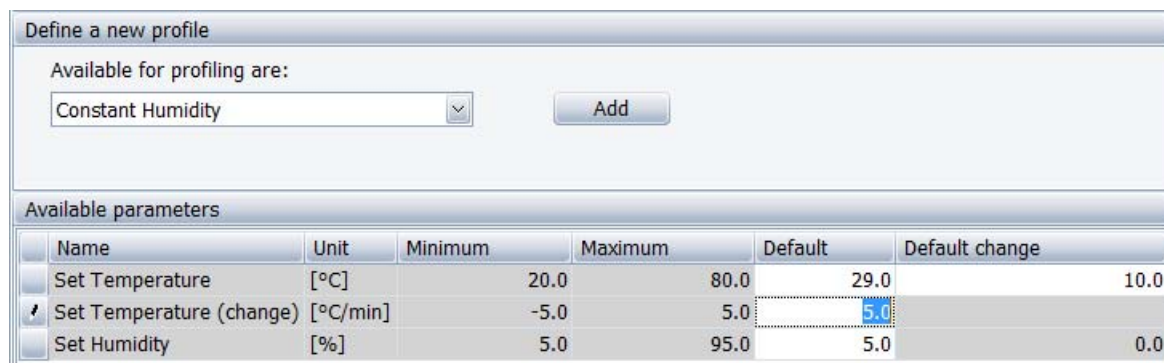
To use the “constant humidity” mode select

**Step #1: choose a profile type**

The modes available are shown in a combo box. Select “constant humidity”.



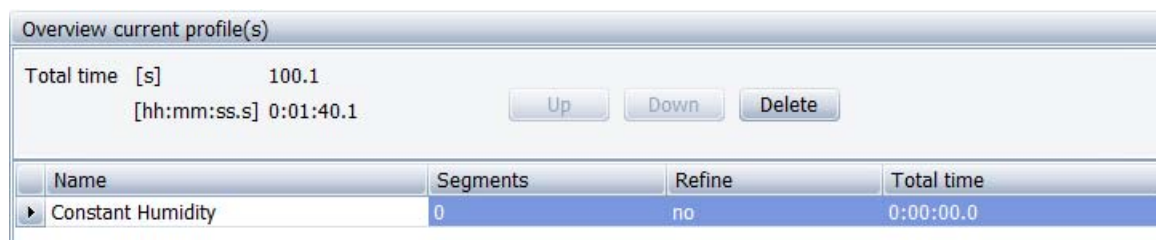
You may then change default parameters.



For instance, you may set the default temperature to 29 [°C], and the default heating rate to 5°/min (a default cooling would be set by a negative rate).

To define the profile using the mode selected in the combo box press .

The profile appears at the top in the settings dialog:

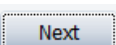


**i NOTE**

Currently, it is not possible to define more than one profile.

To change to another mode it is necessary to delete the profile using the button.

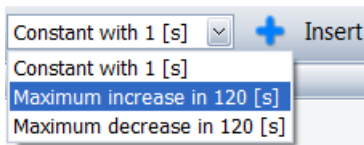
So far, we have defined the profile but it is empty, i.e. it has no segments. For this reason, the total time is given by the current scan.


Press  to switch to the table editor:

**Step #2: add segments and measurements using the Table Editor**

The table editor provides a list of segments and segment items.


First; select an increasing segment.



Then, press  to append it to the profile: a constant segment is added to the table:

Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0

For each parameter, columns are added for its Start value, its End value and the Rate. In our example of a “Constant Humidity” profile, the humidity exhibits only a start value.

Press  once again to add a further segment:

Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5.0	10.0

The second segment automatically starts at the end of the first one (here, at 39 [°C] and 10 [%]). The start values can be edited for the first segment only. If these values are changed all following segments are shifted accordingly.

Now, we want to add a constant segment with several measurements. To do so, switch back to constant and press the append button:

Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5.0	10.0
3 (const.)		0:04:00.0	240.000	1.000	241.000	49.0	49.0	0.0	10.0

By default, the constant segment uses a duration of 1 [s].

To add a measurement, press  :

Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5.0	10.0
3 (const.)		0:04:00.0	240.000	100.100	340.100	49.0	49.0	0.0	10.0
	Measurement	0:04:00.0	240.000	100.100	340.100				

As can be seen, the duration of the constant segment is automatically adapted to the duration of the measurement method selected (here, to 100.1 [s]).

Press  to add a delay and then again  :

Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5.0	10.0
3 (const.)		0:04:00.0	240.000	205.200	445.200	49.0	49.0	0.0	10.0
	Measurement	0:04:00.0	240.000	100.100	340.100				
	Delay	0:05:40.1	340.100	5.000	345.100				
	Measurement	0:05:45.1	345.100	100.100	445.200				

As a result, we get a segment with two measurements separated by a delay. The delay can be changed to 20 [s], for instance:

Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5.0	10.0
3 (const.)		0:04:00.0	240.000	220.200	460.200	49.0	49.0	0.0	10.0
	Measurement	0:04:00.0	240.000	100.100	340.100				
	Delay	0:05:40.1	340.100	20.000	360.100				
	Measurement	0:06:00.1	360.100	100.100	460.200				

We may now view the profile in the graphical editor. Press Next to go to the

**Step #3 : View in the Graphical Editor**

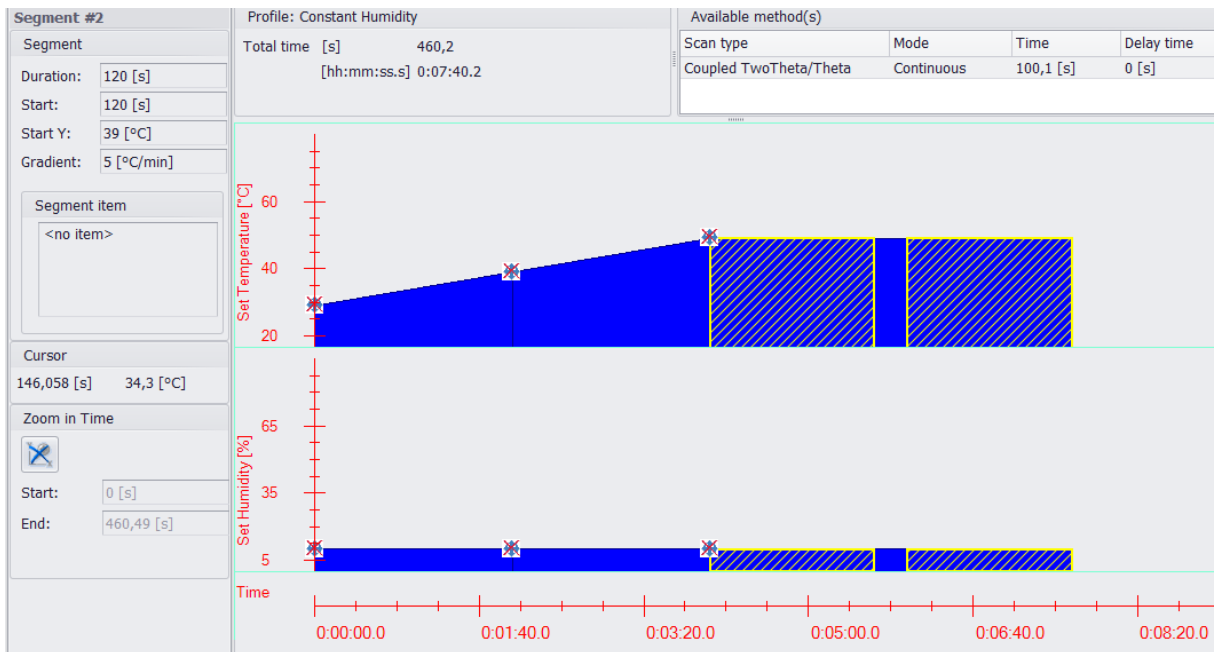


Fig. 14: Graphical profile editor

**The Table and Graphical Editor**

**Common Layout**

In the upper part of the window, both the table and the graphical editor share the same layout:

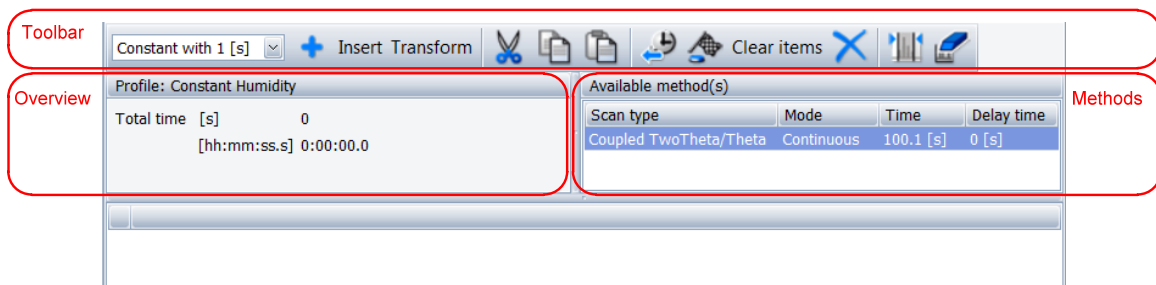


Fig. 15: Profile editors: common headers

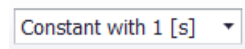
It is grouped into three parts:

**Toolbar**

The toolbar serves to select the next segment and action to append, insert, copy, paste etc.

It is organized into three groups:

**Segment group**



Insert

Transform



**Segment items group**



Clear items



**Profile group**



Combo box with default segments; usually a constant, an increase and decrease of the parameters with maximum speed

Append a new segment of the type selected in the combo box

Insert a new segment of the type selected in the combo box

Transform the current segment into a constant one

Cut the marked segments (together with their segment items)

Copy the marked segments (together with their segment items)

Paste the marked or copied segments before the currently marked segment

Append a delay in the current segment

Insert a sample position change (chambers with internal sample changer only)

Append the currently marked method(s) in the current segment

Clear all items (delays or measurements) in the current segment

Delete the marked item

Optimize the whole profile in time. This operation tries to minimize the duration of the profile

Clear the whole profile

How to select the current segment and mark segments depends on the editor used (table or graphical) and is described below.

**Overview**

The overview summarizes the current profile.

**Available methods**

To the right, the available methods are listed. Currently, only one method is defined (if we had defined more methods in the Basic module above, these methods would appear in the list).

**Profile toolbar**



**Table editor**

The tabular representation of a profile lists information on segments and segment items together with all their parameters. For each parameter, the start value creates one column, and – if appropriate – the end value and/or the rate (or gradient).

Segment info						Parameter #1			Parameter #2	
Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]	End Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5	10.0	
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5	10.0	
3 (const.)		0:04:00.0	240.000	220.200	460.200	49.0	49.0	0	10.0	
	Measurement	0:04:00.0	240.000	100.100	340.100					
	Delay	0:05:40.1	340.100	20.000	360.100					
	Measurement	0:06:00.1	360.100	100.100	460.200					

Segment item info

**Current segment:**


In the table editor the current segment is the one with

▶ 2		0:02:00.0
-----	--	-----------

**Marking segments:**

To mark more than one segment in the table editor, click on the first row, then keep the Shift button pressed and click on the last row: the marked segments are shown in blue:

2		0:02:00.0
3 (const.)		0:04:00.0
	Measurement	0:04:00.0
▶	Delay	0:05:40.1
	Measurement	0:06:00.1


The marked segments can be pasted after the current segment using .

**Chambers with sample changer**

Some chambers provide a built-in sample changer (like the MHC). This allows to change the sample while measuring a profile rather than from the StartJobs plugin (and restarting the profile as a whole).

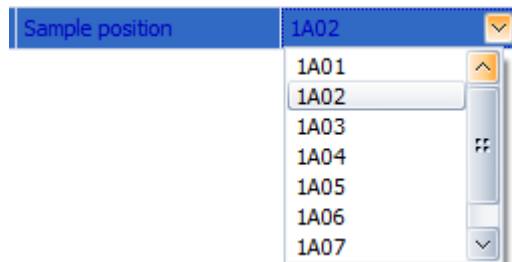
For these chambers, an additional column appears in the table editor:

Segment	Segment item	Sample pos.	Start time
1 (const.)			0:00:00.0

Press the  button on the toolbar to add sample position segment item:


▶	Sample position	1A02	0:00:00.0
---	-----------------	------	-----------

The sample position can then be selected from the available positions listed in the combo box:

**Graphical editor**

The graphical editor shows all segments versus time. For each parameter one track is displayed. In the example above, these are humidity and temperature.


The panel to the left shows information about cursor position and the current segment. This panel can be docked to the left or right or it can be made floating: just click on its head line and drag it while keeping the left mouse button pressed.

Segment #2	
<b>Segment</b>	
Duration:	120 [s]
Start:	120 [s]
Start Y:	39 [°C]
Gradient:	5 [°C/min]
<b>Segment item</b>	
<no item>	
<b>Cursor</b>	
152.839 [s]	39.2 [°C]
<b>Zoom in Time</b>	
	
Start:	0 [s]
End:	460.49 [s]


In the upper part the segment duration, start values and gradient are displayed. If the mouse cursor hits a segment item this information is displayed, too.

### Zooming

It is possible to zoom the profile in time. Press the left mouse button and move the cursor to the left: the zoom fields in the lower part of the panel are updated:

Zoom in Time	
	
<b>Zoom mode</b>	
Start:	72.795 [s]
End:	60.244 [s]

If you release the left mouse button, the time interval shown in Start and End is used for the display.

To deactivate the zoom you can press the button  at any time. Moving the mouse from right to left (with the left mouse button pressed) will do the same.

**XY positions**

The **XY positions** module provides three module items: the definition for XY positions, the setup for an alignment and the Camera, which is an optional module.

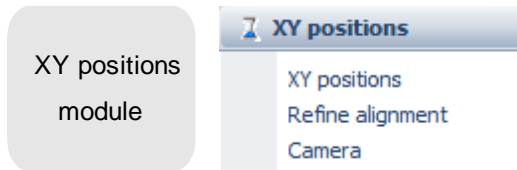


Fig. 16: WIZARD XY positions module

**XY positions form**

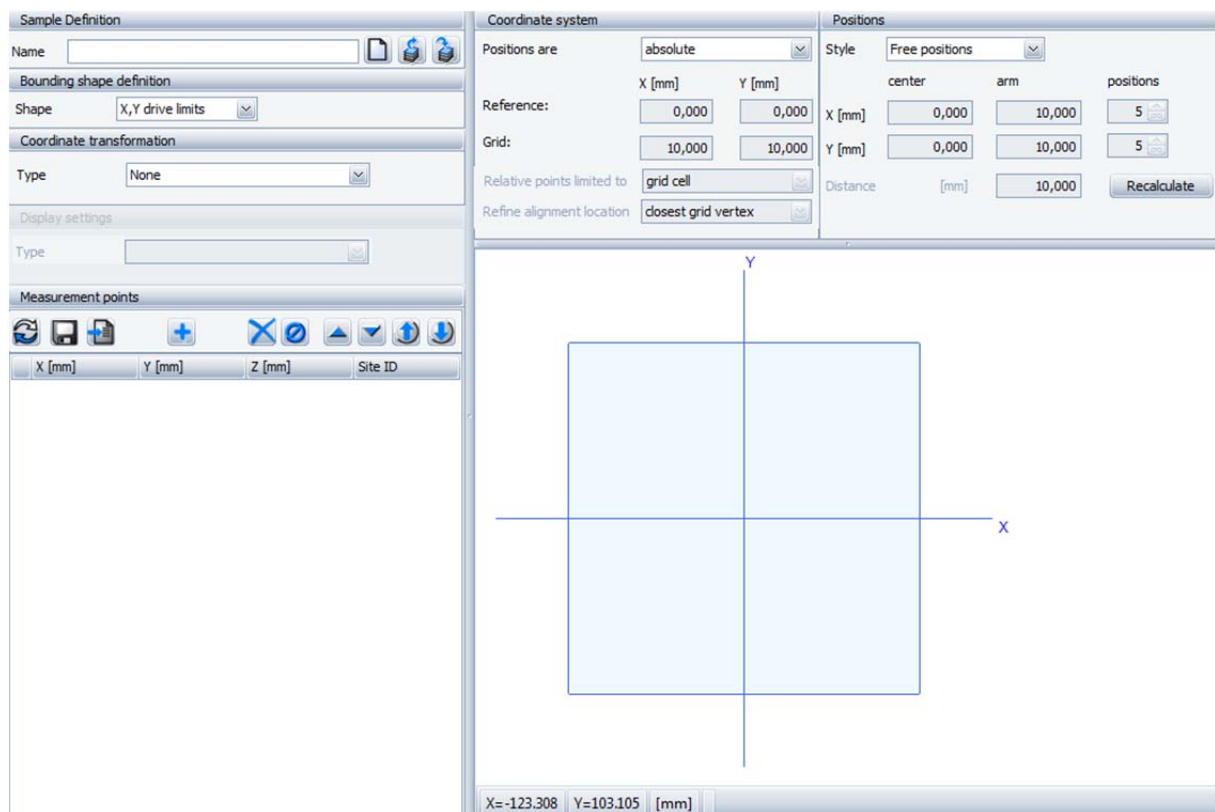


Fig. 17: XY positions display

**Sample definition**

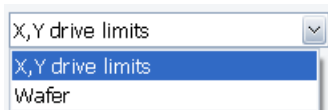
Allows to save and load sample definitions to and from the database.

Sample definition consists of sample shape, size and coordinate system. Please note that it does not include measurement positions. When a sample definition is loaded, respective fields on the form become disabled. To enable editing of the shape, size and coordinate system again, press “Create new” button.

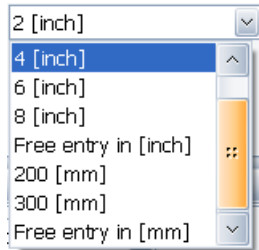
**Bounding shape definition**

Different shapes of your sample can be selected.

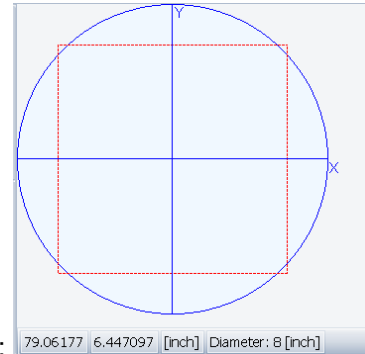
Shapes which are currently available are as follows:



- *X, Y drive* limits select a rectangular shape where the limits are prescribed by the X and the Y drive.
- *Wafer* selects either predefined wafer diameters in [inch] or [mm] or defines a free wafer diameter:



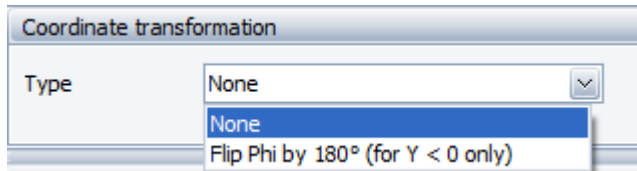
The X,Y positions display changes accordingly:



The red dashed rectangle indicates the X,Y drive limits.

**Coordinate transformations:**

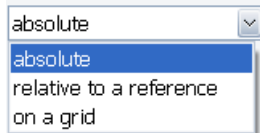
Coordinate transformations are applied during the measurement (they do not affect the graphics display to the right). The availability of the transformations depends on the stage used.



Flip Phi by 180° (for Y<0 only)

Choosing this transformation will avoid usage of the negative Y drive positions: all negative Y positions are reached by using a Phi=180° instead.

**Coordinate system: absolute and relative coordinates**

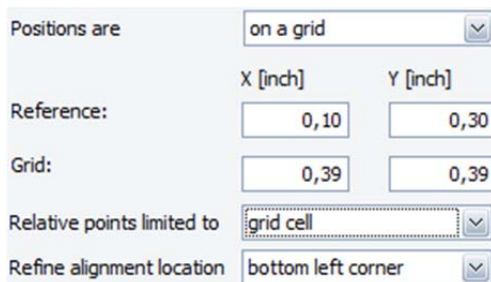


Three coordinate systems are available:

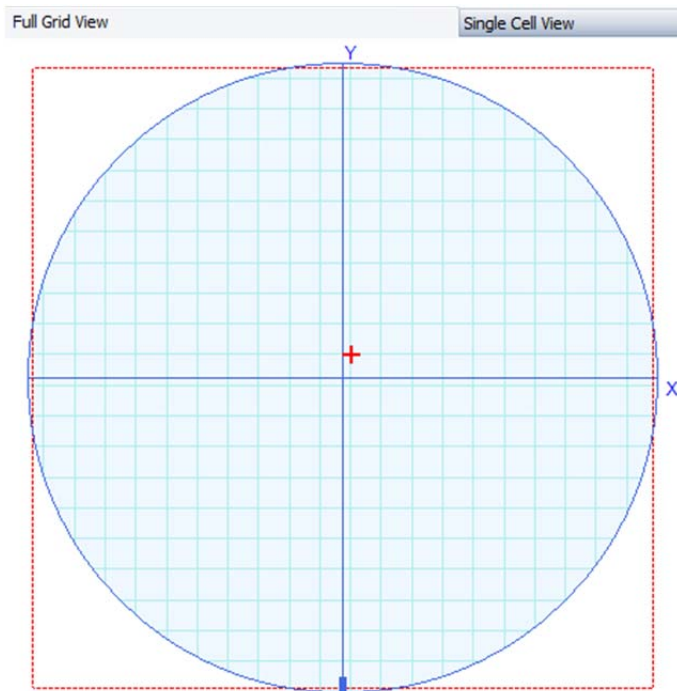
- *Absolute* is the default. All points are defined as absolute positions of the x and y axes.
- *Relative to a reference* defines an offset position. All points are defined as positions relative to the offset position. This offset position may be changed by the measurement script.
- *On a grid* defines a set of cells relative to the offset position and a set of points within each cell. All cells are relative to the offset position, while points are relative to one of the cell vertices.

Example:

Select *on a grid* and define an offset and the grid:



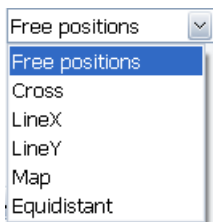
The graphics display changes accordingly:



The red cross defines the new offset. Note that a wafer in [inch] has been chosen. Therefore, all coordinates are shown in [inch].

### Positions

Different predefined styles are offered to specify a set of positions (or a set of grid cells):



- *Free positions*: the user can enter X and Y positions in the table (add button) or on the graphic display (double click)
- *Cross* defines an X,Y cross
- *LineX*, *LineY* defines a line in either X or Y with an offset in the other coordinate
- *Map*: a rectangular map
- *Equidistant*: an almost equal distribution over the whole area.

To “add”, “delete”, “delete all” or to move positions up and down click on the appropriate buttons in the table’s toolbar:



The position corresponding to the row selected in the X,Y positions table is marked by a dark red cross in the graphical display.

Example: Cross without a grid

Choose the positions relative to a reference and select the Cross style. The X,Y fields will be enabled. As a result, the user can enter the centre for the cross and its arm lengths in X and Y.

The screenshot displays the DIFFRAC.WIZARD software interface. The interface is divided into several panels:

- Sample Definition:** Includes fields for Name, Bounding shape definition (Shape: Wafer, Wafer diameter: 8 [inch]), Coordinate transformation (Type: None), Display settings (Type: ), and Measurement points.
- Coordinate system:** Includes a dropdown for 'Positions are' (relative to a reference), Reference: X [inch] (0,10) and Y [inch] (0,30), Grid: X [inch] (0,39) and Y [inch] (0,39), Relative points limited to (area around grid vertex), and Refine alignment location (bottom left corner).
- Positions:** Includes a dropdown for 'Style' (Cross), center X [inch] (0,00) and Y [inch] (0,00), arm (1,00), positions (5), and a Recalculate button.

The main display area shows a circular wafer with a grid and measurement points. The grid is centered at (0,0) with a diameter of 8 inches. The measurement points are marked with 'x' symbols. The status bar at the bottom indicates X=-0.94, Y=-0.81 [inch], Diameter: 8.

