DIFFRAC.SUITE

User Manual

DIFFRAC.WIZARD

Original Instructions

Innovation with Integrity

XRD

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1 WIZARD

1.1 General

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

Experiments currently available are:

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

1.2 Screen Layout and Operation

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

1.2.1 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.

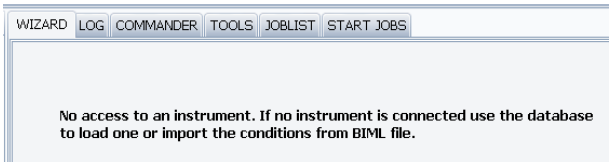
Note

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

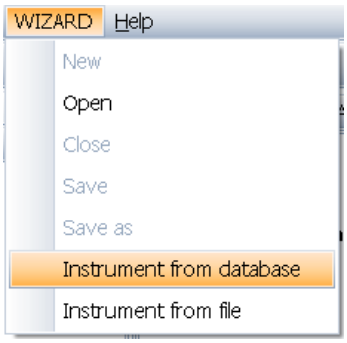
All previously created experiment will not be affected. Experiments loaded from a disk will use its own instrument.

1.2.1.1 Offline Operation

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

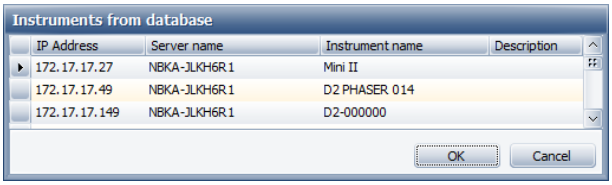


1. The user must load instrument conditions from the database or from a file using the WIZARD menu:



1.2.1.2 Instrument from Database

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



1. Select one instrument here.

1.2.1.3 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.

1.2.2 Menu Overview

Menu	Toolbar	Action
New		Create a new experiment. See section *Creating a New Experiment [▶ 9]*
Save		Save an experiment as a *bsml* file.
Save as		Save an experiment as a *bsml* file under a new name
Open		Open an existing *bsml* file
Open from database		Open an existing *bsml* from database
Open from database (signed only)		In CFR21/Part11 only: Open an existing *bsml* 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.

Menu	Toolbar	Action
Print a report		Print a tabular view of the experiment, see *Summary [▸ 42]*
Close		Close the experiment
Instrument from database		Read the instrument definition from the database (see *Instrument from Database [▸ 8]*)
Instrument from file		Read the instrument definition from a *biml* file (see *Instrument from Database [▸ 8]*)
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.

1.2.3 Creating a New Experiment

1. 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).

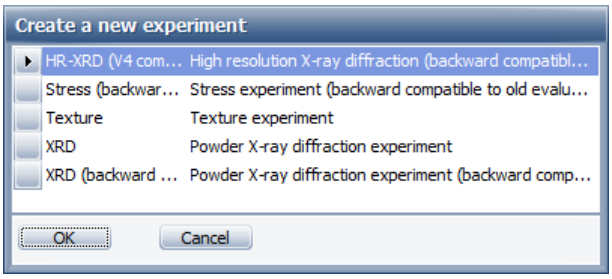


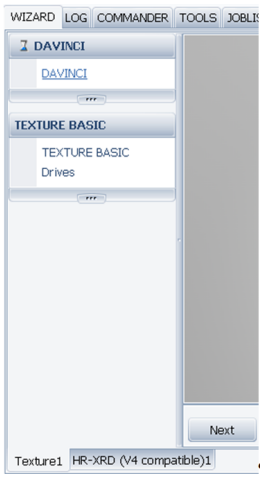
Figure 1.1: Create experiment dialog

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 DIFFRAC.TEXTURE, respectively.

1.2.4 Screen Layout

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

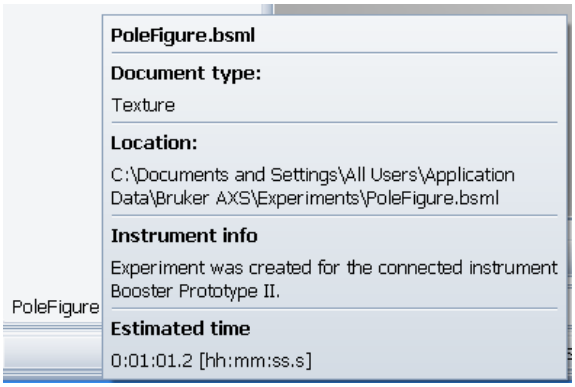


If the experiment has not yet been saved it will automatically numbered using the experiment type, for example, **Texture1**.

1.2.4.1 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:



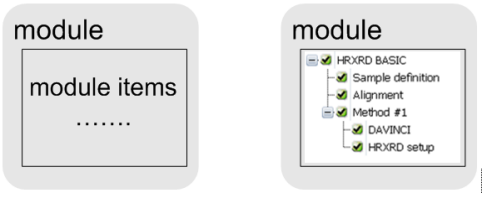
The tooltip states the experiment template used (in the section *Creating a New Experiment [▶ 9]*), the location where the file was stored (or loaded from), the instrument used to create the file and the experiment's estimated measurement time.

1.2.4.2 Module Design

All experiment layouts in the WIZARD plugin follow a general design:

Figure 1.2: General 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.

Figure 1.3: WIZARD module design

1.2.4.3 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):

1.2.4.4 Module Status

The status of a module is indicated by an icon:

	content is valid
	module is currently edited
	content is invalid

1.2.4.5 Modules in Different Experiment Templates

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

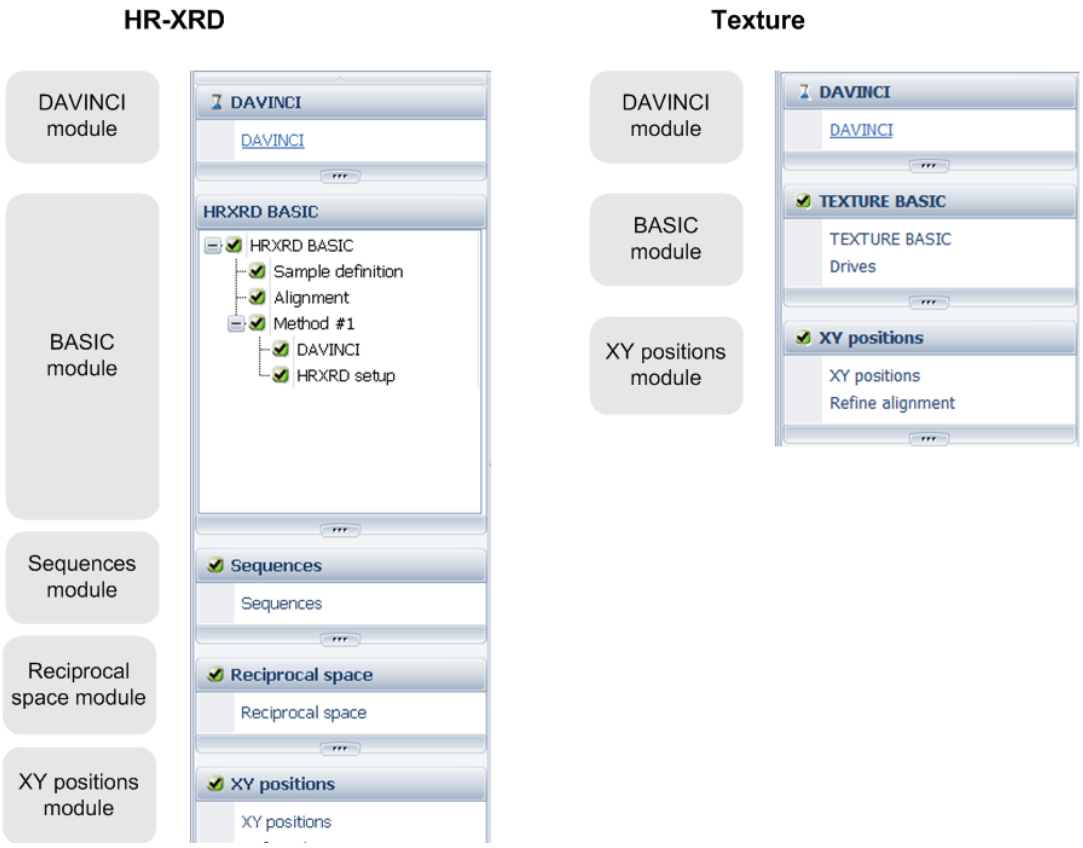


Figure 1.4: Module design for HR-XRD and Texture

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.

2 Basics of WIZARD

The following terms are used for the WIZARD plugin:

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 plugin. 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 LYNXEYE detector:

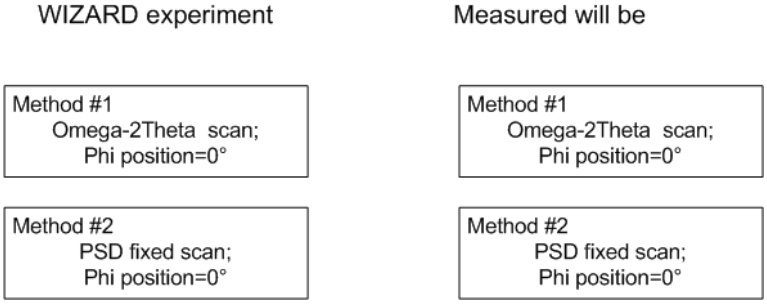


Figure 2.1: WIZARD created experiment without a sequence

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°.

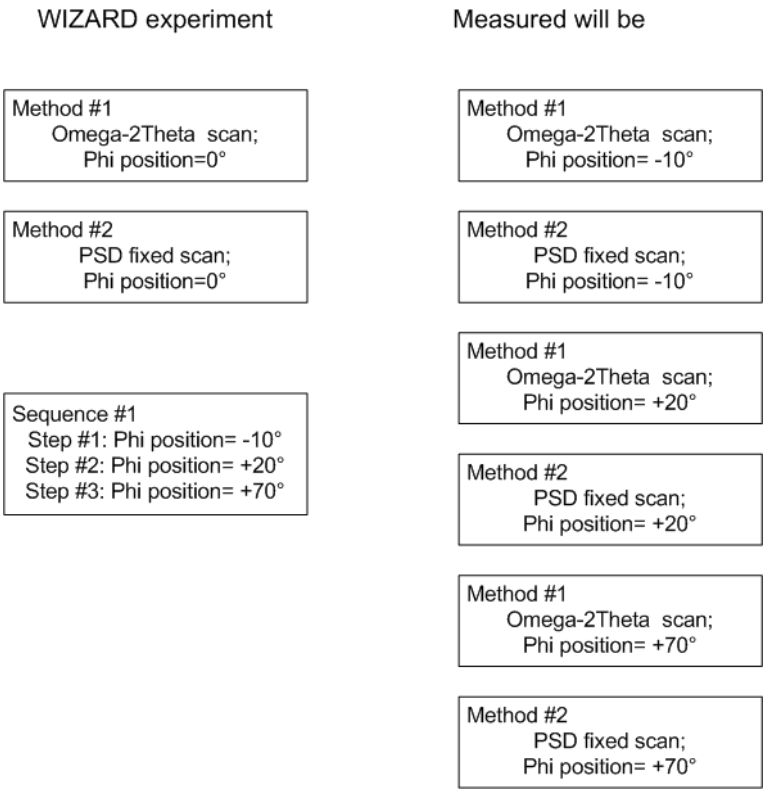


Figure 2.2: WIZARD created experiment with one sequence

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 [▶ 17]*.

2.1 Common modules

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

2.1.1 DAVINCI

Figure 2.3: 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.)