X [inch]	Y [inch]	Z [mm]	Site ID
-1,00	0,00	0,0000	
-0,50	0,00	0,0000	
0,00	0,00	0,0000	
0,50	0,00	0,0000	
1,00	0,00	0,0000	
0,00	-1,00	0,0000	
0,00	-0,50	0,0000	
0,00	0,50	0,0000	
0,00	1,00	0,0000	

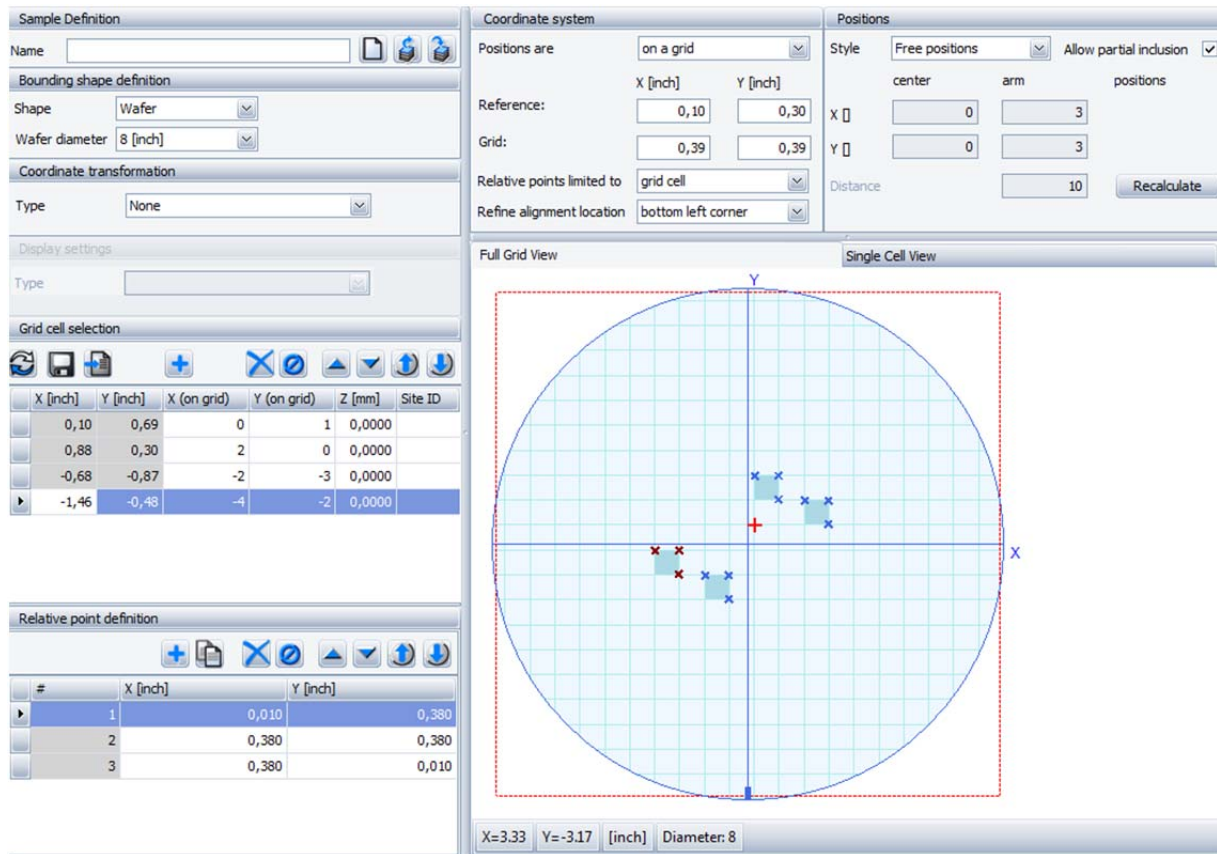
**Hint:** If the style is set back to *free positions* it is possible to add or delete single points from the cross.

**Example:** Free positions on a grid

Choose the on a grid option in the Coordinate system control and select the Free positions style in the Positions control.

Sample display area will change and the Full Grid View tab will be selected by default. Double click on the grid to select grid cells. To select measurement points switch to the Single Cell View tab and double click anywhere in the cell area. Grid cells and points can also be specified in the Grid cell selection and Relative point definition tables respectively.

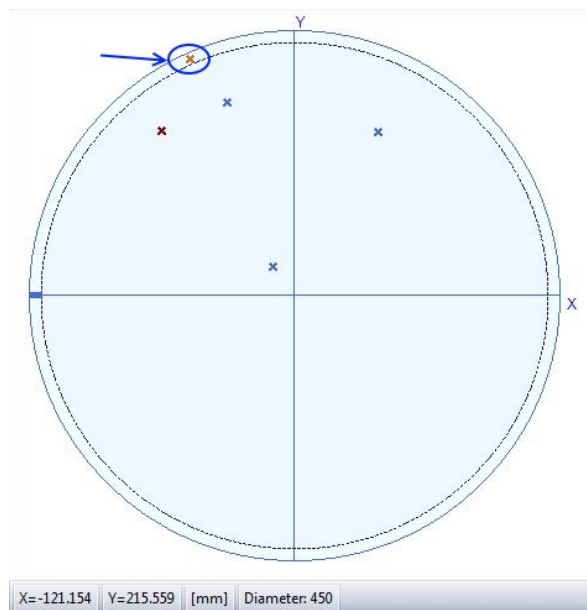
Please note that no measurement is possible unless at least one grid cell and at least one relative point are defined.



For this example refined alignment will be performed 4 times at the bottom left vertex of each cell. "Relative points limited to" and "Refine alignment location" in the Coordinate system control offer several options for the alignment location and relative point grouping

**Edge Exclusion**

Some measurement techniques (e.g. TXRF) are sensitive to the edge of the wafer. The results are influenced when the X-ray beam is not entirely on the wafer anymore. In order to warn the user for this edge exclusion, an extra circle in a dashed line is drawn that marks the zone that can be analysed without problems. The user can add points that are within the dashed circle and the wafer edge, but the points will appear as orange, as shown in the figure below. The results from this zone are to be considered with caution.



**Refine alignment form**

The form allows defining an alignment.

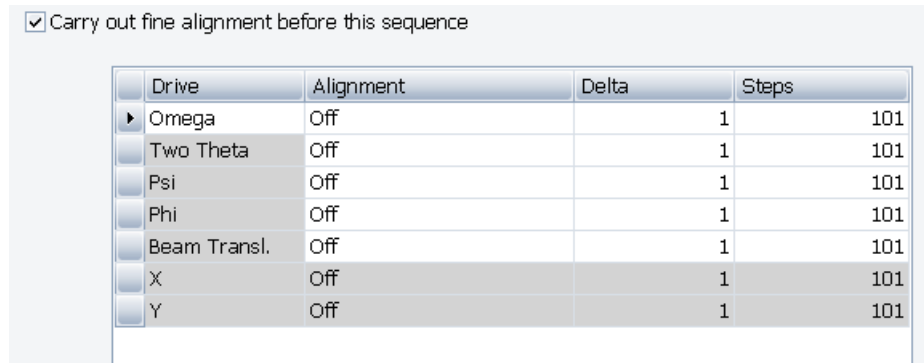
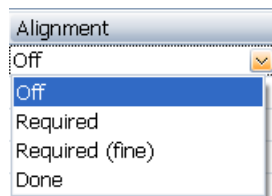


Fig. 18: Refine alignment form

An alignment is carried out at each X,Y position and can be defined for each drive (except for X or Y) if the box is checked at the top left in the form. Click on the list in the *alignment* column:



The following are defined as:

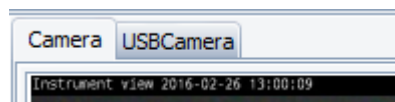
- Off                      No alignment done
- Required                The drive will receive an alignment
- Required (fine)        The drive will receive a fine alignment
- Done                     No alignment has been performed and the drive is considered aligned.

**i NOTE**

How the alignment is done depends on the used measurement script.

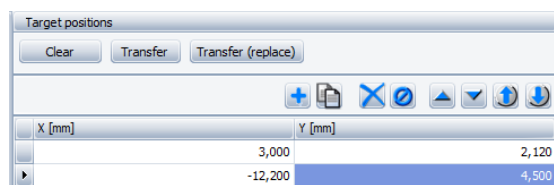
**Camera**

If one or more cameras are available and the application supports them they are shown on a tabbed form: one tab per camera:



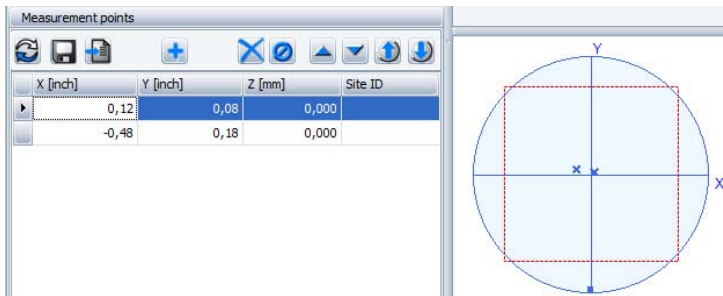
The camera control itself is described in detail in the Measurement Center User Manual.

You may then use the "Measure here" with a right click on the camera image to add X, Y positions to the target positions table to the right:



Note: if there is a camera available but no X-Y stage is mounted the control remains empty.

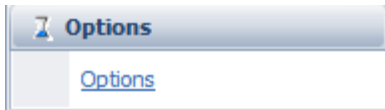
To transfer the positions in the table to the XY positions form press **Transfer** or **Transfer (replace)**. Using the first button will add new positions, the second one will replace all existing X, Y positions. You can see the positions transferred if you click on *XY positions* in the module:

**NOTE**

To transfer points it is necessary to choose the coordinate system *Absolute* and the style *Free positions* in advance.

**Options**

The module allows to set measurement specific options and consists of one module item:



Currently, settings are available for the (optional) video camera(s) and the shutter close only:

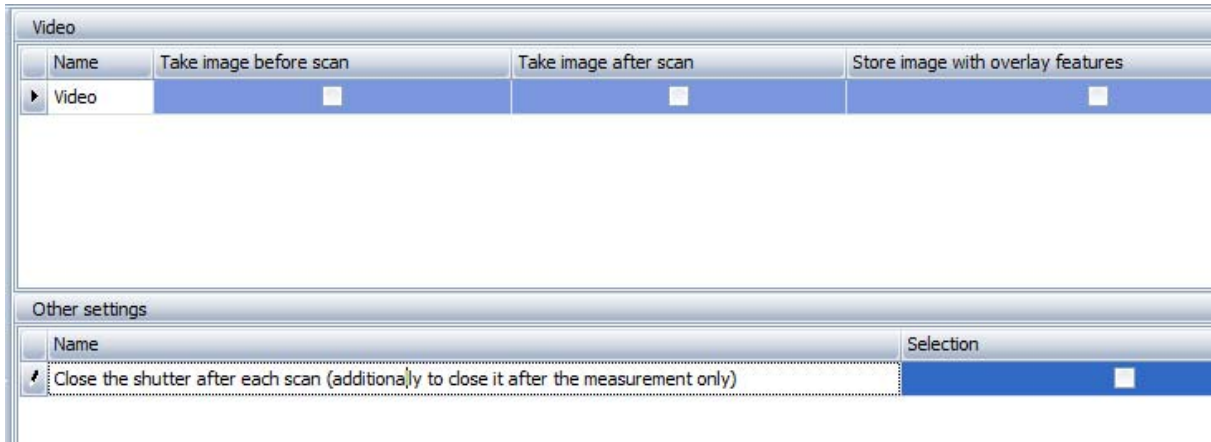


Fig. 19: Options module

Each video system can take an image just before the scan starts and after the scan finished. The images are stored as Jpeg files.

In addition, it is possible to define whether the shutter is closed between two scans inside the same experiment. This option is useful to avoid X-Ray illumination of the sample while, for instance, the sample is heated for a longer time before the next measurement starts at a new temperature.

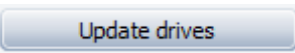
**Fixed drives**

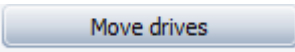
Certain applications (like Stress and Texture) provide a specific form to control drive positioning and oscillation.

This form allows the user to enter parameters (positions and oscillations) for all drives which are not used by the scan or the measurement setup.

Update drives		Move drives							
Drive	Optional	Position	Unit	Osc.	Amplitude	Unit	Speed	Unit	
▶ Beam Transl.	<input type="checkbox"/>	0,00	[mm]	<input type="checkbox"/>	0,00	[mm]	0,0	[mm/s]	
TrackDistance	<input type="checkbox"/>	149,6	[mm]	<input type="checkbox"/>	0,0	[mm]	0,0	[mm/s]	
X	<input type="checkbox"/>	0,000	[mm]	<input type="checkbox"/>	0,000	[mm]	0,0	[mm/s]	
Y	<input type="checkbox"/>	0,000	[mm]	<input type="checkbox"/>	0,000	[mm]	0,0	[mm/s]	
Z	<input type="checkbox"/>	0,000	[mm]	<input type="checkbox"/>	0,000	[mm]	0,0	[mm/s]	

Fig. 20: Fixed drives form

Press  to update the default drive positions with the current positions on the instrument.

Press  to position the drives according the values entered. Oscillations are not transferred.

### Oscillations

To actually use an oscillation it is necessary to check the oscillation box and to specify a non-zero amplitude and velocity.

### Optional drive

A drive may be marked to be optional, i.e. during job execution this drive is allowed to be not available on the actual instrument.

## Summary

The summary module provides a tabular view of the whole experiment.

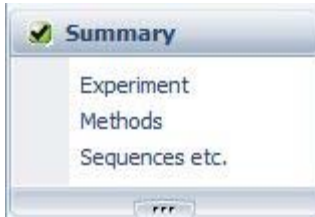


Fig. 21: Summary module

There are three sections: the first one (Experiment) gives an overview of the whole experiment, the second one (Methods) list all base methods: scan setup, fixed drives, optic settings etc.. A final section lists information about optional sequences (like XY maps, profikes etc.).

## Printing a report

Regarding printing, definition of your own layout, and print preview, please see the chapter 10.2.25, Results Manager, in the Measurement Center User Manual.

## Application specific modules

### XRD

This application provides several modules which can be used to define experiments with a single XRD scan up to complex measurements involving profiles (for instance: non-ambient measurements) and wafer mapping.

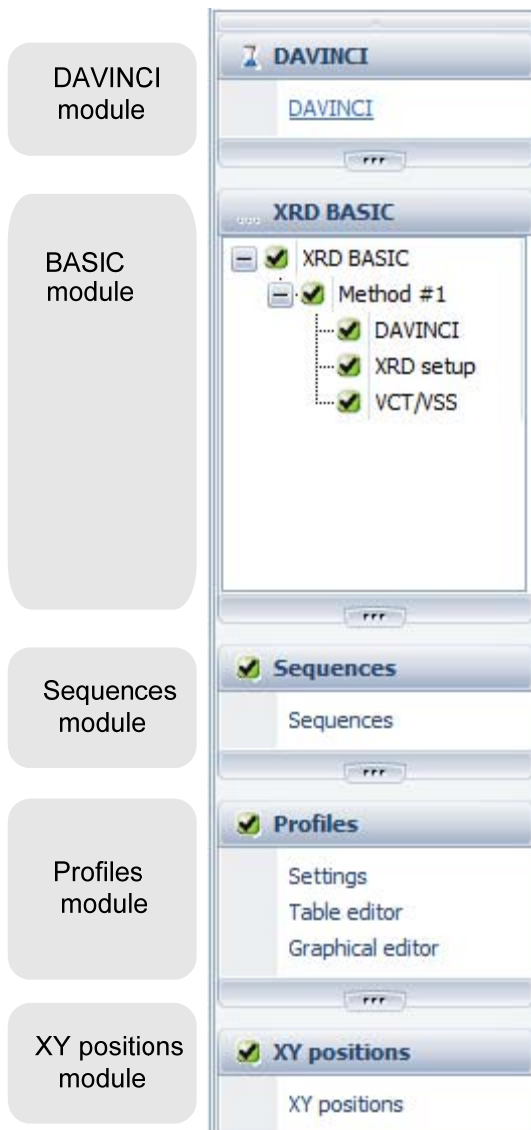
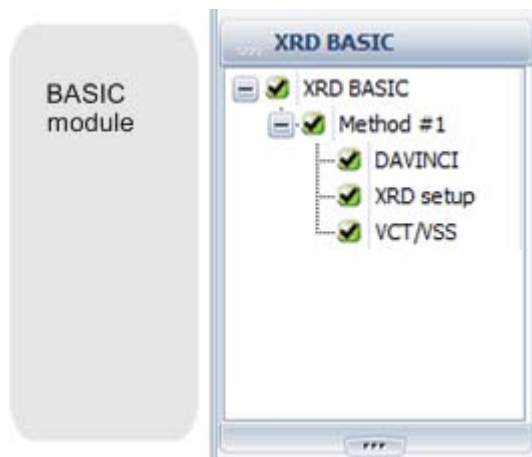


Fig. 22: XRD modules

### DAVINCI module

For this module, see the description on page 9.

## The basic module: XRD BASIC



In comparison to most other modules, this module consists of a tree view rather than of module items. The tree contains at least one base method. It is possible to add, copy or delete methods using the context menu.

In the following sections each tree node is described. The organisation of the nodes guides the user step by step through the set-up procedure.

### XRD basic

This view describes the measurement:

User	Lab Manager
Sample ID	TEST material
Comments	<input type="text"/>

Fig. 23: Sample definition form

The *User* field cannot be edited. It contains the name of the user logged-in into the shell. A free text can be entered into *Sample ID* and *Comments*.

### Method

Method overview	
Detector(s) used:	Selected detector(s): SCINTI using 1 discriminator(s).
Tube(s) used:	Cu tube with 1.54184 [Å]. Generator at 20 [kV] and 5 [mA].
Scan type and mode:	Coupled TwoTheta/Theta as Continuous.
Total time [s]	2501
	[hh:mm:ss.s] 0:41:41.0
Comments:	<input type="text"/>

## DAVINCI

The **DAVINCI** display is fundamentally similar as the display in the DAVINCI module. However, it is possible to change motorized optics only. These changes are method specific.

### XRD scan setup

This form defines the scan setup, and all parameters needed to carry out the measurement.

The default scan setup is a Coupled TwoTheta/Theta scan but may vary according to the detector, which has been selected. See table on p. 88 for an overview on available scan types.

The screenshot shows the XRD scan setup interface with three main sections highlighted by red boxes:

- Scan setup:** Contains fields for Scan type (Coupled TwoTheta/Theta), Time/step [s] (1,00), Delay time [s] (0,0), Scan mode (Continuous), Steps (2501), and Estim. time [s] (2501).
- Scan axes:** A table with columns: Scan axis, Unit, Abs. start, Abs. stop, and Increment.
 

Scan axis	Unit	Abs. start	Abs. stop	Increment
ZTheta	[°]	5,0000	55,0000	0,0203
Theta	[°]	2,5000	27,5000	0,0102
- Fixed axes:** A table with columns: Drive, Optional, Position, Unit, Osc., Amplitude, Unit, Speed, Unit.
 

Drive	Optional	Position	Unit	Osc.	Amplitude	Unit	Speed	Unit
Psi	<input type="checkbox"/>	0,000	[°]	<input type="checkbox"/>	0,000	[°]	0,0	[°/min]
Phi	<input type="checkbox"/>	0	[°]	<input type="checkbox"/>	0,000	[°]	0,0	[°/min]
Beam Transl.	<input type="checkbox"/>	0,00	[mm]	<input type="checkbox"/>	0,00	[mm]	0,0	[mm/s]
X	<input type="checkbox"/>	0,000	[mm]	<input type="checkbox"/>	0,000	[mm]	0,0	[mm/s]
Y	<input type="checkbox"/>	0,000	[mm]	<input type="checkbox"/>	0,000	[mm]	0,0	[mm/s]
Z	<input type="checkbox"/>	0,000	[mm]	<input type="checkbox"/>	0,000	[mm]	0,0	[mm/s]

At the bottom of the interface are two buttons: "Update drives" and "Move drives".

### Basic scan setup

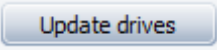
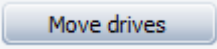
The **scan setup** is found at the top of the form. It serves to select scan type, scan mode, time per step, the number of steps and an optional delay time. The estimated time is calculated automatically.

### Scan axes

All of the axes used for the scan setup are listed in the upper left. A scan axis can be a real drive axis (in the example: the 2Theta and the Theta axis) or a logical axis. The scan parameters may be either Start, Stop and Increment or a Fixed value.

### Fixed drives

All of the axes except those used for the scan themselves are listed here. It is possible to specify a position and/or to define an oscillation.

You may press  to transfer the current instrument drive positions to the Positions column in the table, or  to position the drives directly.

To use an oscillation it is necessary to check the oscillation box and to specify a non-zero amplitude and velocity.

### VCT/VSS

For 0D and 1D detectors, it is possible to split a scan into several sub-scans with different time or increment in each sub-scan.

Fig. 24: VCT/VSS setup

The top of the form shows a summary of the currently defined scan limits (they are identical to those defined in XRD setup form before).

The middle shows the details of the VCT/VSS methods and a list of resulting sub-scans (empty in the figure above).

At the bottom, a graphical representation is shown.



#### NOTE

It is not possible to combine variable scan parameters with any other scan type than a Locked coupled, Unlocked coupled or a Detector scan.

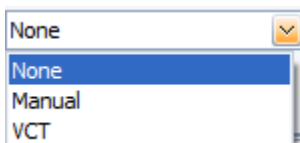
For XRD backward compatible experiments, it is not possible to combine variable scan parameters with sequences or with more than one method.

Two methods are available for defining the splitting:

- VCT: Automatic calculation of an optimum time/step by compensating the intensity variation caused by the Lorentz-Polarisation effect
- VCT/VSS manual: the number of sub-ranges can be defined by the user and both time/step and the step size can be entered for each individual sub-range

By default, no VCT/VSS is selected.

The mode is chosen from the top left combo box:



**NOTE**

After variable scan parameters have been defined, the basic scan should not be changed. If modified (for example, step size, time/step scan mode and so on) the VCT/VSS information is deleted and must be redefined.

**VCT**

The minimum time/step is always the time/step defined in the base range (0.1 s in our example). If the time/step calculated from the formula doubles or halves the time/step of the base range (or of the preceding sub-range), a new sub-range with a longer or shorter measurement time is created.

By default, the program will spend 10% of the total measurement time using the minimum time/step given. The remaining available time (90% of the total by default) is allowed to vary in accordance with the VCT regime. This ensures that adequate statistics are accumulated in the background regions of the low angle regions by avoiding excessive measurement times spent at higher angles.