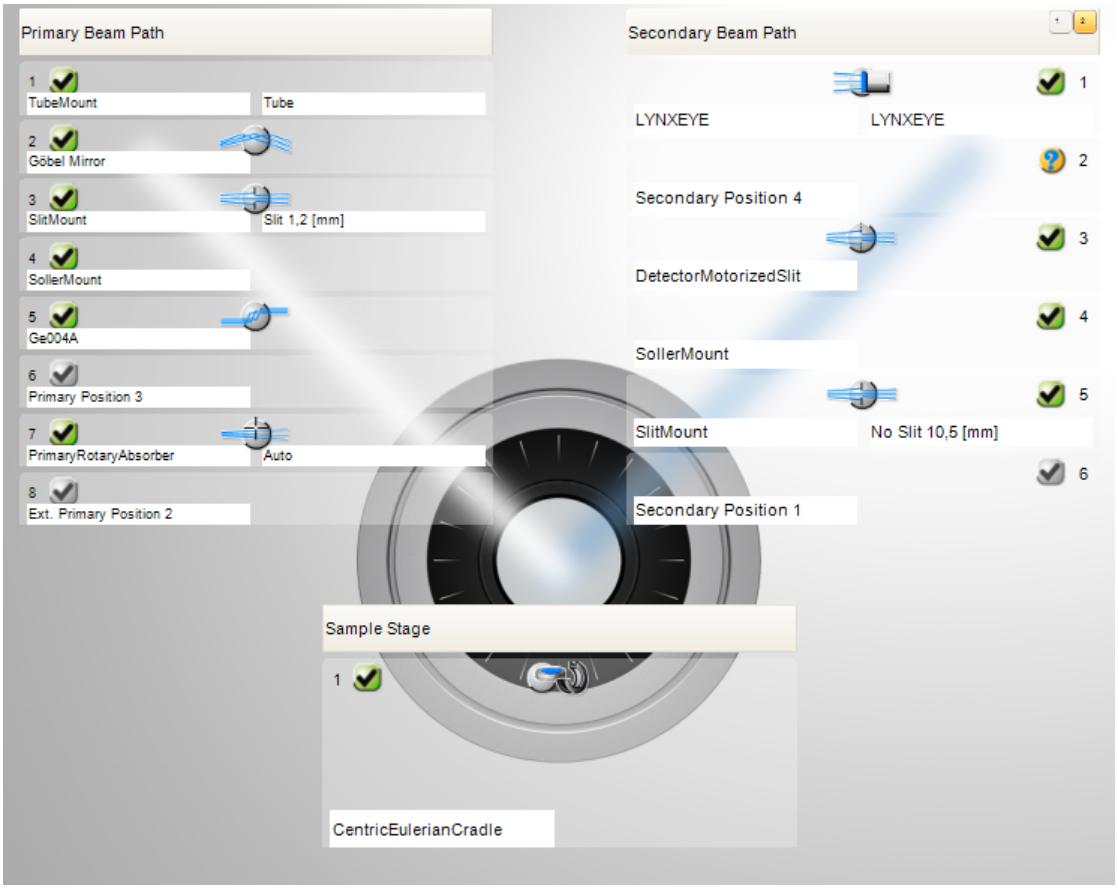
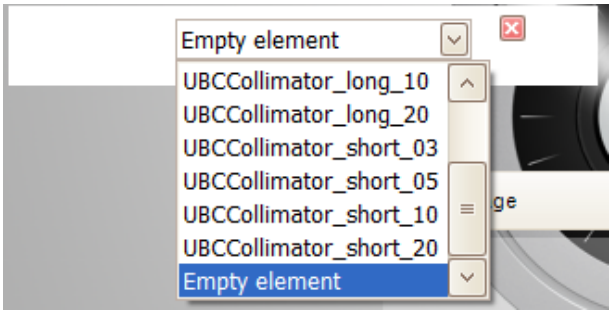


Figure 2.4: DAVINCI display

2.1.1.1 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:

1. In the virtual goniometer, click on the last item to change the **Primary position 2** from an **Empty Element** to an **UBC Collimator**:

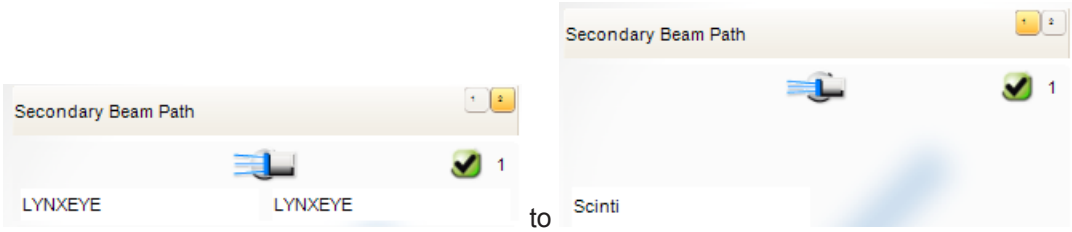


For instance, to:

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 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**):



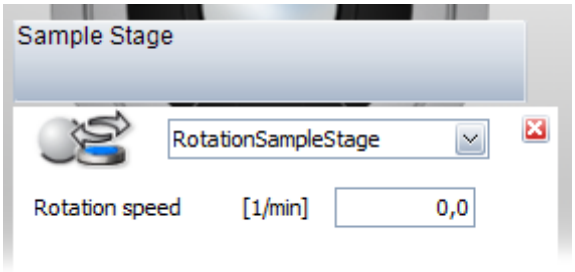
Note

If the instrumental conditions stored with the experiment do no match the current conditions when the bsml file is started in a job, the validation undertaken by the START JOB plugin 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.

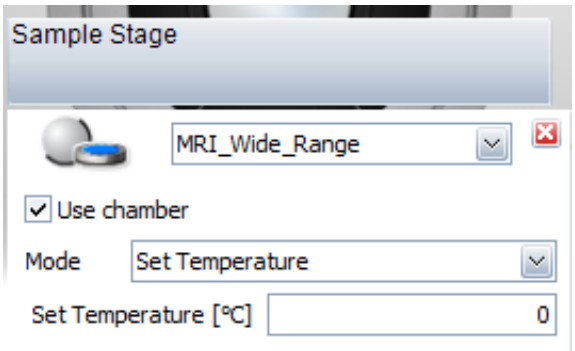
2.1.1.2 Rotation and Non-Ambient Settings

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.

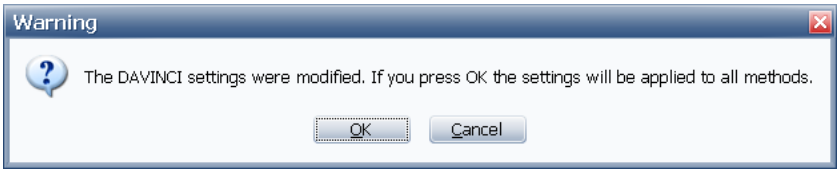
If a non-ambient stage is connected temperature and other parameters can be set. For instance:



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

2.1.1.3 Confirmation

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



Note

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.

2.1.2 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 in section *Basics of WIZARD [▶ 13]*.

Figure 2.5: 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 [▶ 13]*).