Apply

If you change one or both parameters you have to press

For a scan from  $2\theta = 5^\circ$  to  $70^\circ$ , you may receive the following:

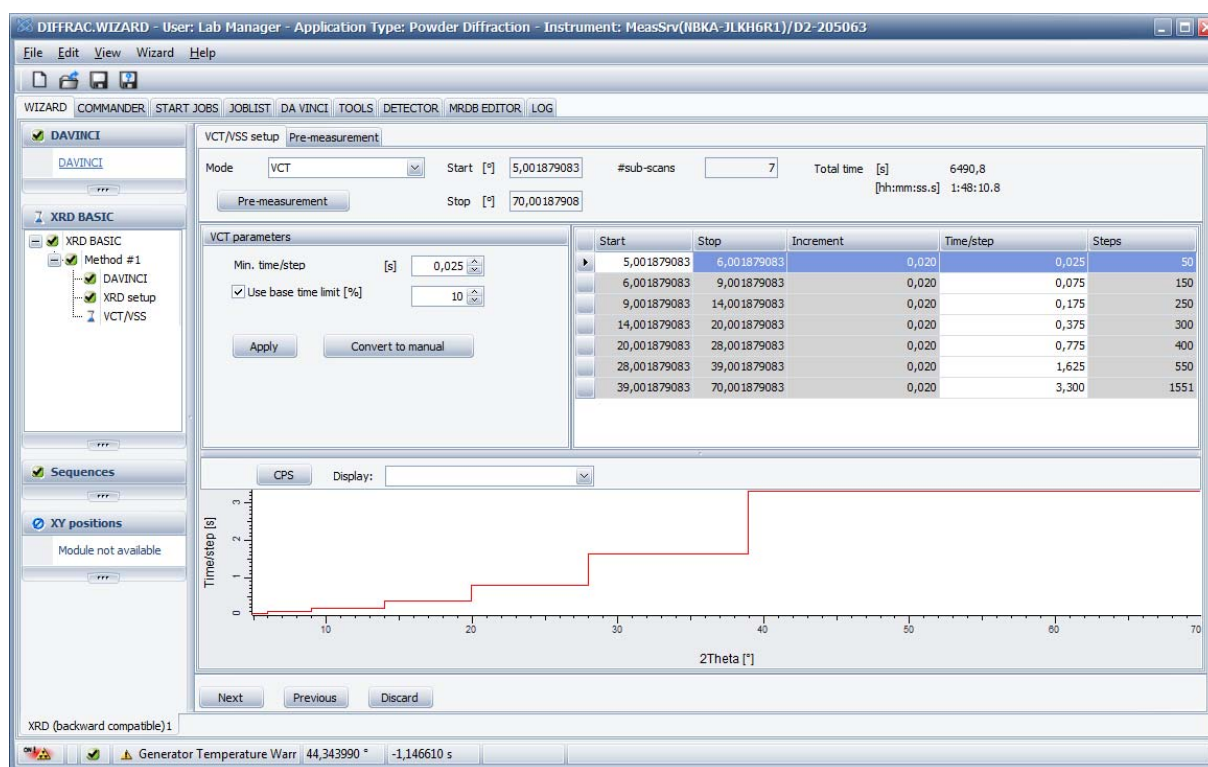
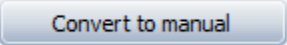


Fig. 25: VCT

**Manual mode**

The standard VCT/VSS from the above example can be easily converted into a manual mode. Click

on . As a result, both increment and time/step can be edited for each sub-scan:

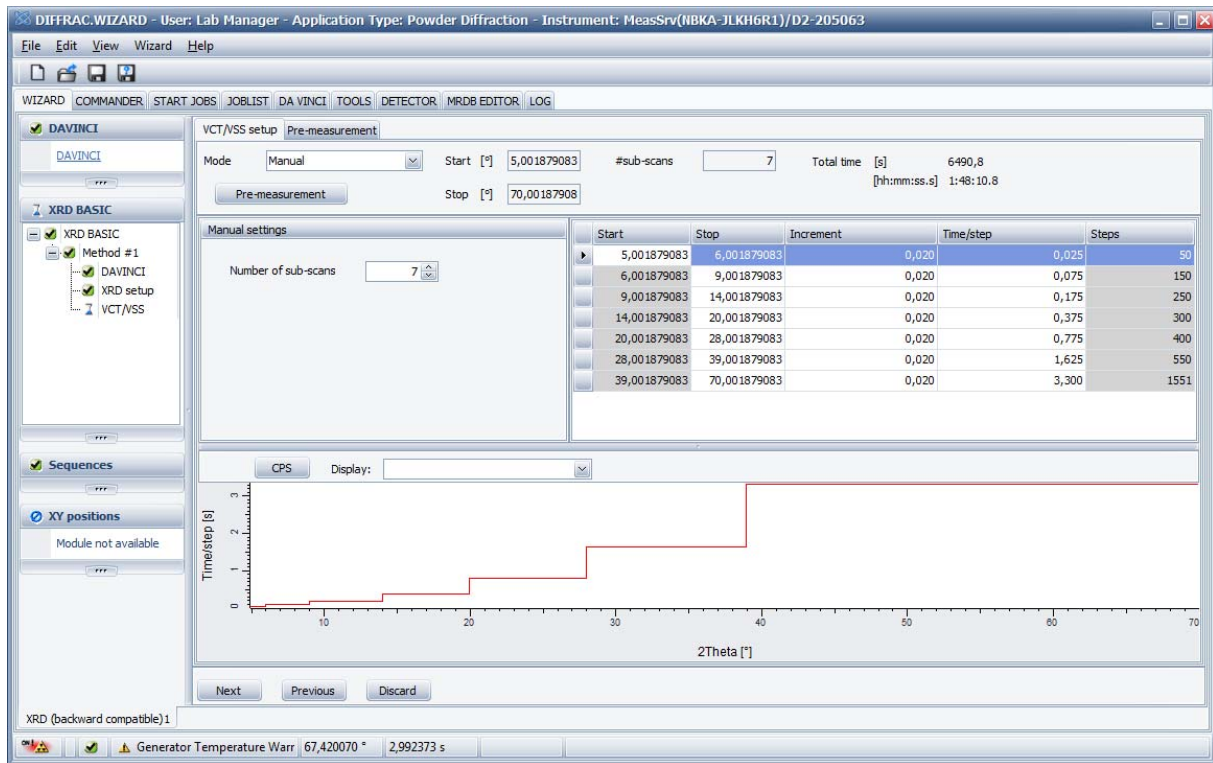
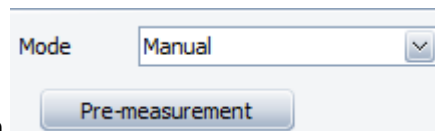


Fig. 26: Manual VCT/VSS

**Pre-measurement**

If you are uncertain where to spend the measurement time you can switch to the pre-measurement tab and execute a fast measurement with the current sample:



Either press the button below the mode selection or click on the second tab.

From top to bottom the tab shows (see next figure): a scan display, scan parameters and at the bottom left a start and stop button.

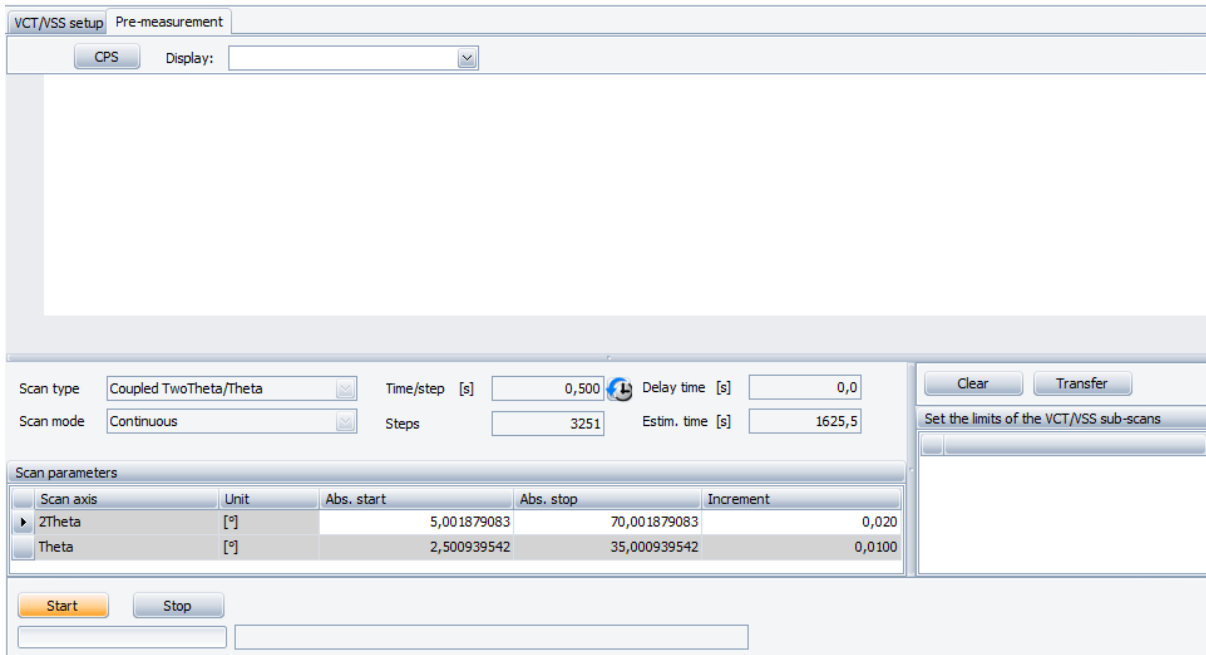

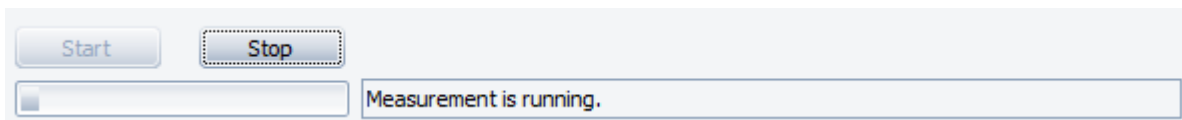


Fig. 27: VCT/VSS pre-measurement

Press the clock button at the right of the time/step field  , to get the fastest possible scan time (it is calculated from the current scan axis increment, the scan mode and the fastest possible detector readout).

After a click on the Start button, the measurement will be executed and progress information is shown below:



**NOTE**

For the pre-measurement the current optic and generator settings are used. If necessary, use COMMANDER to change them.

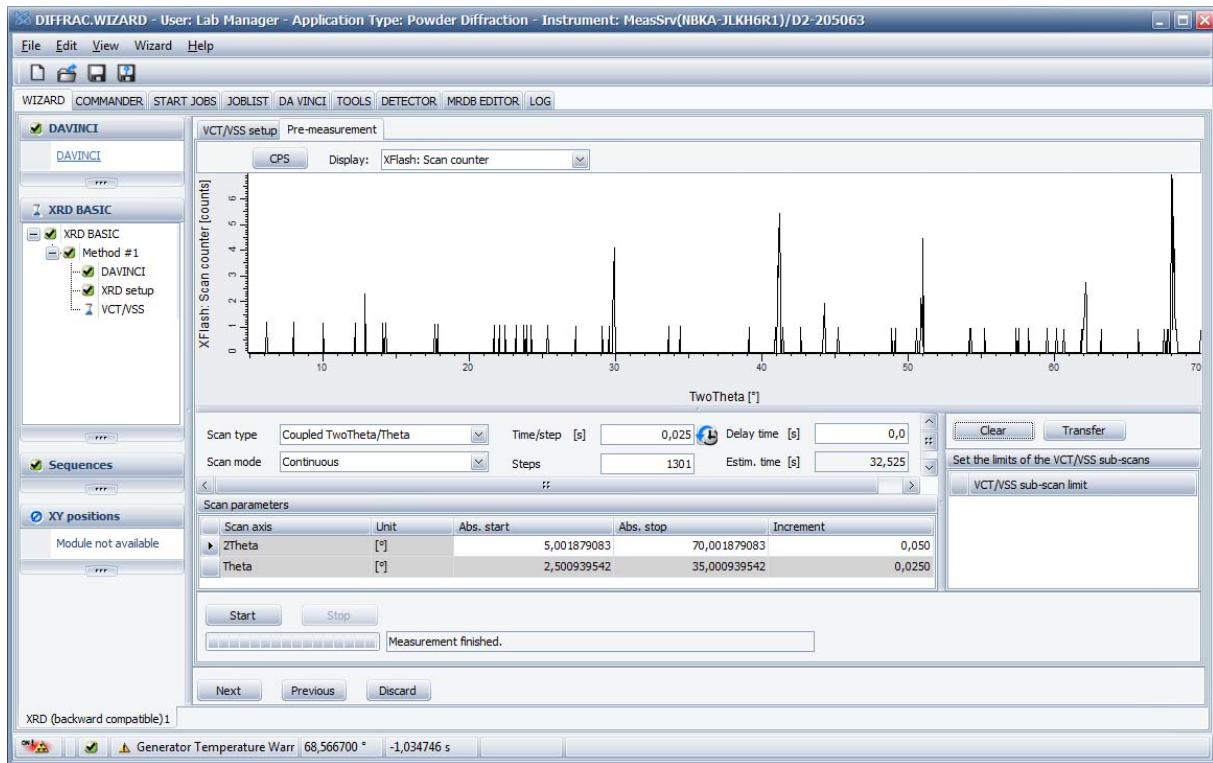
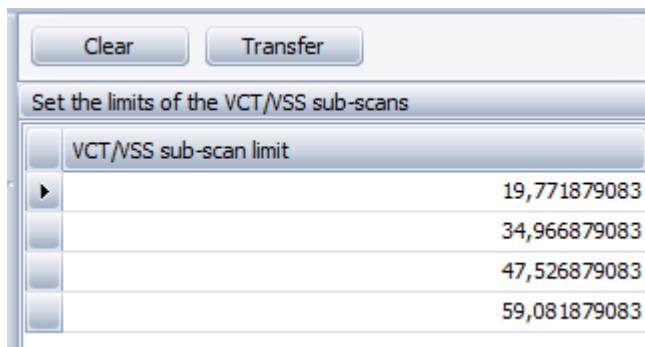


Fig. 28: VCT/VSS pre-measurement executed

A click with the left mouse button into the scan display allows to define sub-scan limits which are shown in the bottom right table, for instance:



Press Transfer and confirm to override your current settings. The program will switch to VCT/VSS setup form and enter the sub-scan limits into a manual mode. The time/step is automatically duplicated for each sub-scan. You may now change increment and time/step as usual.

The current scan is also shown in the manual setup:

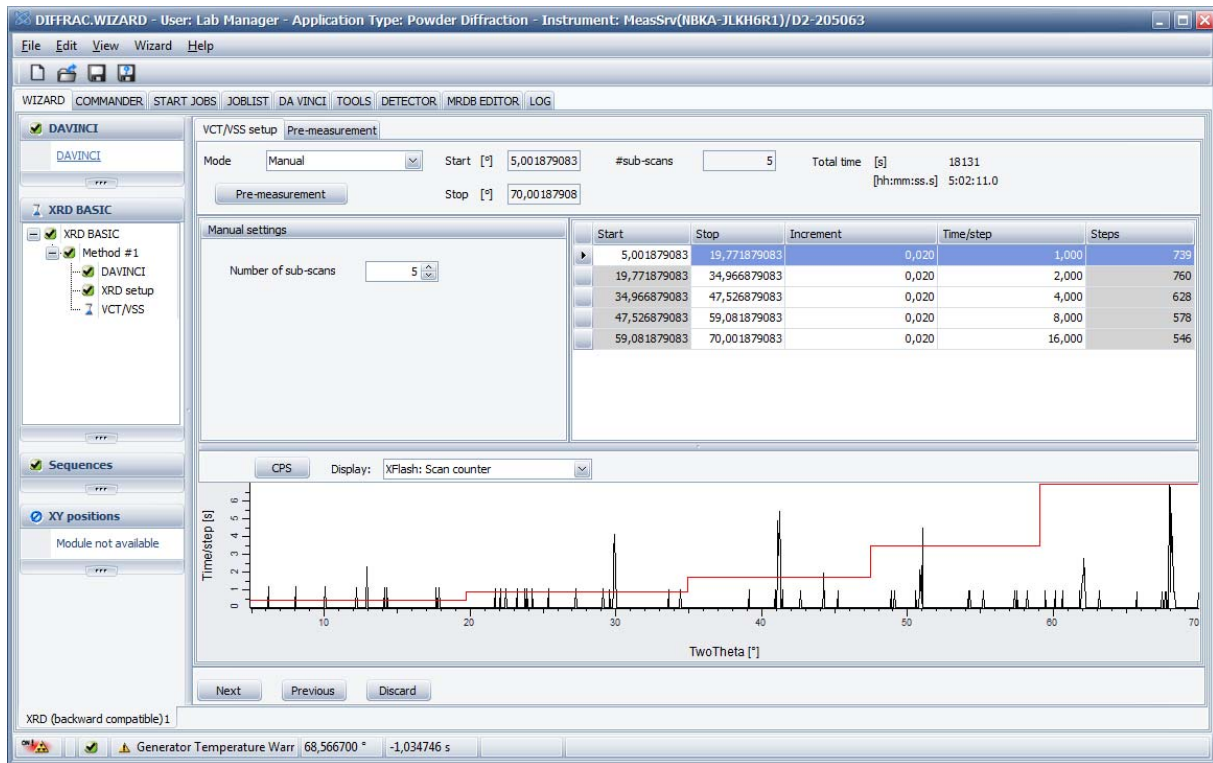


Fig. 29: Using the pre-measurement to define sub-scans

## High resolution XRD

This application provides several modules which can be used to define experiments with a single HR-XRD scan up to complex measurements involving reciprocal space maps and wafer mapping.

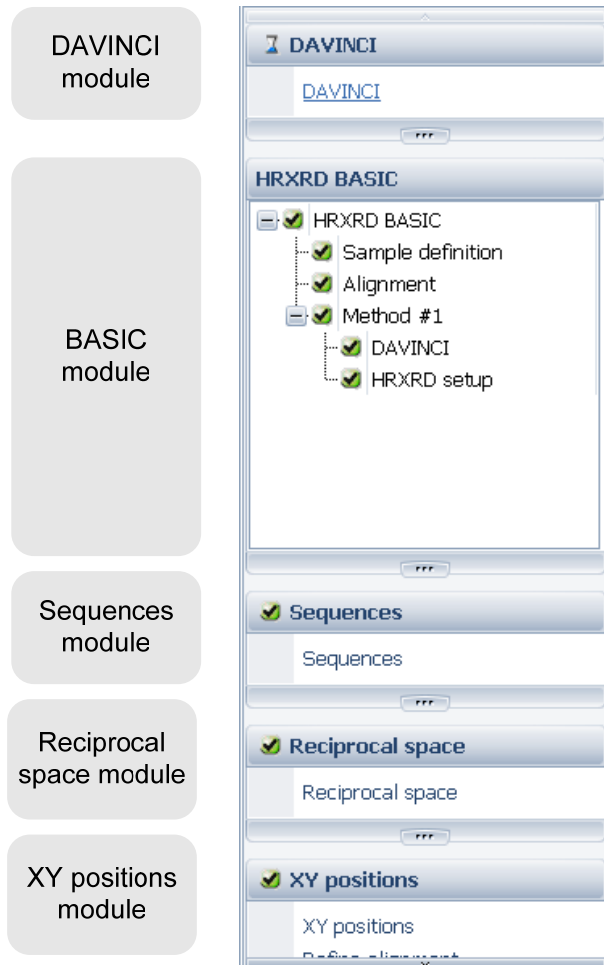
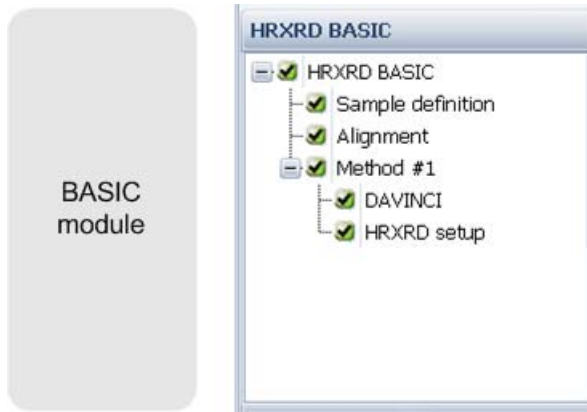


Fig. 30: Modules in HR-XRD

## DAVINCI module

For this module, see the description on page 9.

## The basic module: HRXRD BASIC



In comparison to most other modules, this module consists of a tree view rather than of module items. The tree contains at least one base method. It is possible to add, copy or delete methods using the context menu.

In the following sections each tree node is described. The organisation of the nodes guides the user step by step through the set-up procedure.

### HRXRD basic

This view describes the measurement:

The image shows a form with three fields. The first field is labeled 'User' and contains the text 'Lab Manager'. The second field is labeled 'Sample ID' and contains the text 'TEST material'. The third field is labeled 'Comments' and is an empty text area with vertical scroll bars on the right side.

Fig. 31: Sample definition form

The *User* field cannot be edited. It contains the name of the user logged-in into the shell. A free text can be entered into *Sample ID* and *Comments*.

## Sample definition

It is necessary to define the sample before defining the scan.

The sample definition form is divided into three sub-windows beginning from top to bottom:

- The material database
- The active sample
- The recently used samples

The screenshot shows the 'Sample definition form' with three sub-windows:

- Material Database:** A table listing materials with columns: Name, Crystal system, a [nm], b [nm], c [nm], Alpha [°], Beta [°], Gamma [°]. Materials include Ga(1-x)In(x)As, Ga(1-x)In(x)As(1-y)P(y), Ga(1-x)In(x)P, GaAs, GaN, GaP, and GaSb.
- Active sample:** A table with columns: Type, Name, Crystal system, Surface normal (nm), Azimuth (deg), Refer to substrate, Cx [], Cy [], Relaxation []. The active sample is Si (Substrate) with a cubic crystal system and surface normal [0,0,1].
- Recently used samples:** A section with 'Choose selected' and 'Delete' buttons.

Fig. 32: Sample definition form

### Material database

At the top of the form you will find the content of the **material database** which is described in the MRDB EDITOR plugin. In comparison to this plugin, the WIZARD is not able to edit materials and store the changes back into the database.



#### NOTE

If the content of the material database is changed using the MRDB EDITOR plug-in, WIZARD will recognize the changes for newly created experiments only. To update an experiment already opened, the user must press the reload button at the lower right of the sub-window.

The WIZARD chooses Silicon as a standard substrate without any layers by default.

In this example, a sample with a GaAs as a substrate with two layers is defined. Mark GaAs in the materials table and press the *Exchange substrate* button:

Name	Crystal system	a [nm]	b [nm]	c [nm]	Alpha [°]
Ga(1-x)In(x)As	Cubic	0,58561	0,58561	0,58561	90
Ga(1-x)In(x)As(1-y)P(y)	Cubic	0,57581	0,57581	0,57581	90
Ga(1-x)In(x)P	Cubic	0,566	0,566	0,566	90
▶ GaAs	Cubic	0,5653	0,5653	0,5653	90
GaN	Hexagonal	0,31891	0,31891	0,51855	90

Buttons: Add selected layer, Exchange substrate

To add a layer, click the “add selected layer” button and choose Ga(1-x)In(x)As and Ga(1-x)In(x)As(1-y)P(y), as shown in the example below.

**Active sample**

An active sample, which is shown in the middle of the form, will appear as shown below:

Type	Name	Crystal system	Surface normal (mno)	Azimuth (pqr)	Refer to substrate	Cx []	Cy []	Relaxation []
Layer	Ga(1-x)In(x)As(1-y)P(y)	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,50...	0,50...	1,0000
Layer	Ga(1-x)In(x)As	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,50...	0,50...	1,0000
Substrate	GaAs	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,50...	0,50...	1,0000

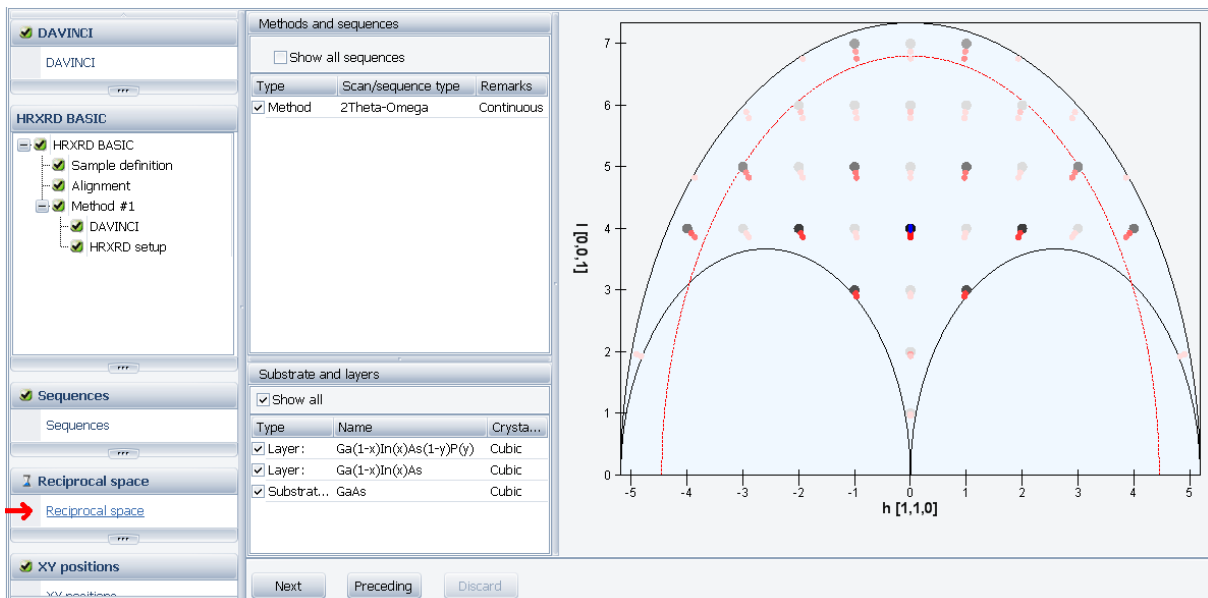


**NOTE**

If the sample just defined will be used in other experiments, it can be stored in the database. (see section Recently used samples, page 48) .

**The sample in reciprocal space**

The sample, which has just been defined using the reciprocal space display can now be controlled. Click on the Reciprocal space module. The module itself is described in detail on page 52.



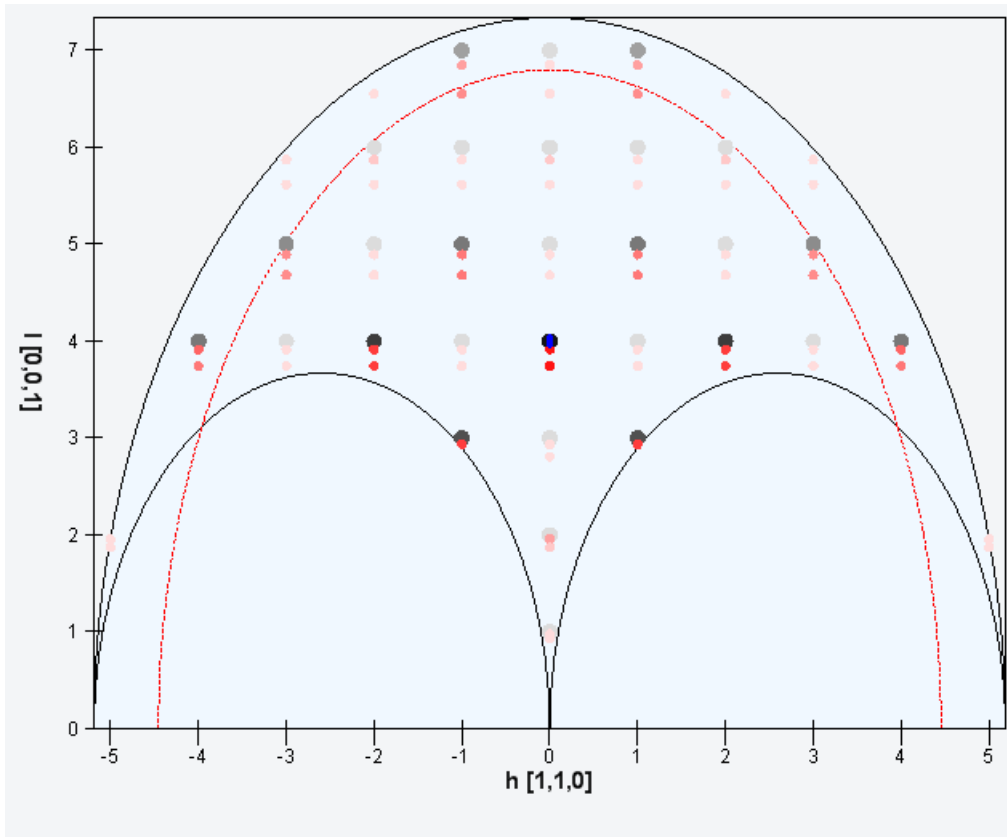
The substrate reflections are shown from black to gray depending on their intensity and the layer reflections are shown from light to dark red.

**Relaxation**

The relaxation of the layers can be altered. To do so, switch back to the Sample definition and change the relaxation of the layers from 1 to 0 in the last column of the sample:

Type	Name	Crystal system	Surface normal (mno)	Azimuth (pqr)	Refer to substrate	Cx []	Cy []	Relaxation []
Layer	Ga(1-x)In(x)As(1-y)P(y)	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,5000	0,5000	0,0000
Layer	Ga(1-x)In(x)As	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,5000	0,5000	0,0000
Subst...	GaAs	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,5000	0,5000	1,0000

Then, switch back to the Reciprocal space module. The picture has now changed:

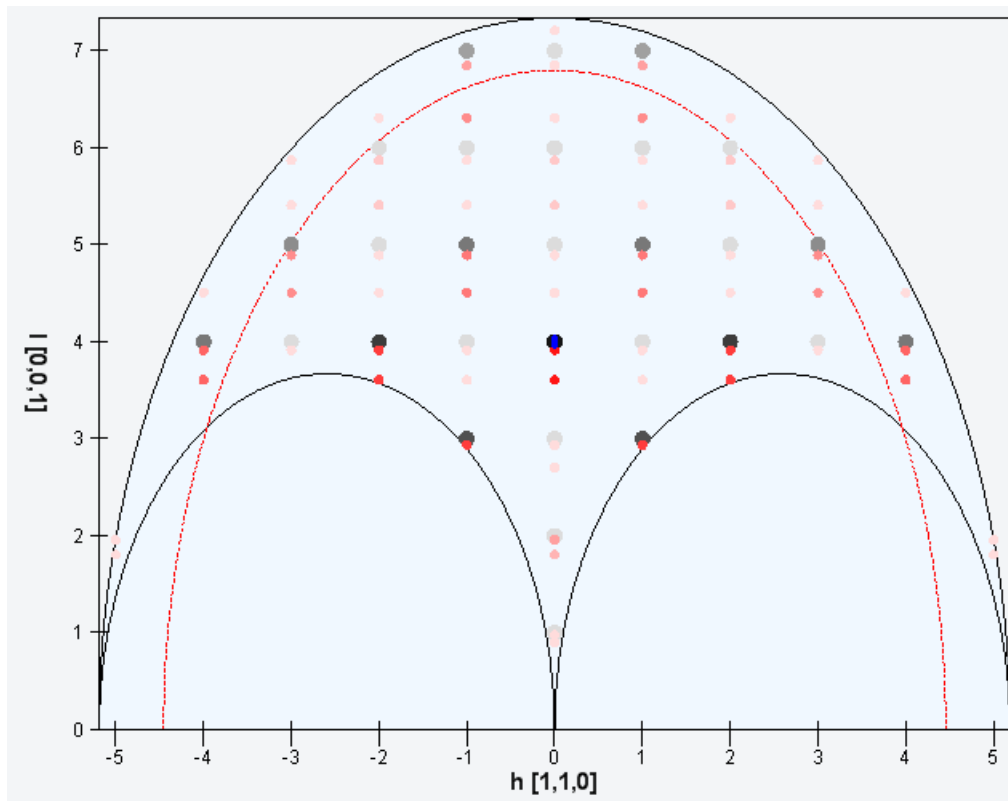


**Concentration**

The concentration can be changed for layers with solid solutions, for example the  $C_x$  for  $Ga(1-x)In(x)As$ :

Type	Name	Crystal system	Surface normal (mno)	Azimuth (pqr)	Refer to substrate	Cx []	Cy []	Relaxation []
Layer	Ga(1-x)In(x)As(1-y)P(y)	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,5000	0,5000	0,0000
Layer	Ga(1-x)In(x)As	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,8000	0,5000	0,0000
Subst...	GaAs	Cubic	[0,0,1]	[1,1,0]	<input checked="" type="checkbox"/>	0,5000	0,5000	1,0000

Switch back to the Reciprocal space module to control the result:

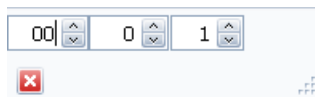


### Refer to substrate

When checked the relaxation will be relative to the substrate. Otherwise, the previous layer will be taken as reference.

### Sample orientation

Surface normal and azimuth can be changed. Click into the cell to open a small dialog:



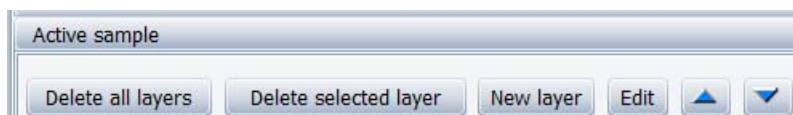
and change the values.

To close the dialog type <Esc> (changes not stored) or <F4> (changes stored). The red button will store the changes.

WIZARD guarantees that surface normal and azimuth are perpendicular if the form is left.

### More options

The buttons at the top of the sample table allow deletion of one or all layers, addition of a new layer (i.e. a manual definition of all parameters), editing of the layers, and moving layers up and down in the sample:



### Recently used samples

To store the samples created for later usage enter a sample name and press *Add to used samples* in the *Active sample* window.



The sample will be stored into the recently used samples at the bottom of the sample form and will be available for later sessions. Click *Choose selected* to use a recently used sample. Used samples also can be deleted.

Recently used samples		
Choose selected    Delete		
Sample name	Substrate	Layers
▶ GaAs sample	GaAs	Ga(1-x)In(x)As(1-y)P(y), Ga(1-x)In(x)As

### Alignment

WIZARD provides the possibility to define the alignment of a sample for a given reflection. This is done together with the COMMANDER plug-in.

Alignment at

Reflection hkl: 0 0 4 s

Calculated substrate positions

Tau(Bragg) [°]	0	Theta(Bragg) [°]	33.0285
Omega [°]	33.0285	2Theta(Bragg) [°]	66.0569

Alignment scan

Reset to defaults

Import from COMMANDER

Export to COMMANDER

Drive	Unit	Position	Offset	Alignment	Delta	Steps
Omega	[°]	33.0285	0	Done		1 101
Theta2-H	[°]	66.0569	0	Done		1 101
Psi-H	[°]	0.000	0	Done		1 101
Phi-H	[°]	0.000	0	Done		1 101
Beam-H	[mm]	0.00	0	Done		1 101
X	[mm]	0.000	0	Done		1 101
▶ Y	[mm]	0.000	0	Done		1 101

Fig. 33: Sample alignment form

If the reflection is modified at the upper left

Alignment at

Reflection hkl: 0 0 4 s

the substrate positions and the corresponding drive positions are recalculated accordingly:

Calculated substrate positions

Tau(Bragg) [°]	0	Theta(Bragg) [°]	34,5646
Omega [°]	34,5646	2Theta(Bragg) [°]	69,1293

Drive	Unit	Position	Offset	Alignment	Delta	Steps
Omega	[°]	33.0285	0	Done		1 101
Theta2-H	[°]	66.0569	0	Done		1 101
Psi-H	[°]	0.000	0	Done		1 101
Phi-H	[°]	0.000	0	Done		1 101
Beam-H	[mm]	0.00	0	Done		1 101
X	[mm]	0.000	0	Done		1 101
▶ Y	[mm]	0.000	0	Done		1 101

### Exchanging positions between WIZARD and COMMANDER

If the reflection has been chosen, the theoretical sample positions can be transferred to the COMMANDER plug-in: Use

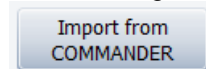
Export to  
COMMANDER

Then, switch to the COMMANDER plug-in:

Omega-H [°]	<b>22,000</b>	34,5646	<input checked="" type="checkbox"/>		
Theta2-H [°]	<b>41,000</b>	69,1293	<input checked="" type="checkbox"/>		

The drives can be moved or the alignment scans can be performed.

After locating the positions, use *Transmit drive positions* from the COMMANDER menu and click



in the WIZARD for the chosen experiment to be updated.

The offsets are updated in the alignment table and the positions are recalculated using the calculated substrate position. Please note the example below:

Drive	Unit	Position	Offset
▶ Omega	[°]	33.0238	0.0046
Theta2-H	[°]	66.9277	-0.8707

## Method

The form offers some information about the current scan setup, tube and detector chosen:

Method overview	
Detector(s) used:	Selected detector(s): PSD in 0D mode with 14,325 [mm] opening.
Tube(s) used:	Cu tube with 1,54184 [Å]. Generator at 20 [kV] and 5 [mA].
Scan type and mode:	2Theta-Omega as Continuous.
Total time [s]	19,7
	[hh:mm:ss.s] 0:00:19.7
Comments:	<input type="text"/>

It is possible to enter method specific comments.

## DAVINCI

The **DAVINCI** display is fundamentally similar as the display in the DAVINCI module. However, it is possible to change motorized optics only. These changes are method specific.

## HRXRD scan setup

This form defines the scan setup and all parameters needed to carry out the measurement.

The default scan setup is a 2Theta-Omega scan but may vary according to the detector, which has been selected. See table on p. 90 for an overview on available scan types.

### Basic scan setup

The **basic scan setup** is found at the top of the form. It serves to select scan type, scan mode, time per step, the number of steps and an optional delay time. The estimated time is calculated automatically.

### Scan axes

All of the axes used for the scan setup are listed in the upper left. A scan axis can be a real drive axis (in the example: the 2Theta and the Omega axis) or a logical axis (in the example: an offset for Omega). The scan parameters may be either Start, Stop and Increment or a Fixed value as in the offset.

In HR-XRD, the scan axes are relative. This means that the scan coordinates refer to the aligned reflection.

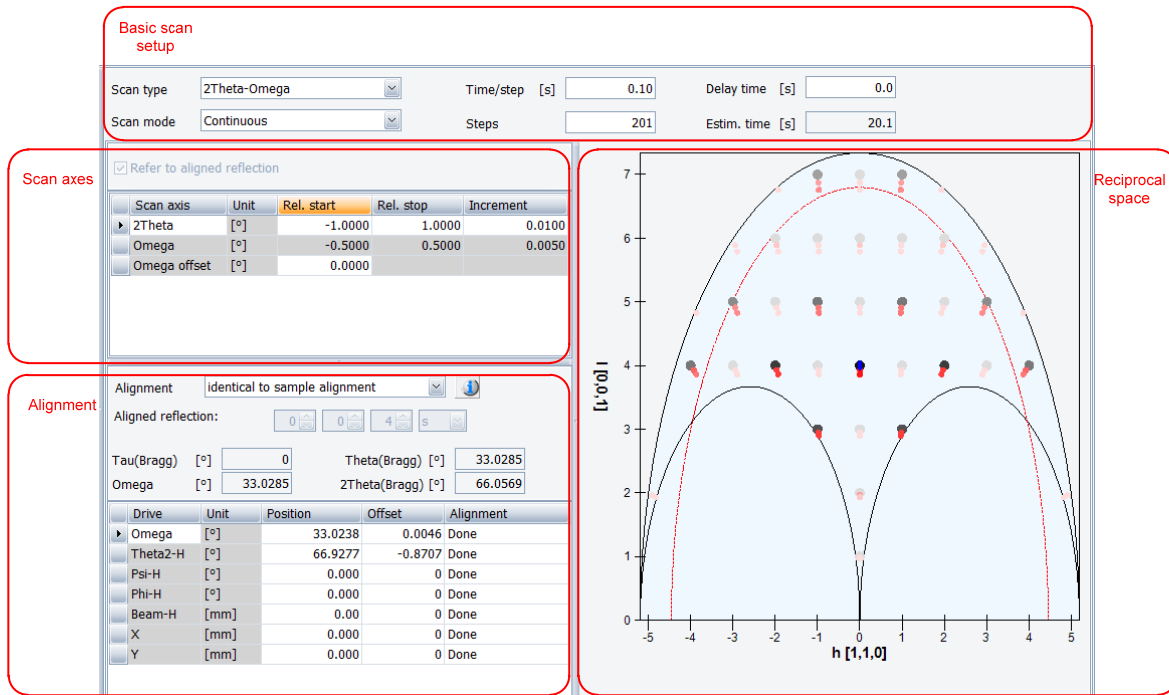
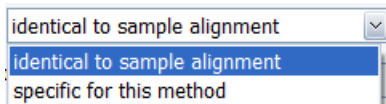


Fig. 34: HRXRD scan setup

**Alignment**

The alignment is identical to the alignment defined in section Alignment on page 49 by default. However, it may be switched to a method specific alignment. This renders the aligned reflection different for each single method.



**Reciprocal space**

The lower right panel shows the current scan in reciprocal space. For further information see the description in Reciprocal space module on page 52.

**Sequences in HR-XRD**

HR-XRD provides several special sequences. For an introduction to the sequences module, see section Sequences on p. 12.

The appearance of HR special sequences is restricted to the scan chosen in the base method. For example, a 2Theta-Omega scan allows an “Omega relative start” sequence but not a reciprocal space sequence.

**Reciprocal space module**

The reciprocal space display shows the reflections of the sample layers, the base methods and the effect of all sequences if they result in a movement in reciprocal space, i.e. in varying 2Theta and Omega values.

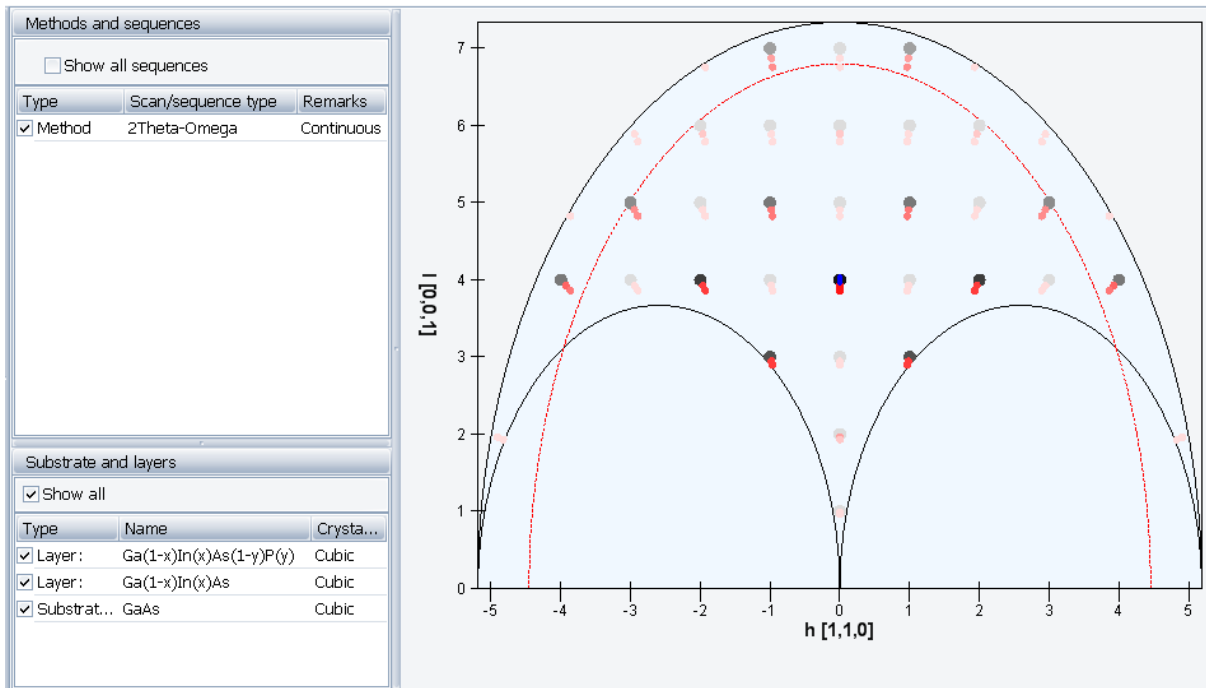


Fig. 35: Reciprocal space display

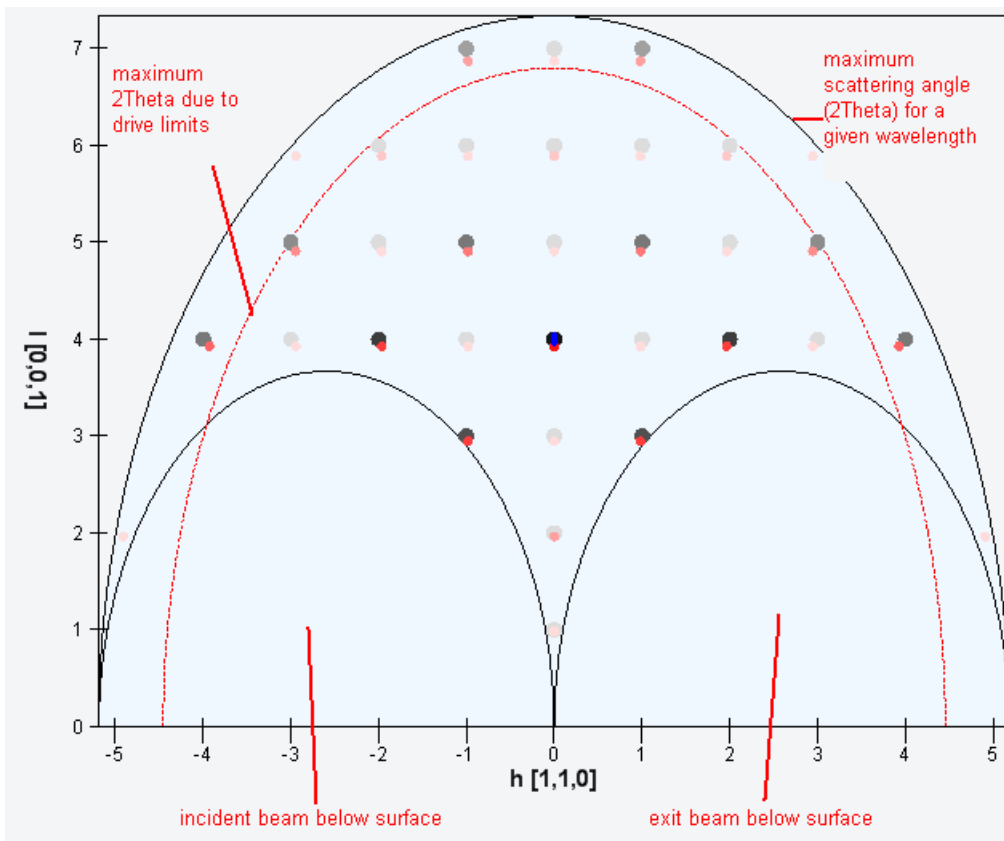
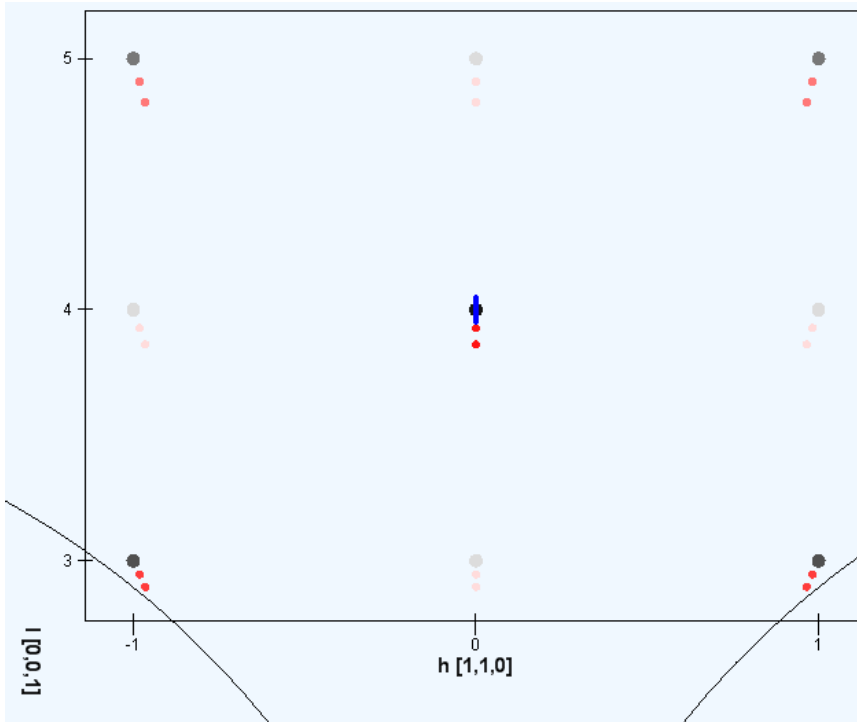


Fig. 36: Reciprocal space limits

The figure shows the GaAs sample defined earlier with a 2Theta-Omega scan.

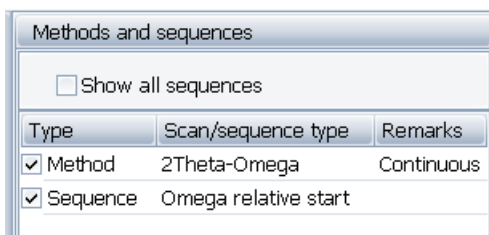
Several regions are not available for the measurement: The location at which the incident and the exit beam are below the sample surface and the location at which 2Theta is out of the drive limits. This is indicated by a red dashed line. If using an instrument with two secondary tracks (i.e. two detectors and perhaps different optics) the 2Theta limit is subject to switching the selected secondary beam path.

The user can zoom into the display. Click on the left mouse button. Move the mouse and release it:



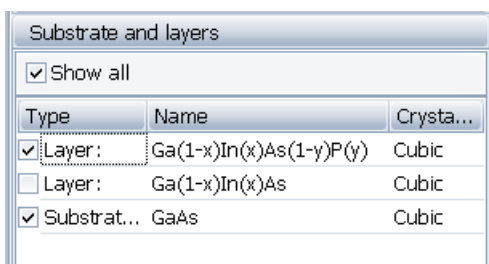
**Select sequences for display**

If sequences have been defined, their effect on the scan in the reciprocal space can be seen by toggling the check box at the upper left:



**Select layers for display**

Check the layer reflections at any time in order to change them.