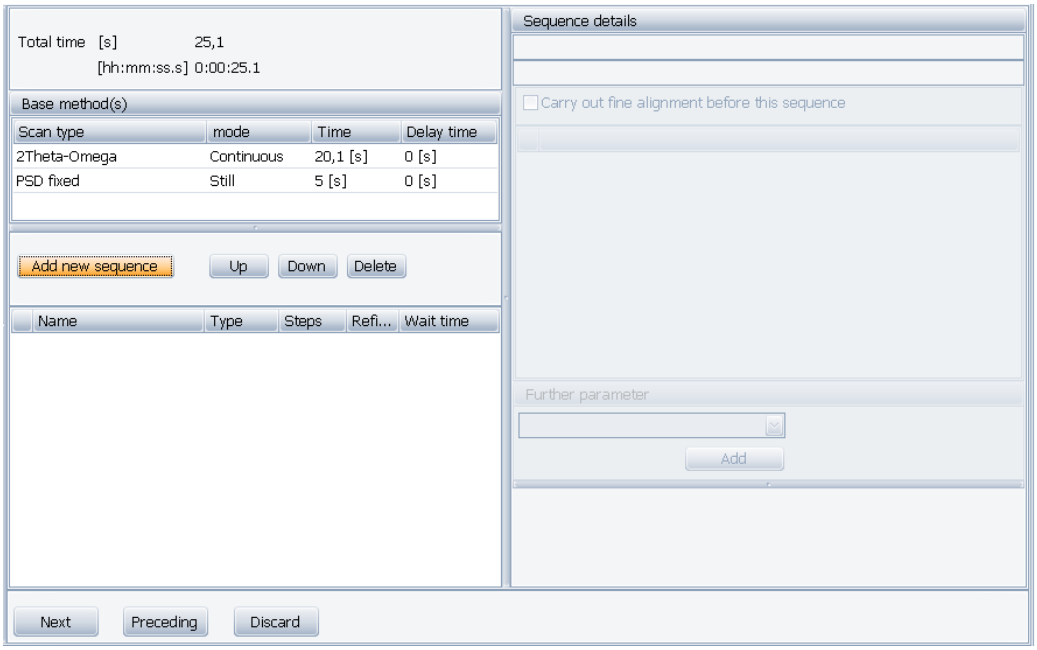
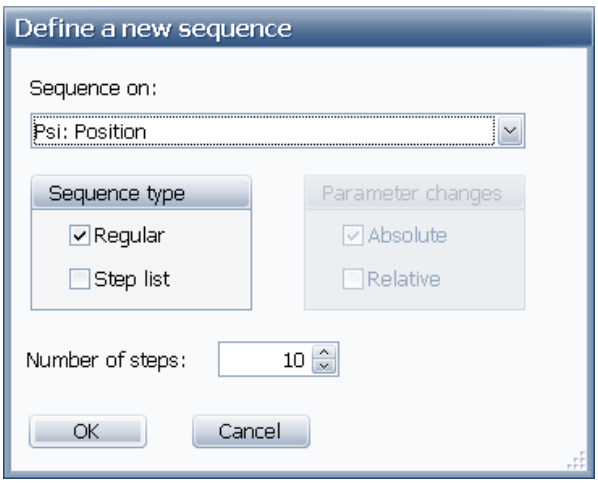


Figure 2.6: Sequences display

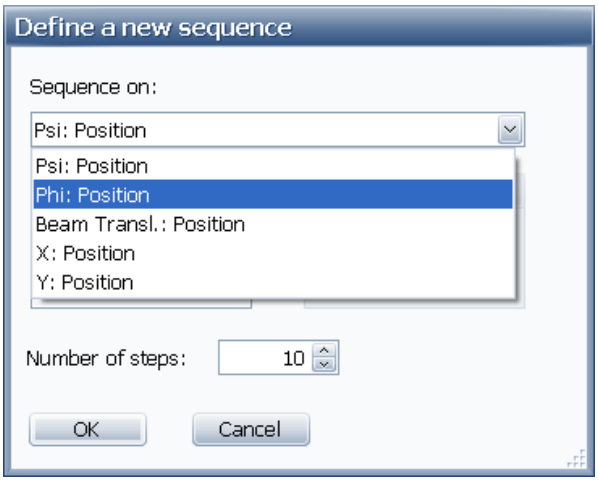
The total time is shown at the upper left of the sequence display, followed by a list of base methods. In this example a 2Theta-Omega scan and a PSD fixed scan is shown.

2.1.2.1 Step List Sequence

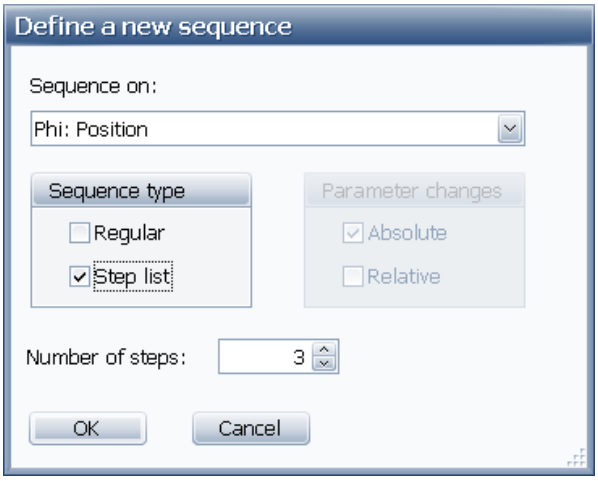
1. To add a new sequence press the button Add new sequence :
   - ➨ A dialog window will open:



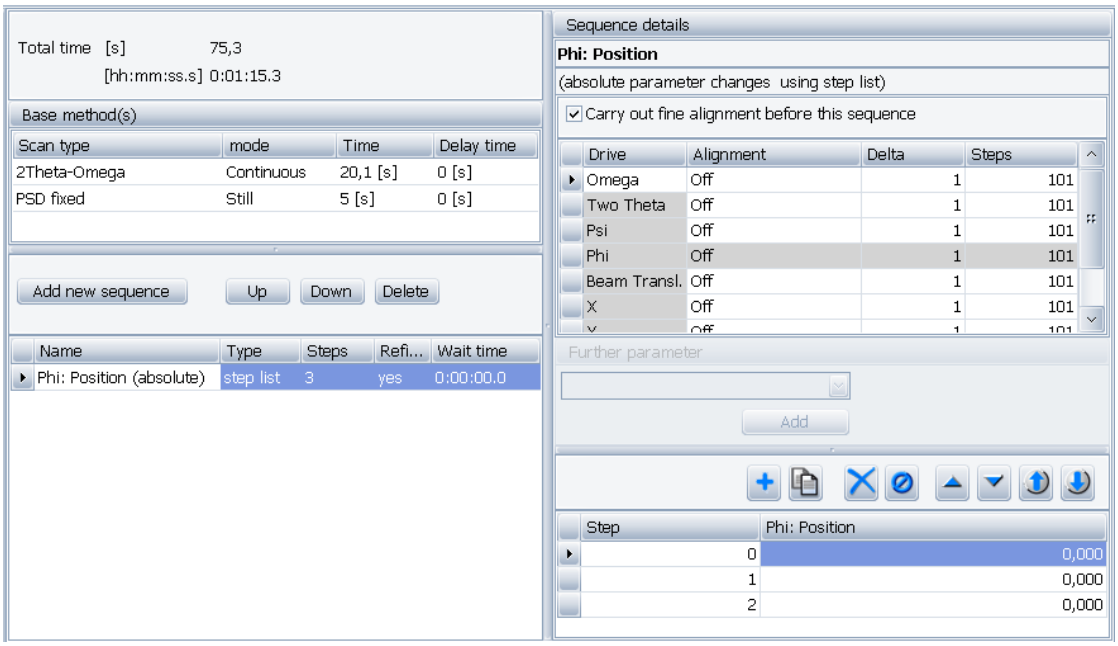
2. Choose **Phi: Position** from the drop-down list of available sequences.



3. Choose a **Step list** sequence with **3** steps:

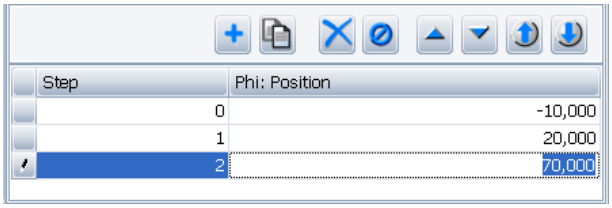


➥ The appearance of the **Sequence** display changes:

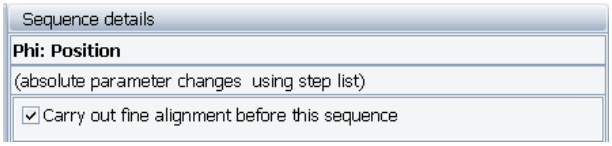


➥ The total estimated time is updated at the top left. The **Sequence** list contains summary information about the new **Phi Sequence** at the lower left.

4. In the **Sequence** details the **Phi position** values can be changed at the lower right:



5. An alignment can be defined in the sequence details in the upper right.
6. This function can be switched off by un-checking the check box:



Note

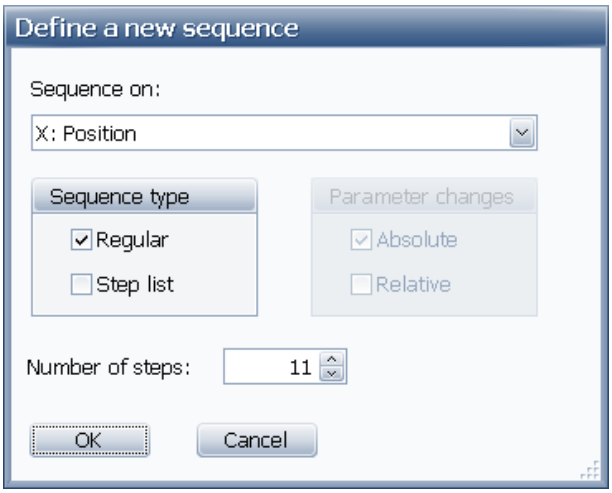
How the alignment for a sequence is used depends on the measurement script.

2.1.2.2 Regular Sequence

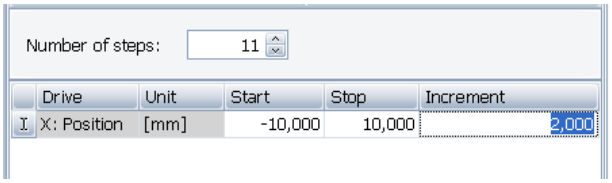
In the following example a further sequence has been added. But now we choose a **regular sequence**. This indicates that the user is specifying a start, stop and increment.

1. Click on the button 

. Then, enter:

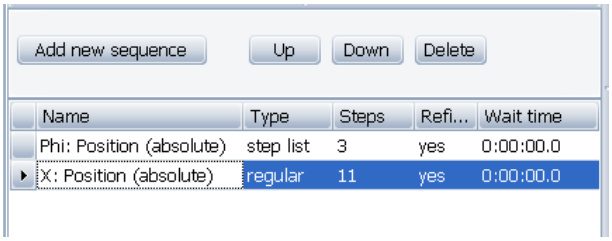


2. Enter the **X** start, stop and increment in the sequence details at the lower right.



2.1.2.3 Changing the Sequence Order

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



2.1.2.4 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.

2.1.3 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**:

Figure 2.7: Profiles module

2.1.3.1 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 **y0** and **y1** 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 **t0** and **t1**), **Segment #2** is an increase from the parameter value **y0** to **y1** (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.