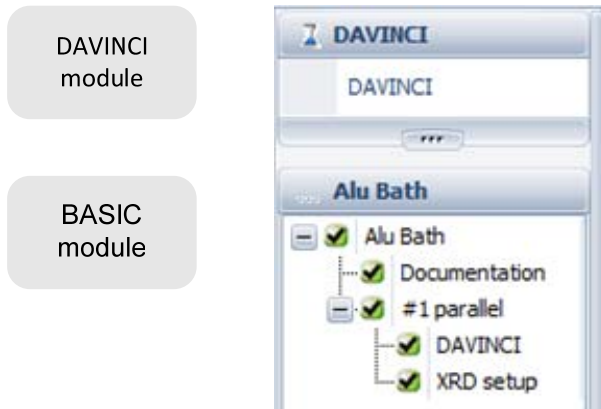
**XY positions module**

For this module, see the description on page 16.

## Alu Bath

Alu Bath allows measurements from a proportional counter either in parallel with another detector (for instance, a LYNXEYE) or one after the other.

This WIZARD provides two modules: one to set-up the primary optical parameters, and one to define the measurement method(s).



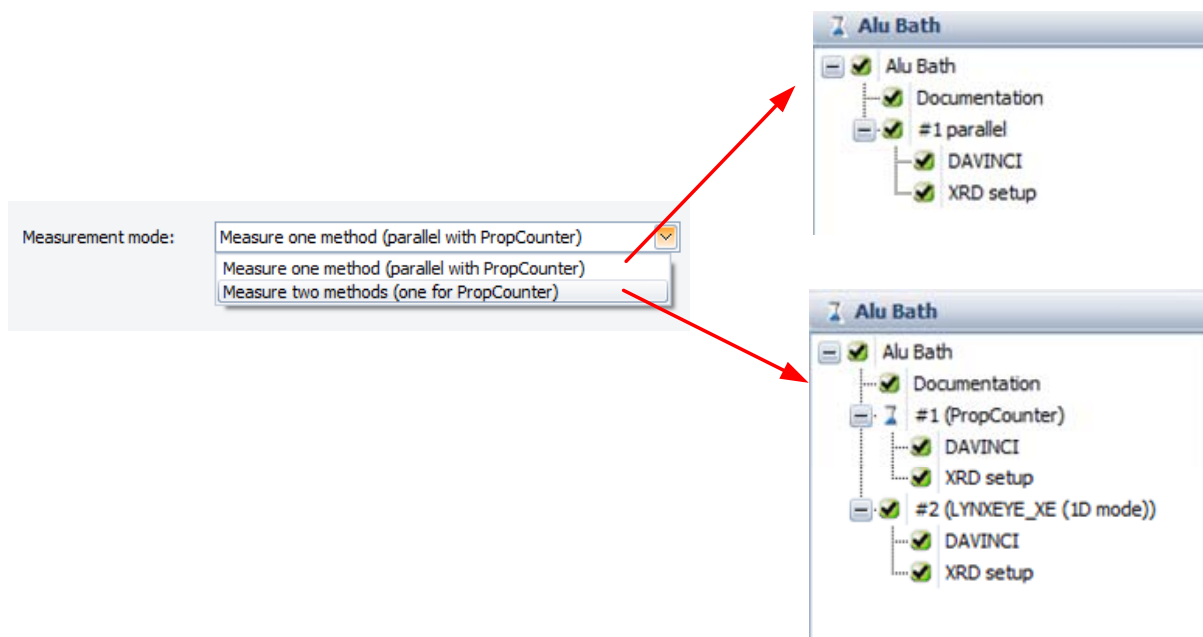
### DAVINCI module

For this module, see the description on page 9.

### Alu Bath module

Either a simultaneous measurement of the primary detector (for instance, a LYNXEYE) and the proportional counter can be carried out or both detectors are measured in sequence.

The measurement mode is selected in the top node of the AluBath setup:



Using the first option, the experiment will carry out one scan while the second option will carry out first the measurement with the proportional counter followed by the primary detector.

Note: Due to the electronics of the proportional counter, the minimum time/step is 25 [ms]. If the parallel measurement is chosen this will restrict the fastest time possible for the LYNXEYE, too.

The scans are defined by the XRD setup as described in XRD scan setup on p. 36.

### Options

Options are described on p. 32.

**SAXS**

The SAXS experiment template allows defining SAXS measurements on a HORIZON system with a 2D detector. Optionally, a VANTEC-1 may be mounted to allow for WAXS measurements. It consists of the following modules:

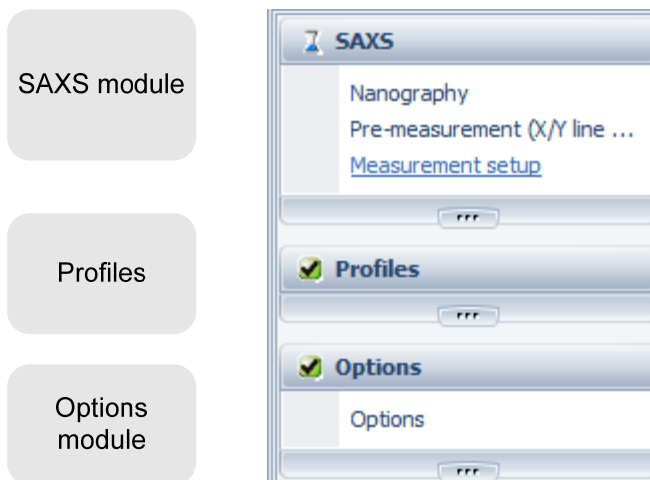


Fig. 37: SAXS modules

The SAXS module not only serves to define the later SAXS measurement but it also allows to carry out the pre-measurements described below.

**Overview: available measurement setups in SAXS**

Type	SAXS measurement setup		Detector involved
Pre-measurements	Nanography		VANTEC-500 in 0-D mode
	X/Y line scan		VANTEC-500 in 0-D mode
Job measurements	Sample measurement		VANTEC-500 (SAXS) VANTEC-1 (WAXS) if available
	Optional measurements		
	Transmission of sample	Sample with glassy carbon	VANTEC-500 in 0-D mode
		Glassy carbon	VANTEC-500 in 0-D mode
	Background		VANTEC-500
	Transmission of background	Background sample with glassy carbon	VANTEC-500 in 0-D mode
		Without glassy carbon	VANTEC-500 in 0-D mode
		Glassy carbon	VANTEC-500 in 0-D mode

Tab. 1: Available measurement setups in SAXS

### Pre-measurements

Two types of pre-measurements are available: a Nanography map and scans along X or Y.



#### NOTE

Pre-measurements taken before the BSML is saved will be stored in the BSML in a special section and copied to the final BRML. Thus, they are available to the evaluation software.

### Nanography map

Nanography maps will scan a complete X, Y rectangle while recording the integral count of the 2D detector.



To start a nanography map click on the  button. This opens the dialog:

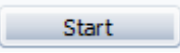
Scan axis	Unit	Use	Abs. start	Abs. stop	Increment
X	[mm]		0,000	82,000	1,000
Y	[mm]		0,0000	100,0000	2,000
Bi-directional		<input type="checkbox"/>			
ReferenceSampleWheel		<input type="checkbox"/>	Glassy Carbon	Glassy Carbon	

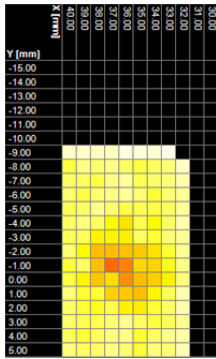
Fig. 38: SAXS Nanography setup dialog

Here, the ranges in X and Y can be entered.

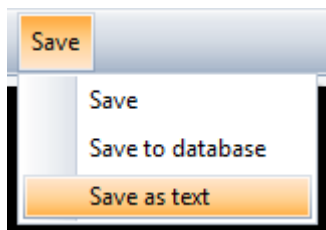
Check the Bi-directional if you want to meander (this saves driving times because Y is then scanned with changing the drive direction if X changes).

It is also possible to measure each X, Y position twice with two different settings of the sample wheel:

If done with the parameter setup, press  to directly start the measurement.



If done, the nanography may be stored as PNG file (using the Export button) or saved as a measurement file:



Save and Save to database will store a complete BRML file to disk or database, respectively. Save as text will store in a text format.



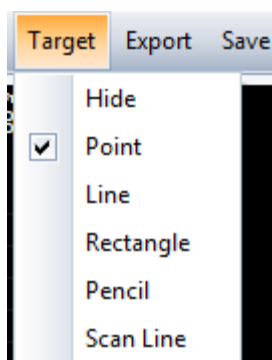
#### NOTE

Pre-measurements (like nanography or X, Y line scans) will be automatically saved within the BSML and are later available in evaluation software.

#### Transfer of positions

X, Y positions can be marked in the nanography and automatically transferred into sample positions for a job measurement.

First, select how to select positions using the Target menu:



Each X, Y position selected is automatically inserted into the table of Target positions at the right:

Target positions	
<input type="button" value="Clear"/> <input type="button" value="Transfer"/> <input type="button" value="Transfer (replace)"/>	
X [mm]	Y [mm]
▶ 3,000	-8,0000
3,000	-7,0000
4,000	-8,0000
4,000	-7,0000
5,000	-8,0000
5,000	-7,0000

The actions to select (point, line, rectangle,...) can be combined. The table allows to delete or move X, Y positions using the standard buttons, please see p.60.

To transfer them to sample measurements press  or . Using the first button will add new positions to the table of sample measurements, the second one will replace all existing X, Y positions. You can see the positions transferred if you click on *Measurement setup* in the module:

#	Sample name	X [mm]	Y [mm]	Detector(s) []	Time [s]	Optional
▶ 1		3,000	-8,0000	SAXS	100,000	
2		3,000	-7,0000	SAXS	100,000	
3		4,000	-8,0000	SAXS	100,000	
4		4,000	-7,0000	SAXS	100,000	
5		5,000	-8,0000	SAXS	100,000	
6		5,000	-7,0000	SAXS	100,000	

Here, you can proceed as described in Sample measurements, on p. 59.

### X/Y line scans

Another type of pre-measurement is a X or Y scan, for instance if the positions of capillaries are searched.

Different scan types are possible to move one drive and keep the other one fixed or to move both:

Scan type	X
Scan mode	X Y X,Y scan
Scan parameter	Still (VANTEC500)

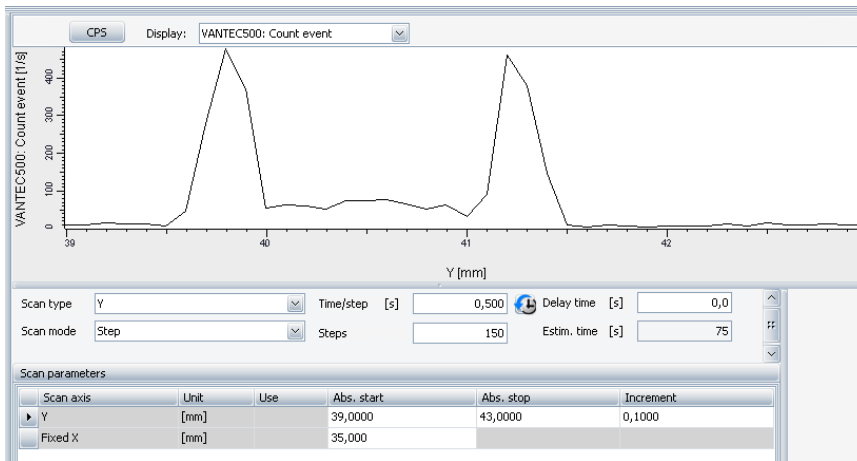
Then, define the drive parameters.



#### NOTE

All other parameters (e.g. generator or optics settings) are taken as they are currently set on the instrument.

Such a scan may give the following result:



The same transfer dialog can be used as described above in the nanography: click on the graphic to define X and Y positions.

### Sample measurements

On this form, the SAXS measurements are defined which are later executed in the job.

Each sample measurement can be combined with optional measurements.

### Definition of a sample measurement

Each row in the table creates a sample measurement:

#	Sample name	X [mm]	Y [mm]	Detector(s) [ ]	Time [s]	Optional
1		0,000	0,0000	SAXS [ v ]	100,000	








Fig. 39: SAXS sample measurement table

**Table entries for sample measurements**

#	The ordinal number of the sample measurement.
<i>Sample name</i>	An optional name of the sample
X	X coordinate
Y	Y coordinate
<i>Detectors</i>	Three selections are possible if both VÅNTEC-500 and VÅNTEC-1 are available:  SAXS: take 2D image  WAXS: 1D measurement from VÅNTEC-1  SAXS and WAXS: simultaneous measurement of both
<i>Time</i>	The exposure time
<i>Optional</i>	Indicators for optional measurements:  T: transmission  Bgrd: background  T(Bgrd): Transmission of background

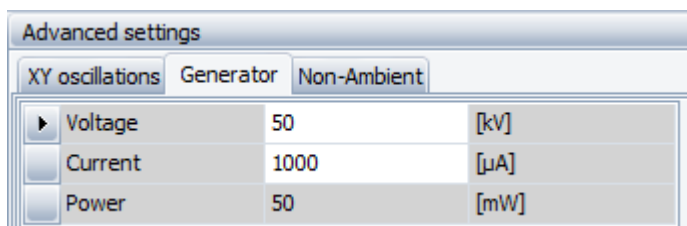
Additional measurements can be created, moved or deleted with the table buttons:



-  Add a new row
-  Delete a row
-  Copy the currently selected row
-  Move the selected row one row up
-  Move the selected row one row down
-  Move the selected row to the top of the table
-  Move the selected row to the bottom of the table

**Advanced settings**

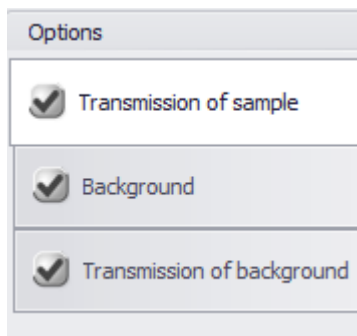
To the top right, it is possible to set X and Y oscillations, generator parameters and Non-ambient parameters (if a non-ambient chamber was mounted):



The advanced settings are specific for each sample measurement, i.e. for table entry.

**Optional measurements**

By default, optional measurements are disabled. This is indicated by greyed check icons on their tabs:



Optional measurements can be enabled for every sample measurement, i.e. for every row in the table to the left.

**Transmission of sample**

To enable this option, check the  Transmission of sample . The tab gets a green check icon:

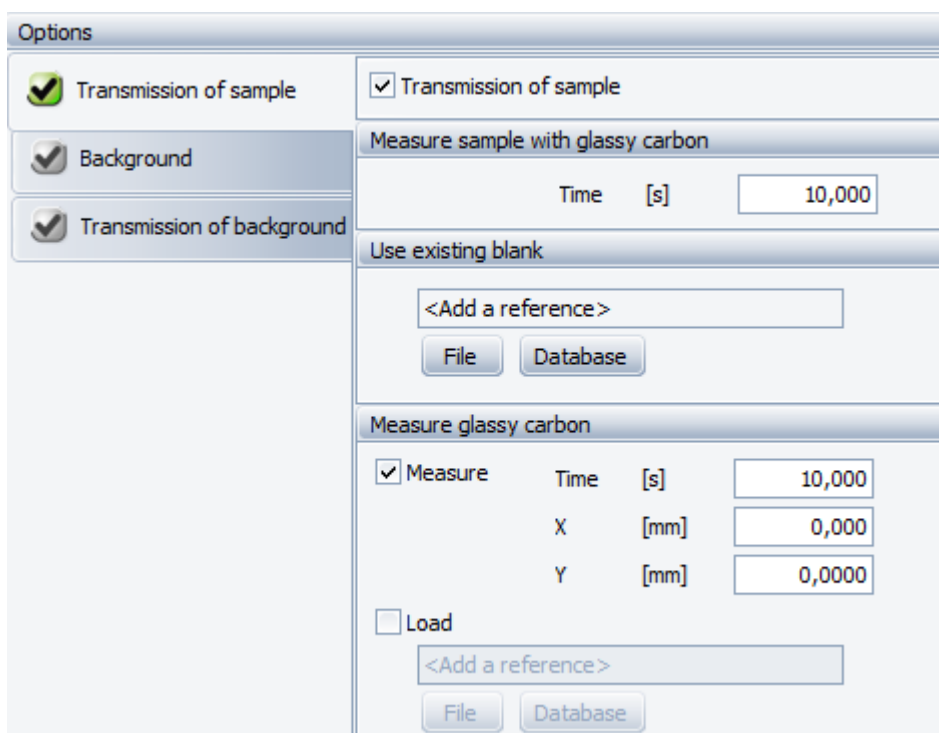


Fig. 40: SAXS optional measurements

The determination of the transmission of the sample requires three measurements:

Measure the sample with glassy carbon	$I_{s+gc}$	only the time can be defined here.
Reference an existing blank measurement	$I_{bg}$	see the section Define a reference to existing measurements, p. 63
Measure the glassy carbon	$I_{gc}$	This can be measured with a specific X,Y position or a previous measurement can be referenced

The measurements allow then to calculate the transmission of the sample using:

$$\tau_s = \frac{I_{S+GC} - \tau_{GC} I_S}{I_{GC} - \tau_{GC} I_{BG}}$$

### Background

The background may be measured or a previous measurement can be loaded (How to load one, please see the section Define a reference to existing measurements, p. 63).

The screenshot shows the 'Options' dialog box with the following settings:

- Transmission of sample
- Background
- Transmission of background
- Background
- Measure
  - X [mm]
  - Y [mm]
  - Time [s]
- Load
- <Add a reference> (text box)
- File Database (buttons)

### Transmission of background

Because the transmission of the background is similar to the transmission of the sample, see the description above.



#### NOTE

This option is only available if the background is also determined in the preceding step.

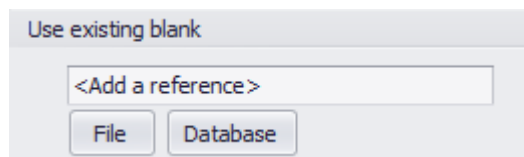
The screenshot shows the 'Options' dialog box with the following settings:

- Transmission of sample
- Background
- Transmission of background
- Transmission of background
- Measure background sample with glassy carbon
  - Time [s]
- Measure blank
  - <Add a reference> (text box)
  - File Database (buttons)
- Measure glassy carbon
  - Measure
    - Time [s]
    - X [mm]
    - Y [mm]
  - Load
  - <Add a reference> (text box)
  - File Database (buttons)

### Define a reference to existing measurements

Certain optional measurements can be or are required to be references to already existing ones.

An example is the blank measurement. In such a case, the form provides the following control:



Measurement references can come from the database or from a file on disk.

Press one of the buttons and the browser dialog opens:

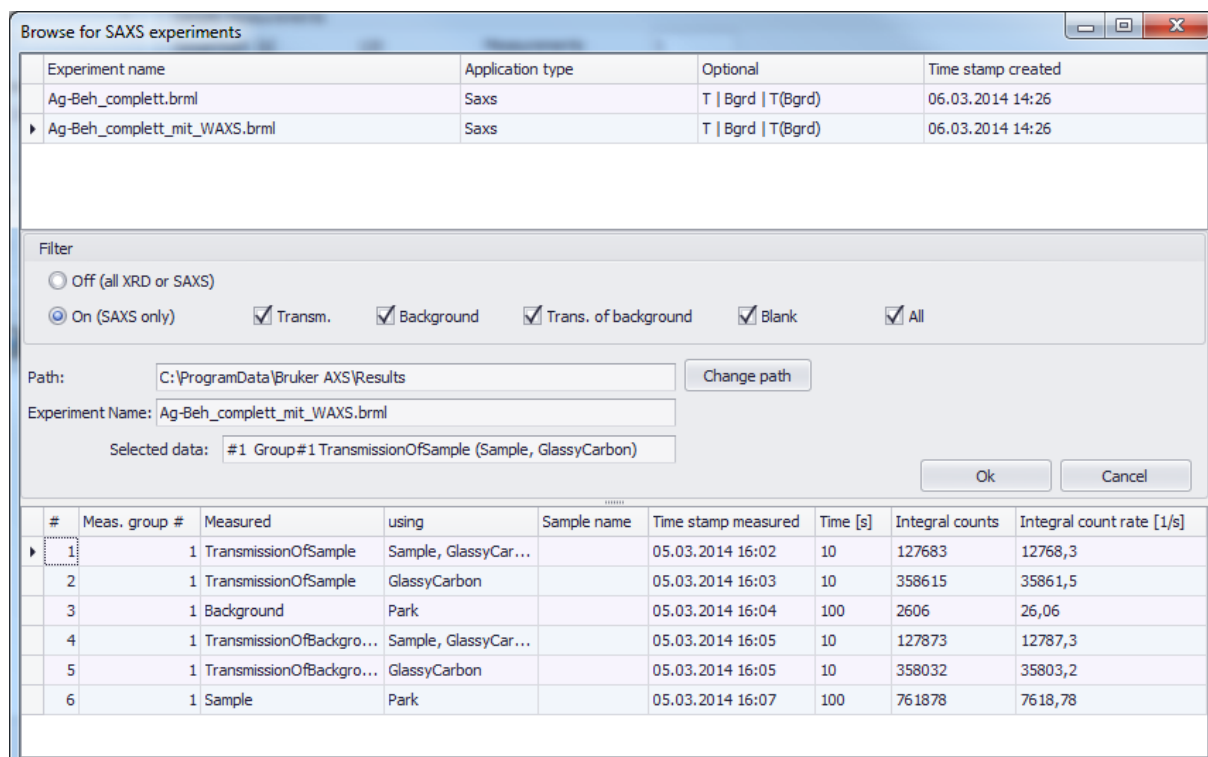


Fig. 41: SAXS BRML browser

Note that you can use the filter options to restrict the search.

The optional measurements (like Transmission or Transmission of background) are indicated by the flags in the Optional column:

T      Transmission

Bgrd   Background

T(Bgrd) Transmission of background

These indicators tell that a BRML contains such measurements but it does not tell how many measurements were done.

However, you need to select exactly one measurement. This is done in the lower part of the dialog.

Selected data: #3 Group#1 Background (Park) Ok Cancel

#	Meas. group #	Measured	using	Sample name	Time stamp measured	Time [s]	Integral counts	Integral count rate [1/s]
1	1	TransmissionOfSample	Sample, GlassyCar...		05.03.2014 16:02	10	127683	12768,3
2	1	TransmissionOfSample	GlassyCarbon		05.03.2014 16:03	10	358615	35861,5
3	1	Background	Park		05.03.2014 16:04	100	2606	26,06
4	1	TransmissionOfBackgro...	Sample, GlassyCar...		05.03.2014 16:05	10	127873	12787,3
5	1	TransmissionOfBackgro...	GlassyCarbon		05.03.2014 16:05	10	358032	35803,2
6	1	Sample	Park		05.03.2014 16:07	100	761878	7618,78

To help with the selection the dialog shows several measurement details (like the optics used, the integral count rate etc.).

The selected measurement is shown to the left of the OK button. Without selected data the dialog can only be closed with the Cancel button.

### Profiles

The profiles module is present if, for instance, a Non-ambient chamber is installed. See the description on pp. 16.

In SAXS, the complete measurement setup can be put on a profile.

### Options

Options are described on p. 32.

### Stress

The Stress experiment template allows defining stress measurements with a 0-D, 1-D or 2D detector. It consists of the following modules:

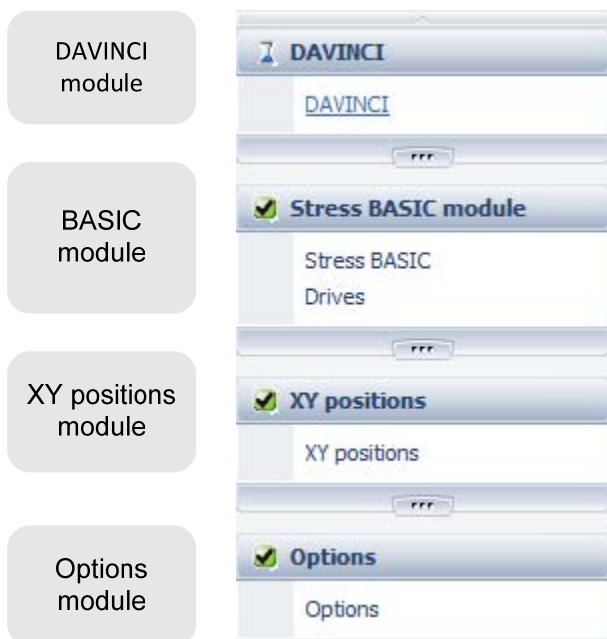


Fig. 42: Stress modules

Apart from the DAVINCI module used to select optics, detectors and other hardware, the complete stress measurement is defined in the Stress BASIC module that we describe below.

### DAVINCI module

For this module, see the description on page 9.

### Stress BASIC module

The basic module has two module items. The first item (Stress BASIC) defines the stress setup. The second item “Drives” is used to modify the settings for all drives independent on the stress measurement itself.

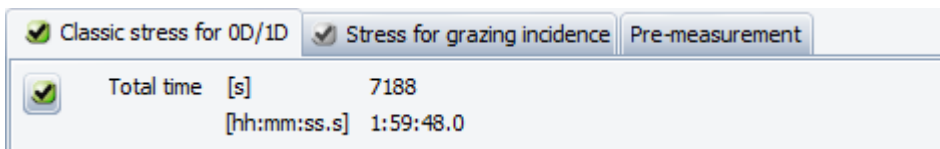
Depending on the Stress application and the detectors used for the measurement setup different setups can be chosen:

- Classic Stress for 0D and 1D detectors
- Grazing Incidence Stress (0D and 1D detectors)
- Stress 2D Side mode
- Stress 2D Iso mode

### Stress measurement setups

Depending on the instrument configuration, different measurement setups exist for Stress. Only those measurement setups are shown which can be used with the given instrument configuration and detector selection in the DAVINCI module.

The following figure shows the Stress measurement setups available if a 0D detector is selected. An overview of all available Stress setups can be defined below on p. 66



Each measurement setup is shown on a single tab. In addition, there may be a pre-measurement tab (if supported by the detector).

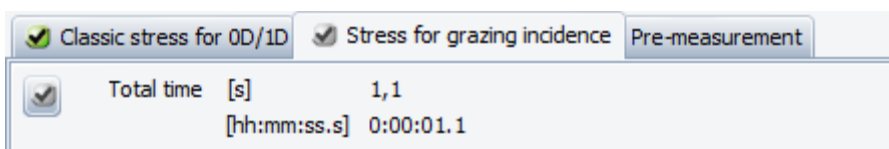



#### NOTE

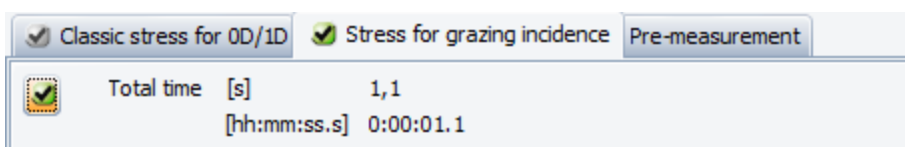
Only one measurement setup can be active at a time. The active setup is indicated in the tab header with a green check mark. To activate a measurement setup, select the corresponding tab and press the select button.

#### Example: activate a measurement setup

In the following figure the “Classic stress for 0D/1D” is chosen while the “Stress for grazing incidence” is displayed:



To activate “Stress for grazing incidence” press the button  in the upper left corner. Now, “Stress for grazing incidence” becomes selected and classic is shown with a grey check mark.



**Overview: available measurement setups in Stress**

Chosen detector	Stress measurement setup	possible scan type(s)	Remarks
0-D detector or Pilatus/1-D detector in 0D mode	Classic stress for 0D/1D	Offset coupled TwoTheta/Theta	
PSD		PSD fixed	
0-D detector or PSD or Pilatus in 0D mode	Stress for grazing incidence	TwoTheta	
2-D detector	Stress 2D Side mode	Phi, Psi	
	Stress 2D Iso mode	Still (VANTEC-500) or still for other 2D detector	

Tab. 2: Available measurement setups in Stress

**Stress measurement setup: Classic Stress for 0D/1D**



**NOTE**

This setup is only possible if a 0D or 1D detector is used for the measurement.

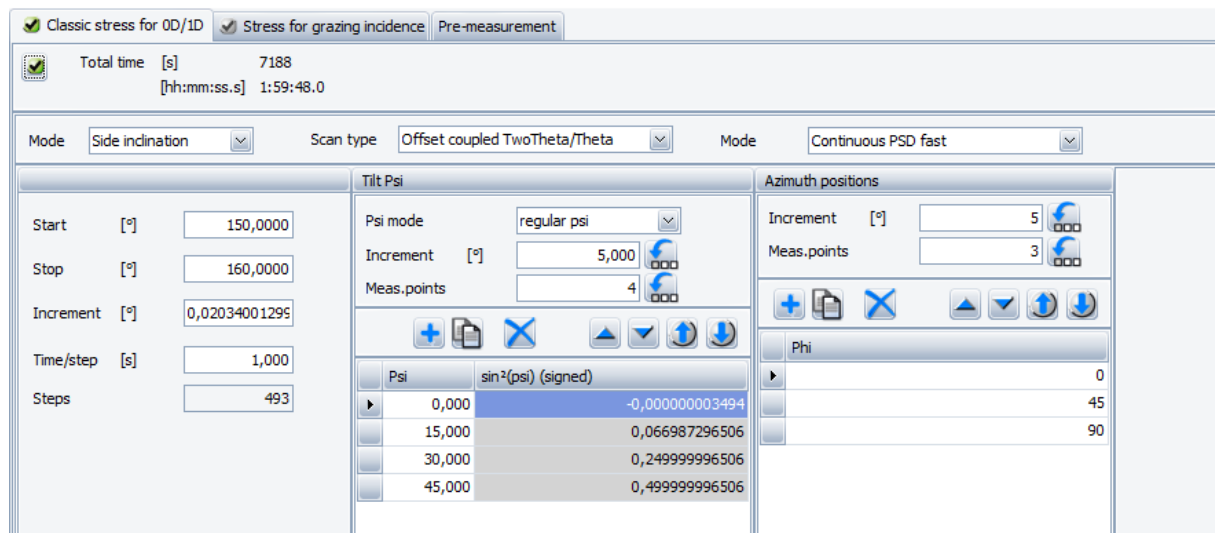
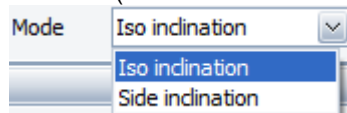


Fig. 43: Classic Stress

In Classic Stress you have to choose between Iso inclination (also called omega mode) and Side inclination (also called Psi mode):



The scan type is fixed to an Offset coupled TwoTheta/Theta scan. The scan modes available depend on the detector chosen. In our example a 1D detector was selected. Therefore, only a Continuous PSD fast scan is possible. 0D detectors may allow choosing between a step and a continuous scan.

In the next step a 2Theta range has to be defined by specifying start, stop, increment plus the time/step. This is done in the left most panel:

2Theta		
Start	[°]	150,0000
Stop	[°]	160,0000
Increment	[°]	0,02034001295
Time/step	[s]	1,000
Steps		493

### **Tilt psi**

In the middle panel the Tilt Psi values can be entered:

Tilt Psi		
Psi mode		regular psi
Increment	[°]	5,00000
Meas.points		2
Psi	sin2(psi)	
0,00005	0,00000000	
15,00005	0,06698730	
30,00005	0,25000000	
45,00005	0,50000000	

In Iso inclination, the Psi values are added to the 2Theta/2 values, in side inclination they are identical to the Psi drive positions of an Eulerian cradle.


Three different entry schemes exist:

regular psi	▼
regular psi	
sin2(psi)	
free entries	

In the regular Psi scheme, you enter Psi values in the left column, the  $\sin^2(\text{psi})$  are calculated.








In the  $\sin^2(\text{psi})$  scheme, you enter values between 0 and 1 in the right column and the Psi are calculated.

Using the scheme free entries, you can enter values in both columns.

Furthermore, using the regular psi and the  $\sin^2(\psi)$  scheme, you can enter an increment or the number of measurement points. Then, press the button : this takes the first and the last Psi (or  $\sin^2(\psi)$ ) value from the table and calculates all others in this range.

The Psi table entries can also be modified with the table buttons:





-  Add a new row
-  Delete a row
-  Copy the currently selected row
-  Move the selected row one row up
-  Move the selected row one row down
-  Move the selected row to the top of the table
-  Move the selected row to the bottom of the table








### ***Azimuth positions***




Finally, enter the azimuth (or Phi) positions in the right most panel:


**Azimuth positions**

Increment [°]  

Meas.points  

	Phi	
		0,000
		45,000
		90,000

The usage of  and the table buttons work is identically to the description above for Psi.

### ***Pre-measurement***

Pre-measurement for Classic Stress

If you are not sure about the sample it is possible to carry out a pre-measurement. To do so, mark the Psi and Phi entry you want to measure with a click on the row. Then, change to the tab Pre-measurement:

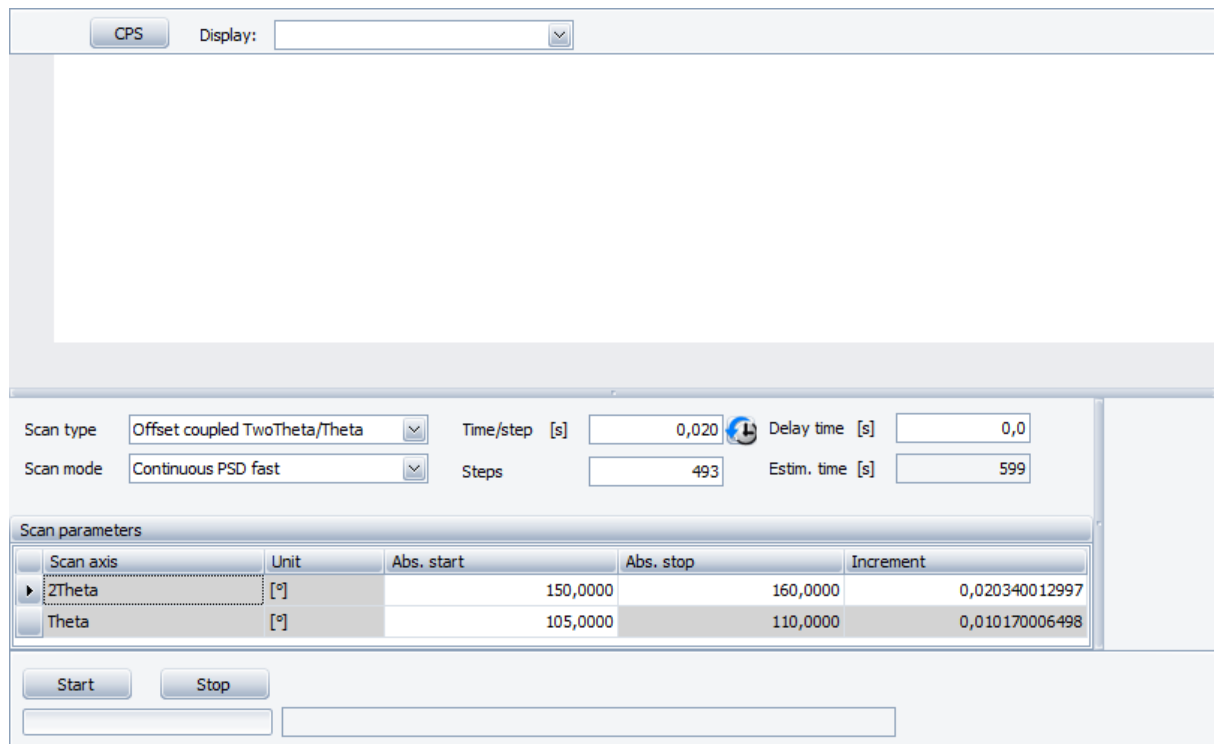

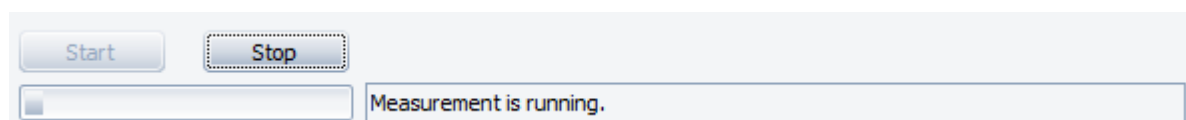


Fig. 44: Stress pre-measurement

You may choose between different scan types and change scan parameters. To get the fastest possible scan time press the clock button at the right of the time/step field

Time/step [s]   , (it is calculated from the current scan axis increment, the scan mode and the fastest possible detector readout).

After a click on the Start button, the measurement will be executed and progress information is shown below:

**NOTE**

For the pre-measurement the current optic and generator settings are used. If necessary, use COMMANDER to change them before.

**Stress measurement setup: Stress for grazing incidence****NOTE**

This setup is only possible if a 0D or 1D detector is used for the measurement.

This stress setup uses 2Theta scans. The scan modes available depend on the detector chosen. In our example a 1D detector was selected. Therefore, only a Continuous PSD fast scan is possible. 0D detectors may allow choosing between a step and a continuous scan.

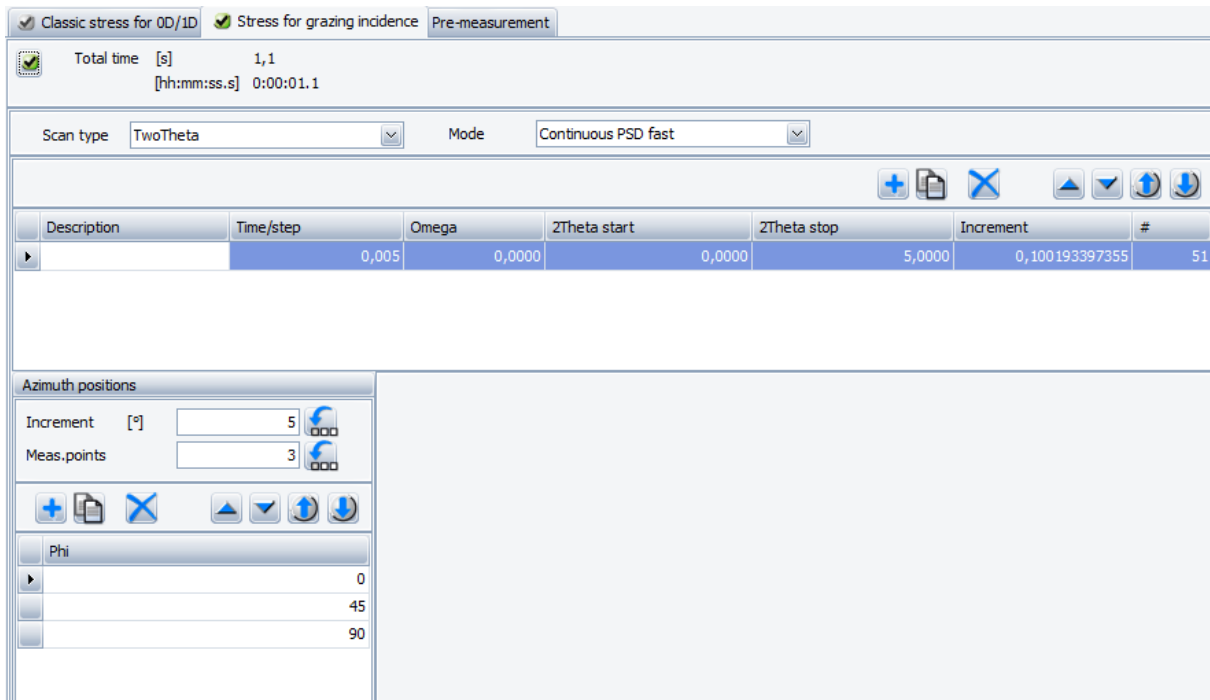











Fig. 45: Stress for grazing incidence

### Reflections

In the table you can define Omega values and 2Theta scan parameters together with the time/step. The description is optional.

Description	Time/step	Omega	2Theta start	2Theta stop	Increment	#
	0,005	0,000	0,000	5,000	0,100193397355	51

It is possible to measure more than one reflection: Just press the  button to add or  to copy the current row.

-  Add a new reflection
-  Delete a reflection. There must be at least one.
-  Copy the currently selected reflection
-  Move the selected reflection one row up
-  Move the selected reflection one row down
-  Move the selected reflection to the top of the table
-  Move the selected reflection to the bottom of the table

### Azimuth positions

For the definition of Azimuth positions, refer to the description of Classic stress above.

### Pre-measurement

Pre-measurement for Grazing incidence Stress

If you are not sure about the sample it is possible to carry out a pre-measurement. To do so, mark the Phi entry you want to measure with a click on the row. Then, change to the tab Pre-measurement. All steps are similar to the pre-measurement described for Classic Stress. Please see there for further details.

### Stress measurement setup: Stress 2D Side mode

A Stress setup for 2D detectors is similar to the pole figure setup used for Texture, see p.80.



#### NOTE

This setup is only possible if a 2D detector is used for the measurement.

A pre-measurement is not possible with a 2D detector.

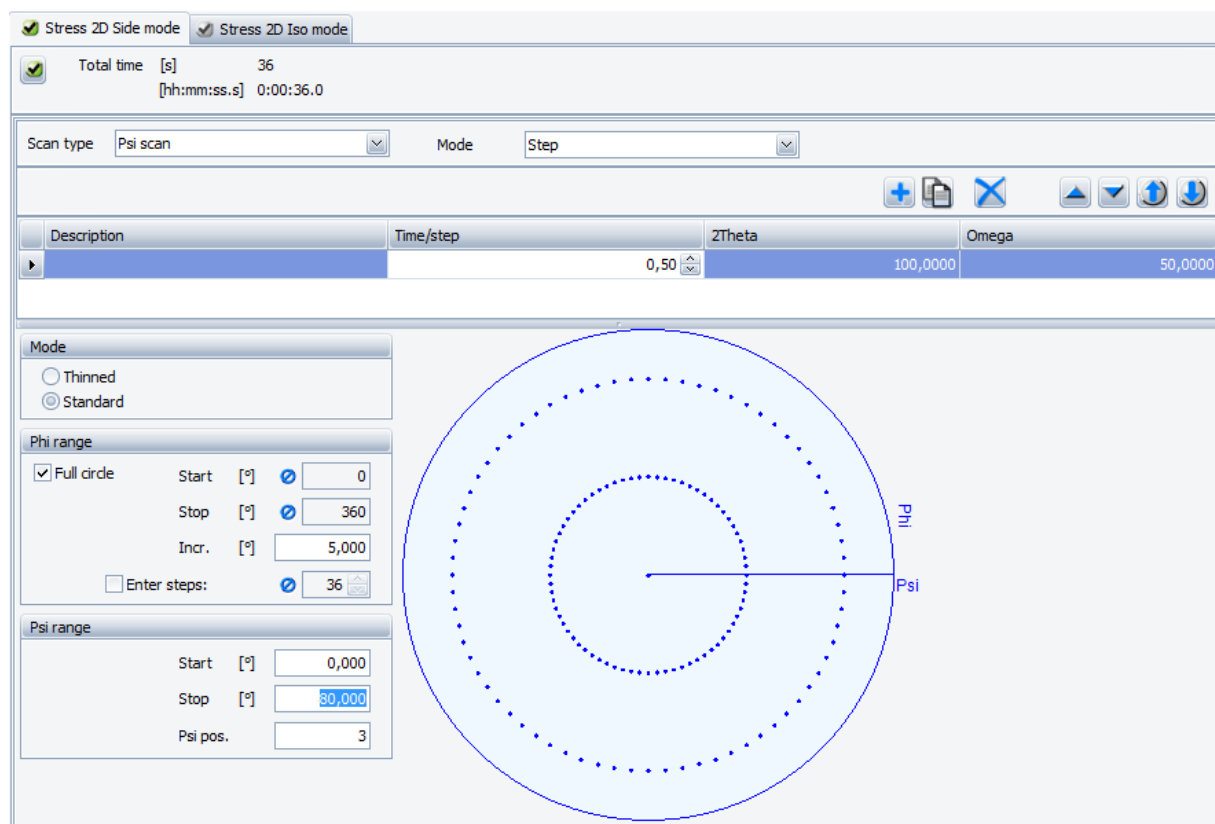


Fig. 46: Stress 2D Side mode

The elements for a 2D setup are the following ones (from top to bottom):

#### Scan types and mode

It is possible to use either Phi scans or Psi scans. Psi scans cannot be combined with a thinned mode. Only step scan mode is possible.

#### Reflections

In the table one or more reflections (i.e. different pairs of 2Theta and Omega) can be defined.

#### Pole figure

Psi and Chi can be set in a thinned or standard mode. The thinned mode cannot be combined with a Psi scan.

It is possible to use either a full Phi circle or to define a Phi sector: To do so, uncheck the check box “full circle”. To specify an increment rather than the number of steps uncheck the check box “enter steps”:

The Psi range can be set with start, stop and the number of Psi positions:

### Stress measurement setup: Stress 2D Iso mode



#### NOTE

This setup is only possible if a 2D detector is used for the measurement.

A pre-measurement is not possible with a 2D detector.

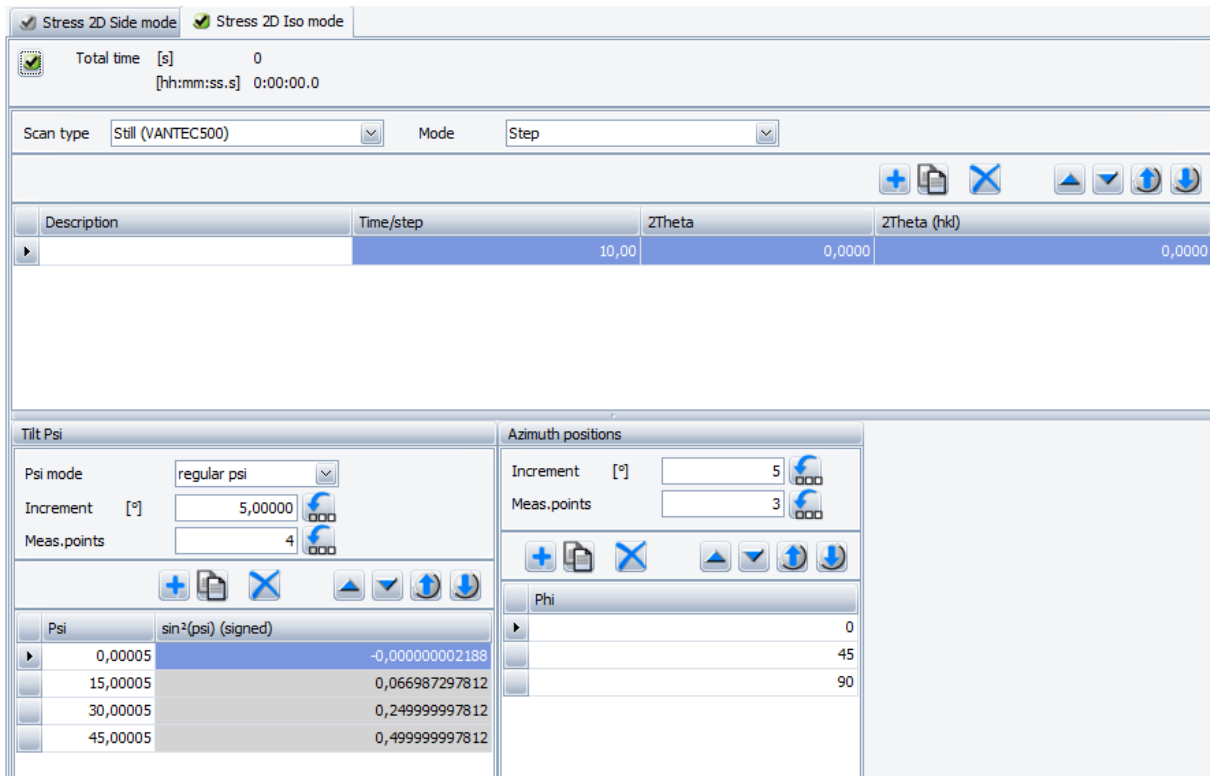


Fig. 47: Stress 2D Iso mode

### Reflections

In the table one or more reflections (i.e. different 2Theta) can be defined. It is also necessary to specify the theoretical 2Theta value,  $2\theta_{hkl}$ .