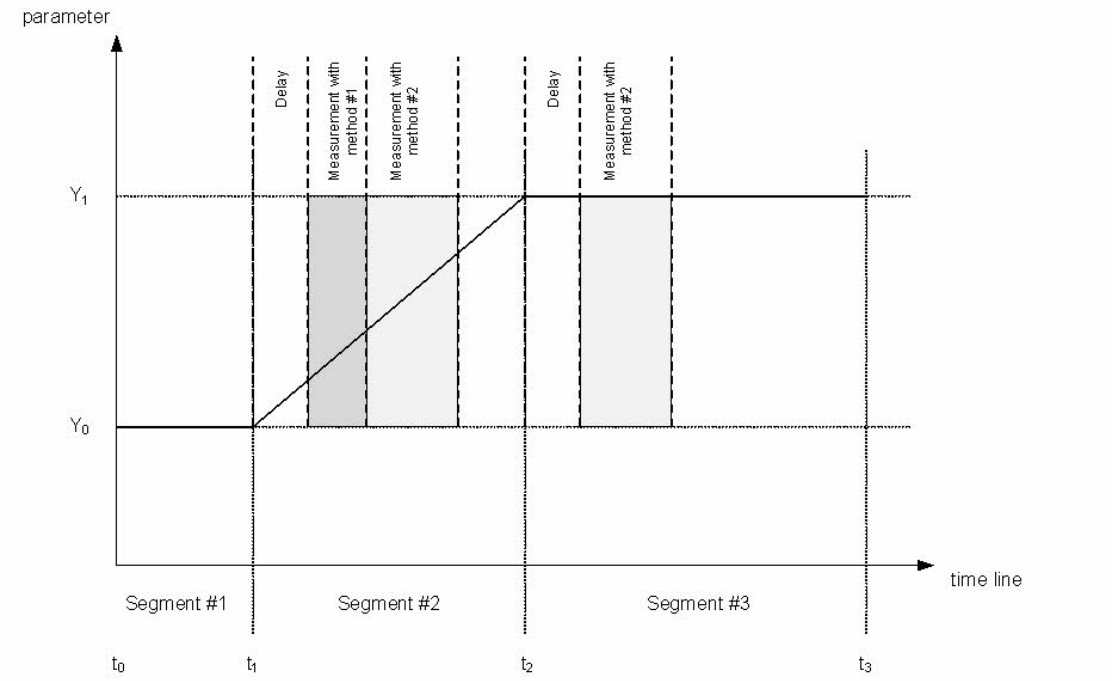


Figure 2.8: Example of a profile with three segments

How would such a profile get executed?

The measurement library will first achieve the point (**t0**, **y0**) 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 **t1**, the parameter will be varied with a constant gradient to **y1**. 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 **t2**, 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 **y0**, the measurement will stop only after **y0** has been reached (if not aborted before).

2.1.3.2 Settings

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

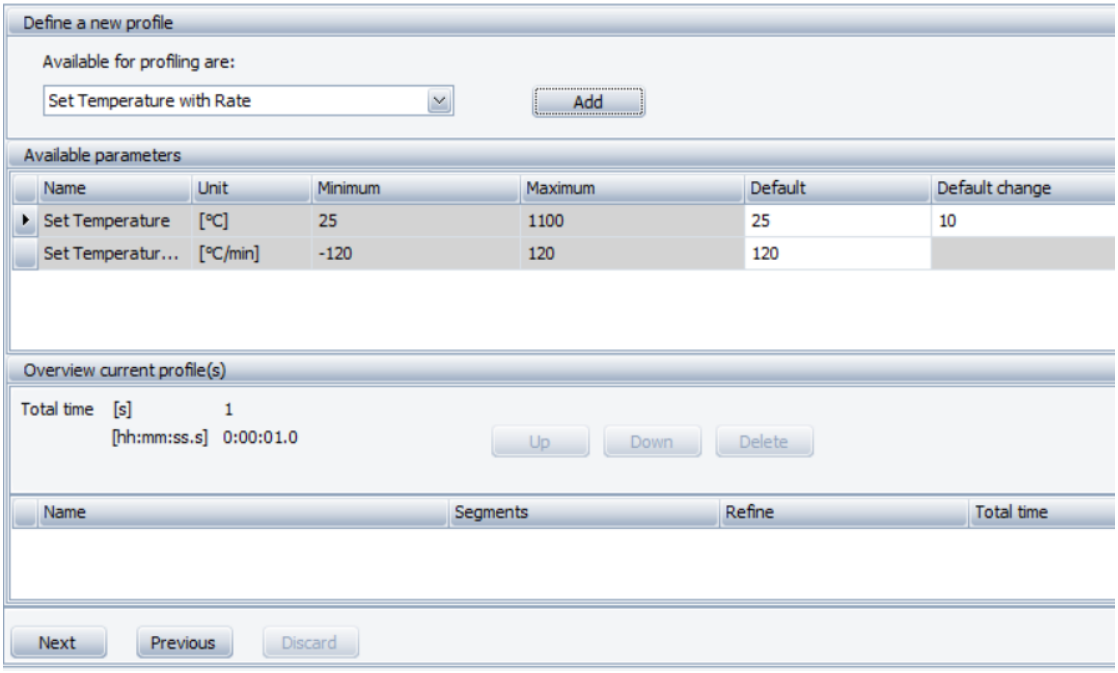
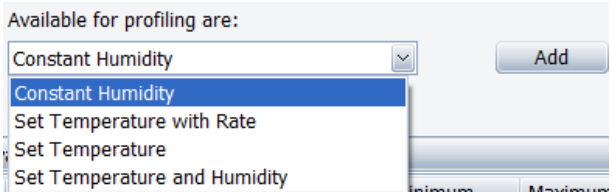


Figure 2.9: Profiles settings

2.1.3.2.1 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.

2.1.3.2.2 Special Cases of Non-Ambient Chambers

Below we give two examples for profiles which can be parameterized.

2.1.3.2.2.1 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.

2.1.3.2.2.2 Stress cell

A TS600 tensile stage provides modes to execute stress on a sample :

Set Elongation

Available parameters

Name	Unit	Minimum	Maximum	Default	Default change
Target Elongation	[%]	0,000	100,000	0,000	10,000
Speed	[mm/min]	0,05	5,00	0,50	4,95

Elongation is specified here as a percentage with a certain speed. The speed default change should be set to a small value or zero to construct profiles.

Set Force

Available parameters

Name	Unit	Minimum	Maximum	Default	Default change
Target Force	[N]	0,00	600,00	0,00	10,00
Speed	[mm/min]	0,05	5,00	0,50	4,95

This defines a certain force executed on the sample with a certain speed. The speed default change should be set to a small value or zero to construct profiles.

Set Position

Available parameters

Name	Unit	Minimum	Maximum	Default	Default change
Target Distance	[mm]	0,000	25,000	0,000	10,000
Speed	[mm/min]	0,05	5,00	0,50	4,95

This defines a movement of the sample with a certain speed. The speed default change should be set to a small value or zero to construct profiles.