### Tilt Psi

The Psi table is described in Classic Stress on p. 67.

For each Psi in the table, omega is calculated from:  $\Omega = 2\theta_{hkl} / 2 + \Psi$ .

Note that Psi must follow the condition:  $|\Psi| > 2\theta_{hkl} / 2$ .

### Azimuth positions

Finally, enter the azimuth (or Phi) positions in the right most panel as described in Classic Stress on p. 68.

### Drives

This form allows the user to enter parameters (positions and oscillations) for all drives which are not already defined by the Stress setup itself. See also Fixed drives, p.32.

### XY positions module

For this module, see the description on page 16.

## Texture

The Texture experiment template allows defining texture measurements with a 0-D, 1-D or 2D detector. It consists of three modules:



Fig. 48: Texture modules

Apart from the DAVINCI module used to select optics, detectors and other hardware, the complete texture measurement is defined in the TEXTURE BASIC module that we describe in the following.

### DAVINCI module

For this module, see the description on page 9.

### TEXTURE BASIC module

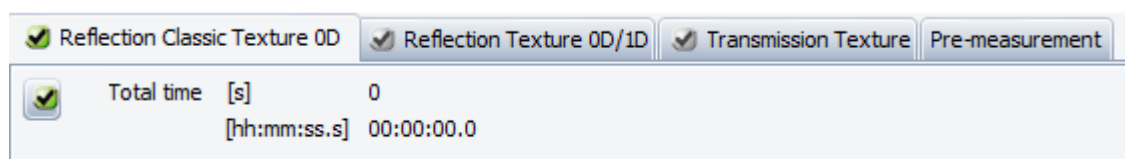
The basic module has two module items. The first item defines the pole figure and the schemes. The second item "Drives" is used to modify the settings for all drives independent on the texture measurement itself.

#### Texture measurement setups

The form defines pole figures, i.e. the coverage of the Phi-Psi space, and the measurement type.

Depending on the instrument configuration, different measurement setups exist for Texture. Only those measurement setups are shown which can be used with the given instrument configuration and detector selection in the DAVINCI module.

The following figure shows the Texture measurement setups available if a 0D detector is selected.



Each measurement setup is shown on a single tab. In addition, there may be a pre-measurement tab (if supported by the detector). The transmission tab might not be available depending on the software version and settings.

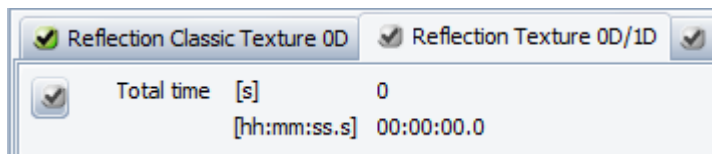


#### NOTE

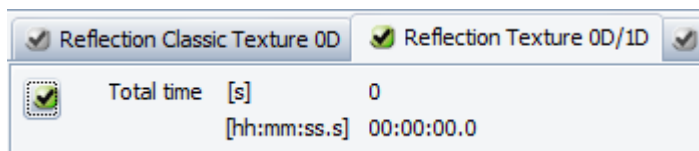
Only one measurement setup can be active at a time. The active setup is indicated in the tab header with a green check mark. To activate a measurement setup, select the corresponding tab and press the select button.

**Example: activate a measurement setup**

In the following figure the “Reflection Classic Texture 0D” is chosen while the “Reflection Texture 0D/1D” is displayed:



To activate “Reflection Texture 0D/1D” press the button  in the upper left corner. Now, “Reflection Texture 0D/1D” becomes selected and classic is shown with a grey check mark.

**Overview: available measurement setups in Texture**

Chosen detector	Texture measurement setup	possible scan type(s)	Remarks
0-D detector or 1-D detector/ Pilatus in 0-D mode	Reflection Classic Texture 0D	Phi scan	
	Reflection Texture 0D/1D	Offset coupled TwoTheta/Theta	Omega remains at half 2Theta plus an optional offset
		Detector	Omega remains fixed
1-D detector	Reflection Texture 0D/1D	Offset coupled TwoTheta/Theta	Omega remains at half 2Theta plus an optional offset
		Detector	Omega remains fixed
		PSD fixed	PSD oriented at 0°
		ThetaF scan	PSD oriented at 90°
2-D detector	Reflection Texture 2D	Phi scan	

Tab. 3: Available measurement setups in Texture

Each single (Phi, Psi) position pair is defined as an orientation. At each orientation a measurement will be carried out. The type of the measurement depends on the detector selected.

The measurement defines the time per orientation and the used 2Theta and Omega positions. The measurements are defined in the table at the bottom (see following figure). It is possible to define more than one measurement.

**Pole figure**

The pole figure display is common to all Texture measurement setups and is located in the lower part of the specific form. The upper part usually contains a table of scheme entries:

Description	Orientations/time	Time/orientation	Scan type	Scan mode	2Theta	Omega	Bckgrd 1	2Theta	time factor
0,0	765	0,100	Phi	Continuous	44,0000	22,0000	<input type="checkbox"/>	0,0000	1,0

Use one pole figure for all entries  
**Mode**  
 Thinned    Delta [°]   
 Standard  
**Phi range**  
 Full circle    Start [°]  0  
    Stop [°]  360  
 Enter steps:  
**Psi range**  
    Start [°]   
    Stop [°]

Fig. 49: Classic Texture 0D



**NOTE**

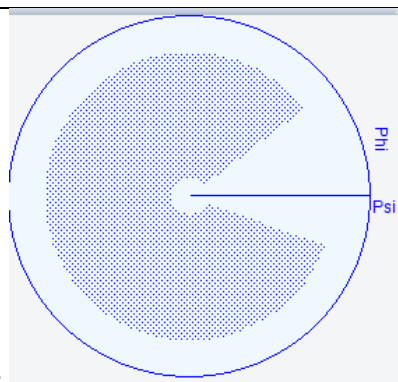
By default, the pole figure is unique for all scheme entries. To allow for different pole figures for each scheme uncheck  Use one pole figure for all entries at the top left of the pole figure control.



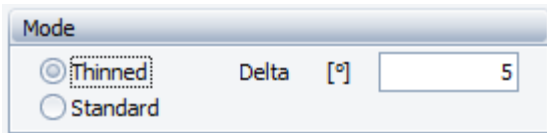
**NOTE**

By default, the pole figure shows one point per orientation. But if the density is high (either there are many orientations or the window covers a small region of the computer screen only) the pole figure coverage is displayed as a hatched region only.

Example:



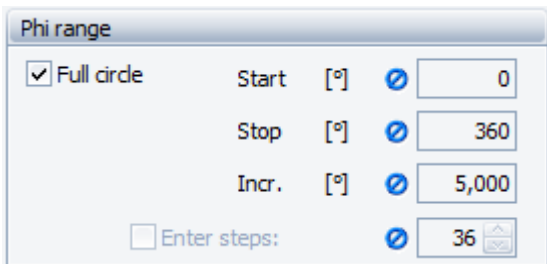
The coverage of the Phi-Psi space can be defined in various ways:



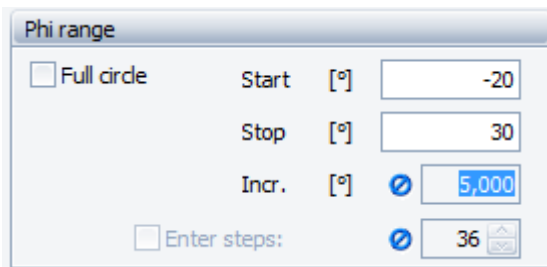
Thinned mode: the orientations are equally distributed, as shown in the figure above.

Standard mode: the number of orientations at a fixed Psi angle is kept constant, i.e. the density of orientations for low Psi angles is higher than for high Psi angles.

The Phi range can be a full circle

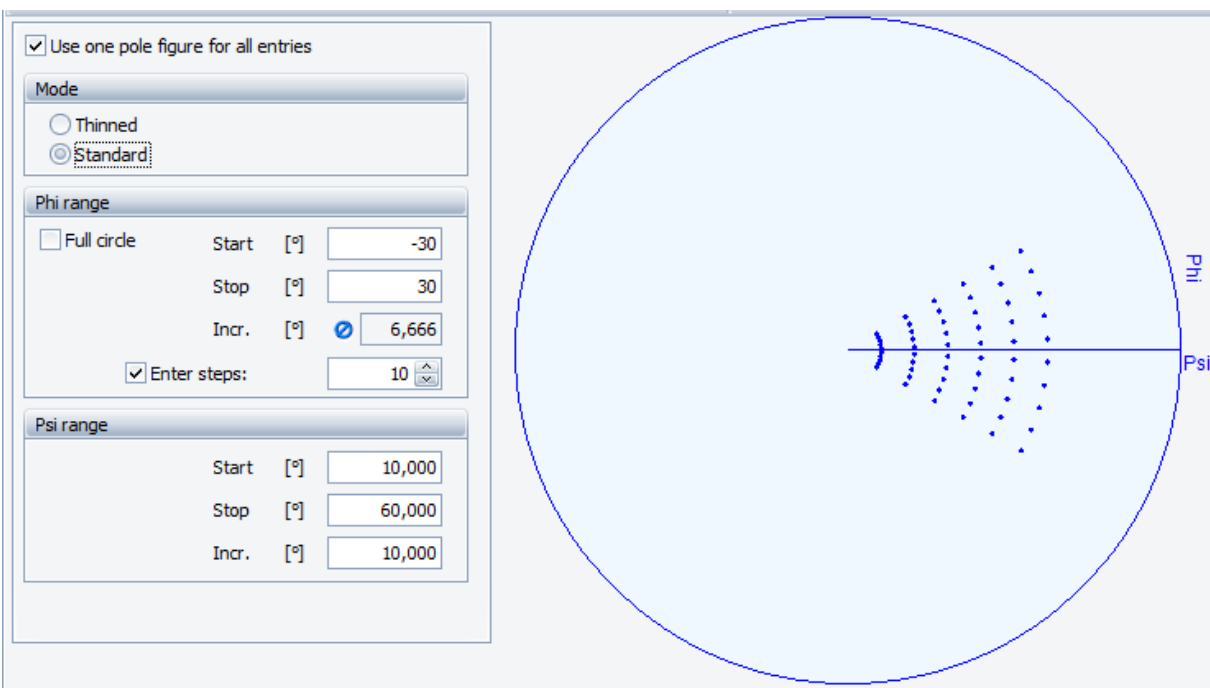


or may define a sector only by un-checking the Full circle check box.



Furthermore, Psi can be restricted.

The example shows a Phi sector in standard mode:



## Orientations

Each single orientation i.e. each (Phi, Psi) point in the pole figure will be covered by the measurement. However, the type of measurement carried out is prescribed by the measurement setup chosen and the detector which was previously selected in the DAVINCI module.

### Measurement setup: Reflection Classic Texture 0D

This measurement setup is only available if either a 0-D detector is configured and selected in the DAVINCI. A 0-D detector can be a scintillation counter or solid state detector. It can also be a LYNX-EYE working in 0-D mode. In any case, the resulting scan type will be a Phi scan either in continuous or in step mode.

The form displayed consists of the pole figure as discussed above and a table specific for the classic mode.

Description	Orientations	Time/orientation	Scan type	Scan mode	2Theta	Omega	Bckgrd 1	2Theta	time factor	Bckgrd 2	2Theta	time factor	One bckgrd per Phi
0,0	764	0,10	Phi	Conti...	44,0...	22,0...	<input type="checkbox"/>	0,0000	1,0	<input type="checkbox"/>	0,0000	1,0	<input checked="" type="checkbox"/>

### Table entries in Reflection Classic Texture 0D

<i>Description</i>	This can be any text.
<i>Orientations</i>	The number of orientations as calculated from the pole figure
<i>Time/orientation</i>	This is the time spent per orientation (please see the note below).
<i>Scan type</i>	In the classic setup this is fixed to a Phi scan.
<i>2Theta</i>	Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
<i>Omega</i>	Enter an Omega value here if the half of 2Theta is not wanted.
<i>Background 1 or 2:</i>	Check the box in the Background 1/2 column to create one or two background measurements. If checked a 2Theta value must be checked in the following column. This value should be distinct from the 2Theta value used for the measurement. A time factor for the background measurement can be entered in the next column.
<i>One background per Phi</i>	If checked, a background measurement will be created, but only if Psi varies.



#### NOTE

The time/orientation entered in the table is a minimum time used for the measurement. If this time leads to a scan velocity which is too fast it will be automatically reduced before the measurement.

### Adding, deleting and moving orientations

The toolbar at the top of the table can be used to modify the number of schemes:







Add a new orientation



Delete an orientation



Copy the currently selected orientation

-  Move the selected orientation one row up
-  Move the selected orientation one row down
-  Move the selected orientation to the top of the table
-  Move the selected orientation to the bottom of the table

### Measurement setup: Reflection Texture 0D/1D

This measurement setup is only available if either a 0-D detector or a PSD in 1-D mode is configured and selected in the DAVINCI.

In this setup the user can choose between different scan types depending on the chosen detector as described on the table of Texture measurement setups on p. 75.

Description	Orientations	Time/orientation	Scan type	Scan mode	2Theta center	2Theta start	2Theta stop	Increment	Meas.points	Omega
I 45,0	764	0,10	Detector	Continuous	45,0000	40,0000	50,0000	0,1000	101	22,5000

#### Table entries in Reflection Texture 0D/1D

<i>Description</i>	This can be any text.
<i>Orientations</i>	The number of orientations as calculated from the pole figure
<i>Time/orientation</i>	This is the time spent per orientation (please see the note below).
<i>Scan type</i>	Depending on the detector chosen, different scan types can be chosen, see overview on p. 75
<i>Scan mode</i>	Depending on the detector and scan type different modes are allowed
<i>2Theta center</i>	Read only for moving scans (detector scan, offset coupled TwoTheta/Theta). For still scans (PSD fixed or ThetaF) enter the 2Theta value here.
<i>2Theta start</i>	Read only for still scans. Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
<i>2Theta stop</i>	Read only for still scans. Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
<i>Increment</i>	For still scans the resolution of the PSD can be changed (this results in a binning of the channels). For moved scans the scan increment can be changed like standard scan parameters in XRD.
<i>Meas.points</i>	For still scans this is fixed. For moved scans it can be entered instead of the increment which is then recalculated.
<i>Omega</i>	This is automatically calculated from the 2Theta center if 2Theta center, start or stop are modified. Enter an Omega value here if the half of 2Theta is not wanted.

### Measurement setup: Reflection Texture 2D

If a 2D detector is selected Phi scans will be created for each Psi. Because of the area coverage the Psi is defined by start, stop and the number of Psi positions:

Description	Orientations/time	Time/orientation	Scan type	Scan mode	2Theta	Omega
	73	0,100	Phi	Step	0,0000	0,0000

Use one pole figure for all entries  
**Mode**  
 Thinned Delta [°]   
 Standard  
**Phi range**  
 Full circle Start [°]    
 Stop [°]    
 Enter steps:  
**Psi range**  
 Start [°]   
 Stop [°]   
 Psi pos.

Fig. 50: Texture 2D setup

#### Table entries in Reflection Texture 2D

<i>Description</i>	This can be any text.
<i>Orientations</i>	The number of orientations as calculated from the pole figure
<i>Time/orientation</i>	This is the time spent per orientation (please see the note below).
<i>Scan type</i>	This is fixed to a Phi scan.
<i>Scan mode</i>	Step or continuous run can be chosen
<i>2Theta</i>	Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
<i>Omega</i>	This is automatically calculated from the 2Theta. Enter an Omega value here if the half of 2Theta is not wanted.

#### Drives

This form allows the user to enter parameters (positions and oscillations) for all drives which are not already defined by the Stress setup itself. See also 32Fixed drives, p. 32.

#### XY positions module

For this module, see the description on page 16.

## TXRF

There are four modules that have to be filled out: *Element file*, *Measurement*, *Calibration* and *XY positions*.

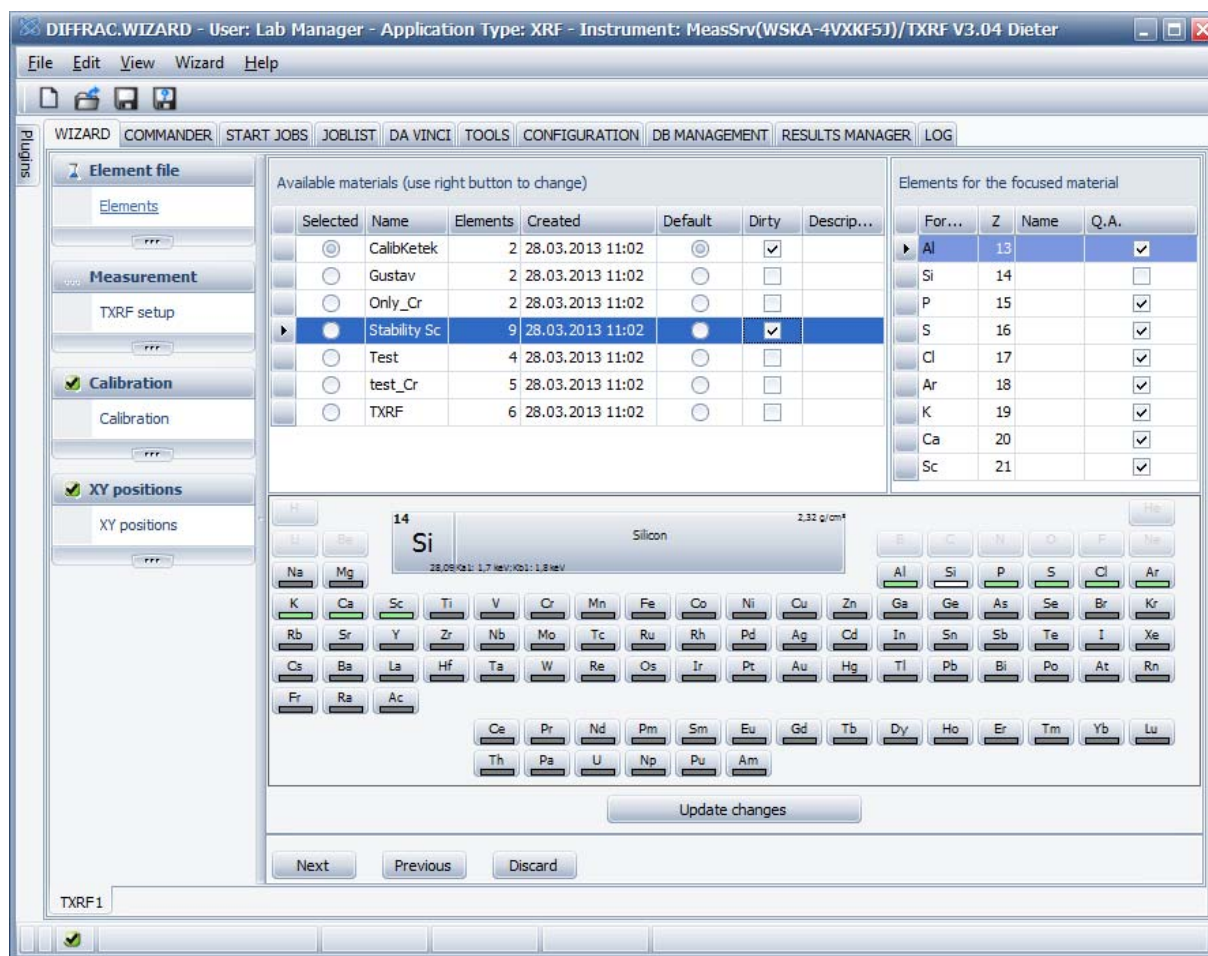


Fig. 51: TXRF setup

### Element file / Elements

In order to start a new measurement a new material (element file) has to be added. A material can be added or removed by right-clicking in the window titled "Available materials".

If there are materials already available in the database of your system, you can select a row, and the window "Elements for the focused material" will show the elemental content of the material. When you create a new material a new line is inserted and you should change the name of the material.

The available materials window has seven columns with the following meaning:

#### *Selected*

The selected material is used for the measurement.

#### *Name*

It identifies the material. It cannot be changed after a measurement is done with this material.

#### *Elements*

Just shows the number of selected elements.

#### *Created*

Shows the date, when the material has been created.

#### *Default*

One material can have the default flag active. If you create a new experiment the default material will have the selected flag.

#### *Dirty*

If the material properties or the elements for a material have changed, the dirty flag is set active and the "Update Changes" button is also usable.

#### *Description*

An additional description can be written to the field.

The window “*Elements for the focused material*” lists all elements that are selected in the periodic table.

A green button in the periodic table, which lead to a checked box entry in the “Q.A.” column in the focused material table, means that the element will be evaluated quantitative (a concentration is calculated). Clicking on a green button changes the color to white. White marked elements are calculated qualitatively only.

All changes to the material are stored in memory until a click on the “*Update Changes*” button will save them to the database. It is recommended to save changes to the database before switching to other tabs.

There are two cases loading saved experiment files concerning materials which should be mentioned (the name of the material and the selected elements are stored inside the file):

1. If you load an experiment containing a material that does not exist, you will be asked to add the material to the database. If you accept it, the material and all containing elements are added. If you deny, then the saved material is used but no material properties can be changed (tab is greyed out).
2. If you load an experiment containing an existing material but with different selected elements, the saved material is used, but the element file tab is greyed out (see picture below).

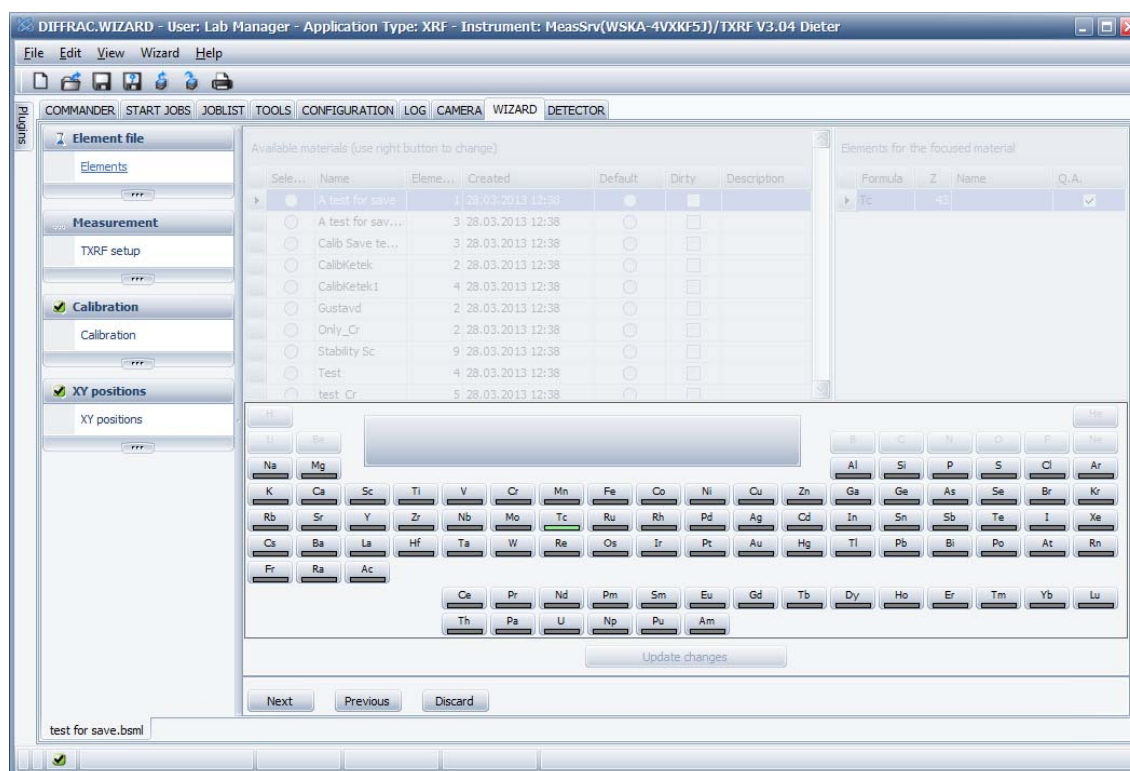


Fig. 52: Element file dialog if material is different from the one in the database

### Measurement / TXRF Setup

In this tab you will find five windows: *Measurement settings*, *Application settings*, *Remeasure settings*, *Element settings*, *Tube-Reference wafer*, and *Periodic table*. This last one is not labeled as such and is basically used to inform the user of the elemental content of the material to be analyzed.

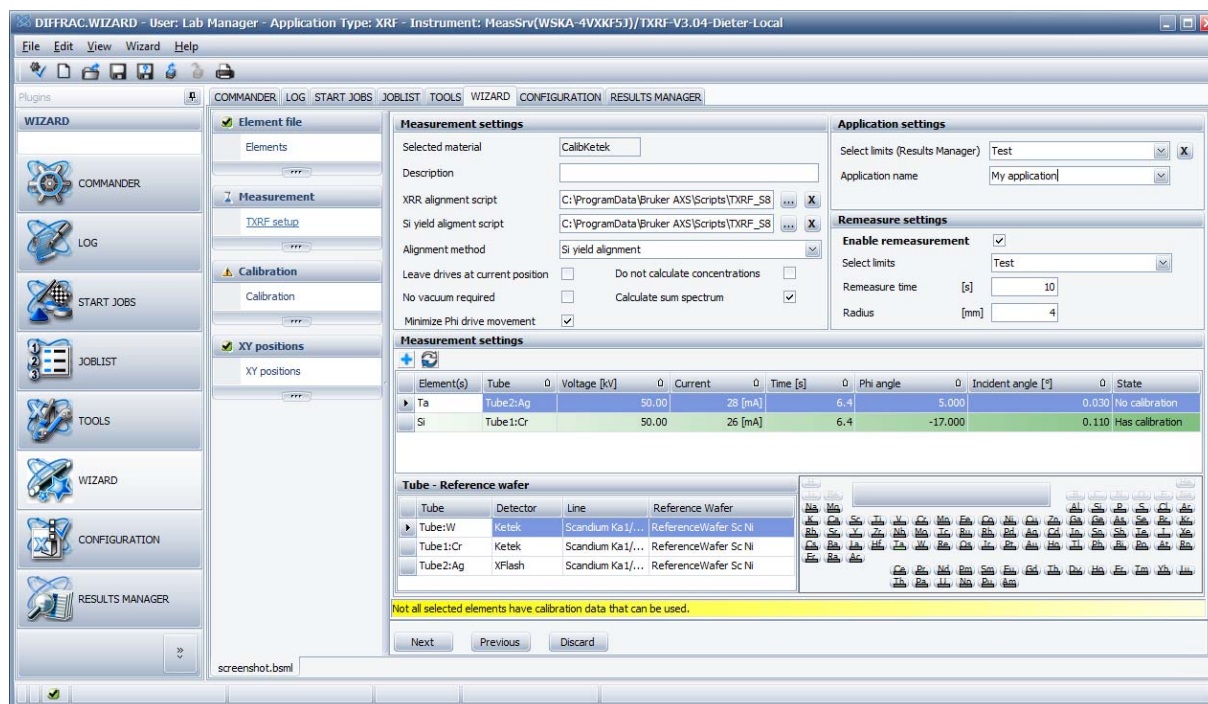


Fig. 53: TXRF Setup dialog

## Measurement settings 1

### *Selected material*

Shows the current selected material name from the “Element file” tab.

### *Description*

Additional description that is stored in the experiment

### *XRR alignment script*

The selected file is called to perform an XRR alignment during the measurement. There are two buttons at the end of the entry window of the Alignment script: “...” and “X”. The former allows selecting a script with file extension “.cs”, and the latter is used to remove the script entry.

### *Si yield alignment script*

The selected file is called to perform an Si yield alignment during the measurement. It is not editable for all alignment methods.

### *Alignment method*

Defines how the alignment is done. See possible entries are described below

### *Leave drives at current position*

No drives are moved during the measurement. This option can be useful when an aligned position of the drives has been found and only still scans are to be measured. Otherwise the box should be unchecked, to allow alignment of the sample of interest.

### *Do not calculate concentrations*

A calibration for all elements with the given conditions must be present to run a measurement and to calculate the concentration. If this option is selected, a measurement without existing calibration is allowed.

### *No vacuum required*

The vacuum sensor is ignored allowing measurements without vacuum.

### *Calculate sum spectra*

The intensities and concentrations for all points are used to calculate a sum entry which is visible in the results manager.

### *Minimize phi drive movement*

If a different tube is selected for a measurement then the wafer must be rotated by a specific angle so that the beam has the same angle to the wafer as the earlier selected tube (phi rotation).

Since this is an “expensive” operation, there is an algorithm which changes the phi angles for other tubes if the value for one is changed so that no phi movement is required.

The following „Alignment methods“ can be selected:

*Keyence sensor alignment:*

This option invokes the script to align the wafer at the center position using the X-ray sources available in the system. All other points to be analyzed will be aligned using the Keyence proximity sensor, an interferometry laser device.

*Fast alignment:*

In this case no alignment is done using the X-rays in XRR mode, only the Keyence is used for alignment purposes of all points on the wafer.

*Full alignment:*

Each point to be analyzed will be aligned using the X-ray beam. The alignment script will be used at every point.

*No alignment:*

No script is used in this mode, and each point to be analyzed is selected using any current position parameters existing in the memory of the system, and all points will be analyzed based on that information.

*Si yield alignment:*

The Si yield alignment script is called in the center after invoking the XRR alignment script. It saves the intensities for Si. The script is called again at each point to adjust the Si intensity to the same value as at the center.


## Measurement settings 2

This table shows the measurement conditions for each element / tube and the current state of calibration.

The table has two view modes which can be switched by using the “+” or in the other view the “-” button. In the detailed view, the measurement settings can be changed for each element.

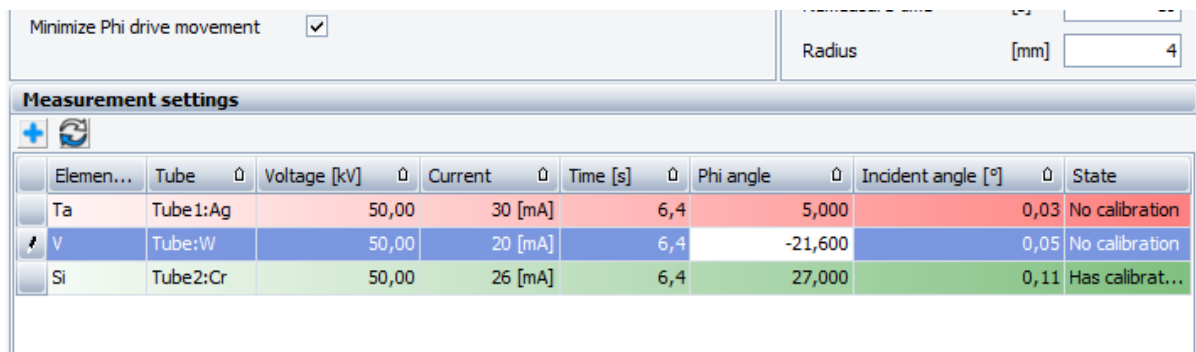
In the combined view all settings apply to all elements in the first column.

In the detailed view the “periodic table” and the “Tube – Reference wafer” window are hidden. The first one is not needed, the second one removed to have more space for the bigger table.

Please use the refresh button  to update the view after changing any of the values.

The colored state in the last columns shows if a calibration is **available**, **not available** (measurement will abort) or **not needed** (see “Do not calculate concentrations” check box above).

If you change the tube in any of the views, the voltage, current and incident angle are adjusted to an existing entry with the selected tube. If none is found, default entries for the new tube are used.



Element	Tube	Voltage [kV]	Current [mA]	Time [s]	Phi angle	Incident angle [°]	State
Ta	Tube1:Ag	50,00	30 [mA]	6,4	5,000	0,03	No calibration
V	Tube:W	50,00	20 [mA]	6,4	-21,600	0,05	No calibration
Si	Tube2:Cr	50,00	26 [mA]	6,4	27,000	0,11	Has calibrat...

Fig. 54: TXRF measurement settings

The picture shows the automatic calculated “Phi angles” with the “Minimize Phi drive movement” optimization and two different calibration states.

A calibration contains the voltage, current, Phi angle and incident angle. If you change any of these values, an existing calibration cannot be used anymore.

**Tube – Reference wafer**

Inside this window you assign a detector and a reference wafer to a tube.

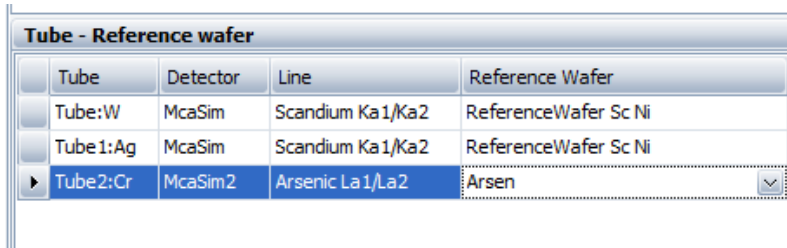


Fig. 55: Tube - Reference wafer settings

It is only possible to change the detector (only usable detectors for the given tube are selectable) and the reference wafer. The used lines for calibration are selected automatically from the tube and reference wafer element.

Reference wafers are defined in the “Calibration” tab.

**Application settings**

Measurements are grouped in the Result Manager by the application name. If no name is entered here, the material name is used as default value.

You can select a limit card (added or changed in the Result Manager) which allows coloring results by warning and error limits (not yet implemented).

**Remeasure settings**

You can select a limit card a remeasure time and a radius in this window to allow remeasurement of single points if some conditions meet.

Only the “Warning high” entry is used for this purpose in the limit card.

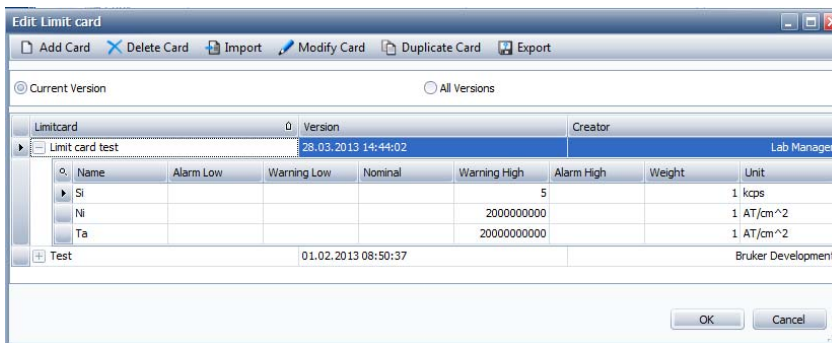


Fig. 56: Limit card settings

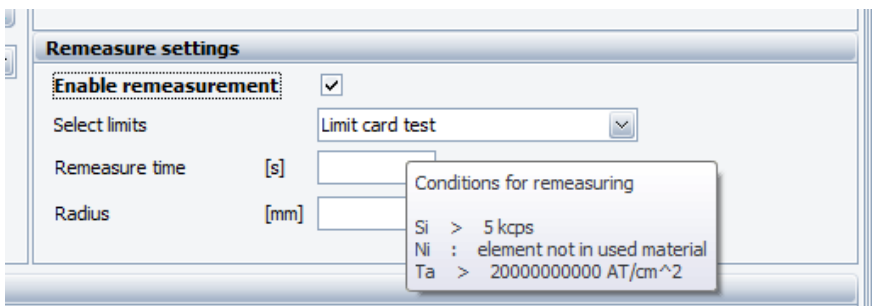


Fig. 57: Remeasure settings

The conditions that are used are shown in a tooltip which is shown, if you leave the mouse a while on the “Select limits” combo box.

The “*Remeasure time*” overrides the measurement time from the measurement setting.

All points (including measurements with different tubes at this point) around the given radius are also remeasured even if the condition is not fulfilled for the point.

## Calibration

The dialog contains multiple windows which allow adding reference wafers and to perform or save calibration measurements for the wafer selected in the left upper window.

Entry type	Tube	Voltage	Current	Incid. an...	Phi Angle	Measure	Calib. line	Usages	Date	Ref. intensity
	Tube:Ag	50,00	30,000	0,03	0,00	<input type="checkbox"/>	Ka1/Ka2	1	21.03.2013	1,295
	Tube:W	50,00	20,000	0,05	0,00	<input checked="" type="checkbox"/>	Ka1/Ka2	1		

Fig. 58: Calibration settings

For adding a reference wafer select a name, an element the density and add it with the given button.

**Be careful!** The reference cannot be deleted later or the density changed at the moment.

Added reference wafers are selectable in the Tube-Reference-Wafer window in the chapter before.

The settings in the table are taken from the measurement settings tab.

You can see at the first (different icons) and last column (value filled in) that there is a calibration for the Ag tube with the given values but none for the tungsten tube.

After setting a measurement time for the calibration and optionally choose different wafer positions for the measurement it is possible to directly start the measurements or save them to an experiment file (\*.bsml) for later or periodic use.

All measurements that have the “Measure” state active will be executed or saved into the experiment file. That can be new (the Measure flag cannot be removed) or already existing ones.

If you decide to directly start the calibration, the measurement can be aborted using the “Abort” button.

The “*Ref.intensity*” values are automatically filled in after successful calibration.

## Scan types overview

The available scan types depend on the instrument hardware (drives, detectors) and on the application type.

The following table applies also to the COMMANDER plugin (but note that some application types are available in WIZARD only).

## Calibration

Scan type	Detectors	Scan modes	Remarks
Single axis scans for specific axes	0D detectors or PSD in 0D mode	Step	
Optic specific scans	0D detectors or PSD in 0D mode	Step	
Detector specific scans		Step	For example: Discriminator scans, HVPlot
Still scans	For every detector	Still	

Tab. 4: Technical scan types

<b>XRD</b>			
Scan type	Detectors	Scan modes	Remarks
For 0D			
Coupled TwoTheta/Theta	0D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	
	PSD at 0°	Continuous PSD fast	
	PSD in 2D mode at 90°	Continuous Step	
Offset coupled TwoTheta/Theta	0D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	
	PSD at 0°	PSD fast scan	
	PSD in 2D mode at 90°	Continuous Step	
Rocking	0D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	
Theta	0D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	Theta/Theta goniometer only. Available in COMMANDER only.
TwoTheta	0D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	
	PSD at 0°	PSD fast scan	
	PSD in 2D mode at 90°	Continuous Step	
For 1D			
Coupled TwoTheta/Theta (VDO) <sup>1,4</sup>	LYNXEYE XE/T <sup>4</sup>	Continuous PSD fast,	Scans with variable detector opening (VDO). <sup>1,4</sup>
Offset coupled TwoTheta/Theta (VDO) <sup>1,4</sup>		Continuous PSD fast (no overtravel) <sup>3,4</sup>	
TwoTheta (VDO) <sup>1,4</sup>			
PSD fixed	For PSDs only	Still	
Still scans	For every detector	Still	
For 2D			

Scan type	Detectors	Scan modes	Remarks
Coupled TwoTheta/Theta	Photon	Continuous Continuous Run (Single Frame)	
Offset Coupled TwoTheta/Theta	Photon	Continuous Continuous Run (Single Frame)	
Rocking	Photon	Continuous Continuous Run (Single Frame)	
Still	Photon	Step (SSD)	
Coupled TwoTheta/Theta	Pilatus	Step	
TwoTheta		Step	
Offset Coupled TwoTheta/Theta		Step	
Rocking		Step  Continuous Run Continuous (exact)	
Still		Step	
Coupled TwoTheta/Theta	VANTEC	Step  Step (with Count Limit)  Cont. Run Continuous Run (Exact)	
Offset Coupled TwoTheta/Theta	VANTEC	Step  Step (with Count Limit)  Cont. Run Continuous Run (Exact)	
Rocking	VANTEC	Step  Step (with Count Limit)  Cont. Run Continuous Run (Exact)	
Still	VANTEC	Step  Step (with Count Limit)	

Tab. 5: Scan types in XRD

**Notes:**

1 VDO

Variable Detector Opening: For a TwoTheta/Theta scan or a TwoTheta scan the opening of the LYNXEYE XE or T can be adapted dynamically

from a start value to an end value at given 2Theta.

- 2 Continuous PSD fast A fast scan with standard overtravel by the half of the detector opening
- 3 Continuous PSD fast (no overtravel) A TwoTheta/Theta scan or a TwoTheta scan without standard overtravel by the half of the detector opening.
- 4 This feature is available only for certain LYNXEYE XE or T hardware sold.

## High resolution XRD

Scan type	Detectors	Scan modes	Remarks
2Theta-Omega	0-D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	
	1-D detector at 0°	Continuous PSD fast	
Omega-2Theta	0-D detectors or Pilatus/1-D detector in 0D mode	Continuous Step	
	1-D detector at 0°	Continuous PSD fast	
Rocking curve	0-D detectors or Pilatus/1-D detector in 0D mode		
	1-D detector at 0°	PSD fast scan	
Reciprocal space	0-D detectors or Pilatus/1-D detector in 0D mode	Step	
PSD fixed	For PSDs only	Still	
Single axis scans for specific axes	0-D detectors or Pilatus/1-D detector in 0D mode	Step	

Tab. 6: Scan types in HRXRD

## Alu Bath

Note: The advanced application type is defined in WIZARD only. These scan types are described Alu Bath, p. 54

## SAXS

Note: The advanced application type is defined in WIZARD only. These scan types are described in SAXS, pp. 54.

Standard measurements are also possible from COMMANDER. The following table lists the possible scan setups.

Scan type	Detectors	Scan modes	Remarks
Still scan	VANTEC-500	Still	
X or Y or XY scan	VANTEC-500	Step	
Still scan	VANTEC-1	Still	

Tab. 7: Scan types in COMMANDER for SAXS

## SCXRD

Scan type	Detectors	Scan modes	Remarks
Coupled TwoTheta/Theta	Photon	Continuous Run (exact) Continuous Run (single Frame)	
Offset Coupled TwoTheta/Theta	Photon	Continuous Run (exact) Continuous Run (single Frame)	
Rocking	Photon	Continuous Run (exact) Continuous Run (single Frame)	
Still	Photon	Step (SSD)	
Phi-Psi	Photon	Continuous Run (exact) Continuous Run (single Frame)	
Coupled TwoTheta/Theta	VANTEC	Cont. Run	
Offset Coupled TwoTheta/Theta	VANTEC	Cont. Run	
Rocking	VANTEC	Cont. Run	
Still	VANTEC	Step Step (with Count Limit)	

Theta-Phi	VANTEC	Cont. Run	
Phi-Psi	VANTEC	Cont. Run frame)	

Tab. 8: Scan types in COMMANDER for SCXRD

### Stress

Note: This application type is defined in WIZARD only.

The different scan types depend on the Stress setup chosen and are described in Stress, pp. 64.

### Texture

Note: This application type is defined in WIZARD only.

The different scan types depend on the Texture setup chosen and are described in Texture, pp. 74 .

### XRF

Scan type	Detectors	Scan modes	Remarks
Still	Amptek	Step Fast Step	Fast Step mode with special hardware (Kodiak), not live time capable in this mode  Use live time capable Only Step Scan
Rocking	Ketek	Step	
Still	Ketek	Step Fast Step	
Rocking and Axis Scans	0D Detectors	Step	
Still	XFlash	Step Fast Step	Use live time capable Only Step Scan
Rocking	XFlash	Step	
Still	XFlash	Step Fast Step	

Tab. 9: Scan types in COMMANDER for XRF

## Index

- Alu Bath 54
- BIML file 2
- BSML file 8
- Experiment 8
  - Base methods 8
  - Regular sequence 9
  - Sequences 8
  - Step list sequence 9
- HR-XRD
  - Alignment 49, 51
- Non-ambient
  - used in DAVINCI 11
- Pre-measurement
  - Classic Stress 69
  - Grazing incidence Stress 71
  - VCT/VSS 39
- Profiles
  - CHC 18
  - MHC 23
  - Segment 16
  - Segment item 16
- Rotation
  - used in DAVINCI 11
- Sample rotation 11
- SAXS
  - Measurement setups 56
  - Transmission of the sample 62
- State file 2
- Stress 65
  - Iso inclination 68
  - Measurement setups 66
  - Side inclination 68
- Texture 76
  - Measurement setups 77
  - Orientation 77
  - Pole figure 76
- VCT/VSS 37
- WAXS 56
- WIZARD plug-in
  - Alignment 49
  - Alu Bath 54
  - DAVINCI module 9
  - Drive positions 75, 82
  - HRXRD BASIC module 44
  - Menu 2, 5
  - Module design 5
  - Profiles module 16
  - Reciprocal space display 51
  - Reciprocal space module 52
  - Sequences module 12, 51
  - Stress BASIC module 65
  - TEXTURE BASIC module 76
  - Toolbar 2
  - tree view 35, 44
  - XRD Basic module 34
  - XRD BASIC module 35
  - XY positions module 25
- XRD 34
  - Scan setup 36
  - VCT/VSS 36
- XY Positions
  - Camera 30
  - Coordinate transformations 27
  - Edge exclusion 28

## Index of Tables

Tab. 1:	Available measurement setups in SAXS.....	55
Tab. 2:	Available measurement setups in Stress.....	66
Tab. 3:	Available measurement setups in Texture.....	75
Tab. 4:	Technical scan types.....	87
Tab. 5:	Scan types in XRD.....	89
Tab. 6:	Scan types in HRXRD.....	90
Tab. 7:	Scan types in COMMANDER for SAXS.....	91
Tab. 8:	Scan types in COMMANDER for SCXRD.....	92
Tab. 9:	Scan types in COMMANDER for XRF.....	92

## Index of Figures

Fig. 1:	Create experiment dialog.....	3
Fig. 2:	WIZARD module design.....	5
Fig. 3:	WIZARD module design.....	6
Fig. 4:	Module design for HR-XRD and Texture.....	7
Fig. 5:	WIZARD created experiment without a sequence.....	8
Fig. 6:	WIZARD created experiment with one sequence.....	9
Fig. 7:	DAVINCI module.....	9
Fig. 8:	DAVINCI display.....	10
Fig. 9:	Sequences module.....	12
Fig. 10:	Sequences display.....	12
Fig. 11:	Profiles module.....	16
Fig. 12:	Example of a profile with three segments.....	16
Fig. 13:	Profiles settings.....	17
Fig. 14:	Graphical profile editor.....	21
Fig. 15:	Profile editors: common headers.....	21
Fig. 16:	WIZARD XY positions module.....	25
Fig. 17:	XY positions display.....	25
Fig. 18:	Refine alignment form.....	30
Fig. 19:	Options module.....	32
Fig. 20:	Fixed drives form.....	32
Fig. 21:	Summary module.....	33
Fig. 22:	XRD modules.....	34
Fig. 23:	Sample definition form.....	35
Fig. 24:	VCT/VSS setup.....	37
Fig. 25:	VCT.....	38
Fig. 26:	Manual VCT/VSS.....	39
Fig. 27:	VCT/VSS pre-measurement.....	40
Fig. 28:	VCT/VSS pre-measurement executed.....	41
Fig. 29:	Using the pre-measurement to define sub-scans.....	42
Fig. 30:	Modules in HR-XRD.....	43
Fig. 31:	Sample definition form.....	44
Fig. 32:	Sample definition form.....	45
Fig. 33:	Sample alignment form.....	49
Fig. 34:	HRXRD scan setup.....	51
Fig. 35:	Reciprocal space display.....	52
Fig. 36:	Reciprocal space limits.....	52
Fig. 37:	SAXS modules.....	55
Fig. 38:	SAXS Nanography setup dialog.....	56
Fig. 39:	SAXS sample measurement table.....	59
Fig. 40:	SAXS optional measurements.....	61
Fig. 41:	SAXS BRML browser.....	63
Fig. 42:	Stress modules.....	64
Fig. 43:	Classic Stress.....	66
Fig. 44:	Stress pre-measurement.....	69

Fig. 45:	Stress for grazing incidence.....	70
Fig. 46:	Stress 2D Side mode.....	71
Fig. 47:	Stress 2D Iso mode.....	73
Fig. 48:	Texture modules.....	74
Fig. 49:	Classic Texture 0D.....	76
Fig. 50:	Texture 2D setup.....	80
Fig. 51:	TXRF setup.....	81
Fig. 52:	Element file dialog if material is different from the one in the database.....	82
Fig. 53:	TXRF Setup dialog.....	83
Fig. 54:	TXRF measurement settings.....	84
Fig. 55:	Tube - Reference wafer settings.....	85
Fig. 56:	Limit card settings.....	85
Fig. 57:	Remeasure settings.....	85
Fig. 58:	Calibration settings.....	86

(intentionally left blank)