2.1.3.3 A Step by Step Example

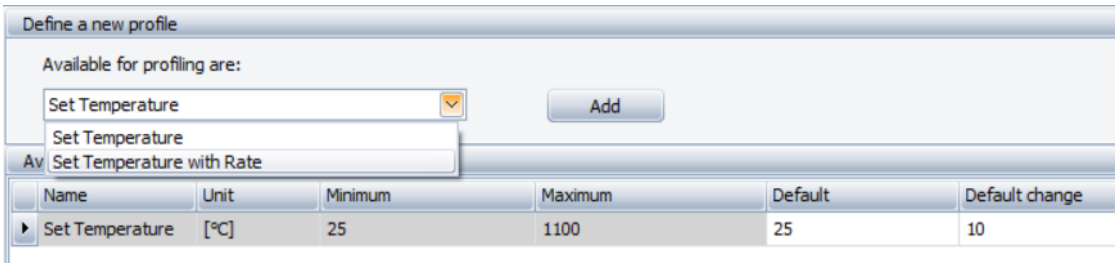
Note

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

Later, we show the parameters for a humidity chamber.

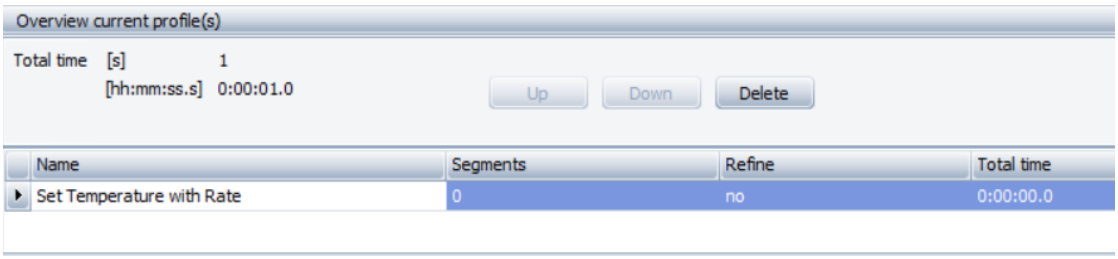
2.1.3.3.1 Step #1: Choose a Profile Type

1. Select **Set temperature with rate** from the combo box with the modi available.



2. You may then change default parameters. For instance, you may set the default temperature to 29 [°C], and the default heating rate to 100°/min (a default cooling would be set by a negative rate).

3. To define the profile using the mode selected in the combo box press Add.
   - The profile appears at the top in the settings dialog:



Note

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

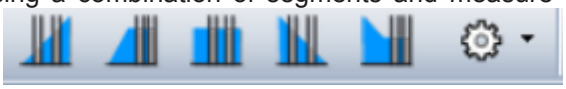
To change to another mode it is necessary to delete the profile using the Delete button.

- So far, we have defined the profile but it is empty, i.e. it has no segments.

4. Press Next to switch to the table editor:

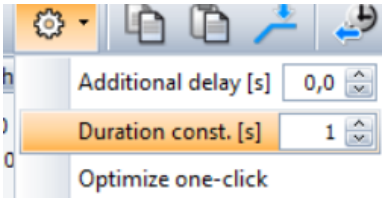
2.1.3.3.2 Step #2: Add Segments and Measurements

2.1.3.3.2.1 Variant 1: Use One-Click Segments

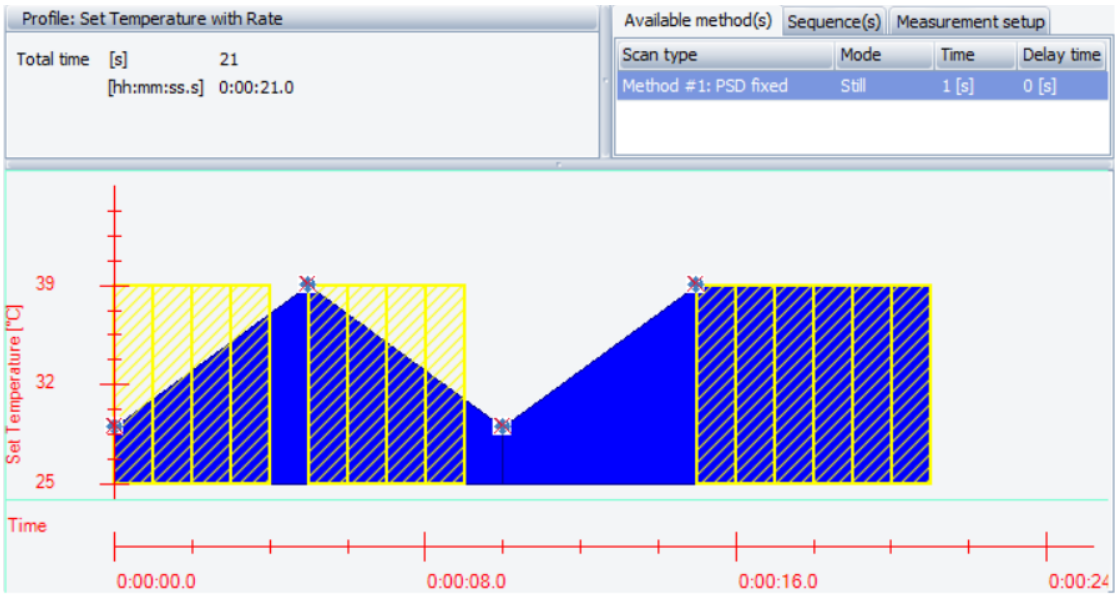
This is the fastest way to define a profile using a combination of segments and measurements. It is accessed via the toolbar buttons  and the measurement(s) currently selected.

Here, we use a PSD fixed scan:

1. Press  to append a ramp completely filled with measurements:
   -  will add a descending ramp filled with measurements:
   - The button  serves to add a step (i.e. a heating followed by a constant segment filled with measurements). Because the default length of a constant segment is 1 [s] and the PSD fixed scan used is 1 [s], too, there would be only one measurement. So, we change the default length of the constant segment using the settings button in the toolbar:
2. Press  to change the duration of the constant:



3. for instance, to 6 [s].
4. Press  , and the step is append to the profile:



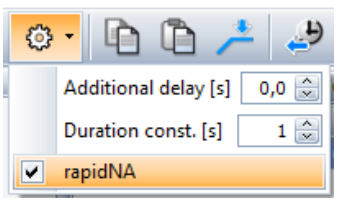
➨ This may be repeated as often as wanted:

Optimization of the Measurement (rapidNA)

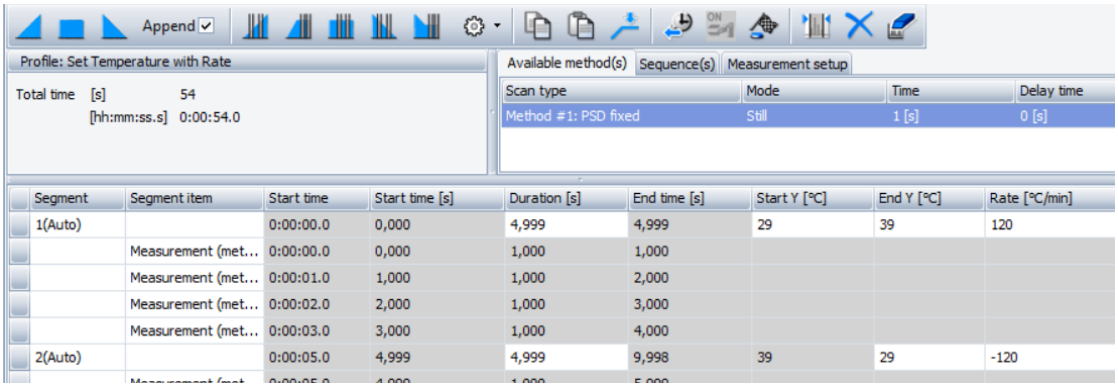
A disadvantage of this type of a profile defined so far is the overhead time needed to execute each single PSD fixed scan. In fact, the first (ramping) segment should have 4 scans before reaching the target temperature. But, the overhead time needed for each single scan may result that the chamber already reached the temperature before the last scan is really measured.

To minimize such effects, some measurement types can be optimized using a rapid Non-ambient measurement. The 4 single scans are combined into one measurement.

1. Select **rapidNA** from the settings toolbar button:

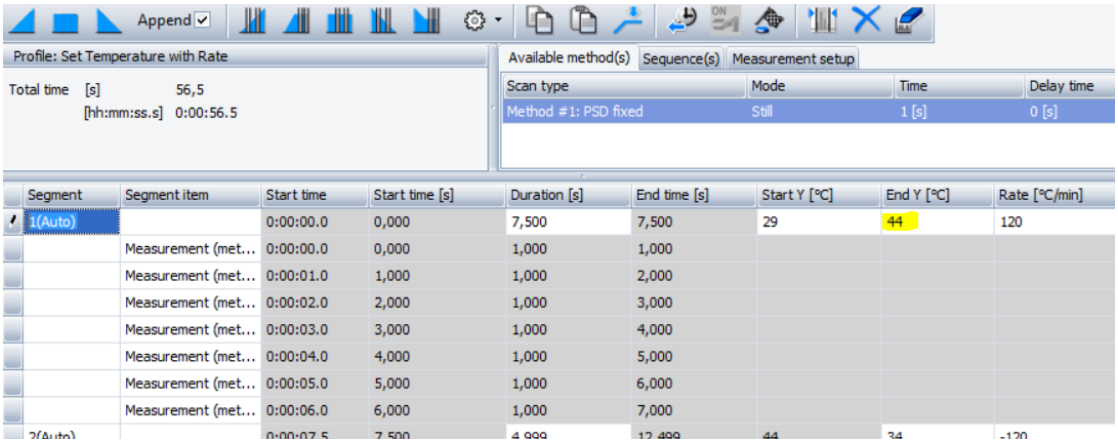


2. Note that this flag is only used for still scans (like the PSD fixed, i.e. no drives moved) and for measurements without any delay times defined on a one-click segment.
   - On the profile **Table editor**, you will note that the one-click segments defined so far are marked with **(Auto)**



Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y [°C]	End Y [°C]	Rate [°C/min]
1(Auto)		0:00:00.0	0,000	4,999	4,999	29	39	120
	Measurement (met...	0:00:00.0	0,000	1,000	1,000			
	Measurement (met...	0:00:01.0	1,000	1,000	2,000			
	Measurement (met...	0:00:02.0	2,000	1,000	3,000			
	Measurement (met...	0:00:03.0	3,000	1,000	4,000			
2(Auto)		0:00:05.0	4,999	4,999	9,998	39	29	-120

   - **(Auto)** marked segments behave differently than “normal” segments: for instance, changing the end temparture here from 39 [°C] to 44 [°C] will auto-fill up the ramp with measurements.



Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y [°C]	End Y [°C]	Rate [°C/min]
1(Auto)		0:00:00.0	0,000	7,500	7,500	29	44	120
	Measurement (met...	0:00:00.0	0,000	1,000	1,000			
	Measurement (met...	0:00:01.0	1,000	1,000	2,000			
	Measurement (met...	0:00:02.0	2,000	1,000	3,000			
	Measurement (met...	0:00:03.0	3,000	1,000	4,000			
	Measurement (met...	0:00:04.0	4,000	1,000	5,000			
	Measurement (met...	0:00:05.0	5,000	1,000	6,000			
	Measurement (met...	0:00:06.0	6,000	1,000	7,000			
2(Auto)		0:00:07.5	7,500	4,999	12,499	44	34	-120

Note: **(Auto)** segments may loose their state if one changes single items (like insertion a delay).

2.1.3.3.2.2 Variant 2: Add Segments Step by Step and Insert Measurements Manually

The **Table editor** provides a list of segments and segment items.

Note: now we choose a humidity chamber in the **Constant humidity** mode: this adds a further parameter: humidity in [%].

1. 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

2. For each parameter, columns are added for its **Start** value, its **End** value and the **Rate**.

3. Press  once again to add a further segment:

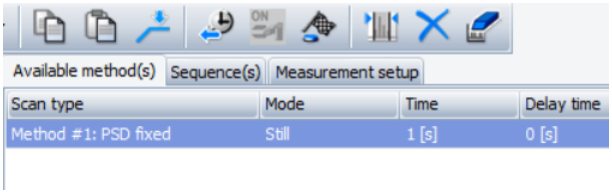
Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5.0	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5.0	10.0

4. 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.
5. 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].

6. To add a measurement, press  .
   ➨ This uses a currently marked method shown on the tab **Available method(s)** to the right below the toolbar:



   ➨ Currently, only one method is defined (if we had defined more methods in the **Basic** module above, these methods would appear in the list).

7. To add it, 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				

8. 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]).
9. 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				

10. We may now view the profile in the **Graphical editor**. Press **Next** to go to the **Graphical editor**

2.1.3.3.3 Step #3 : View in the Graphical Editor

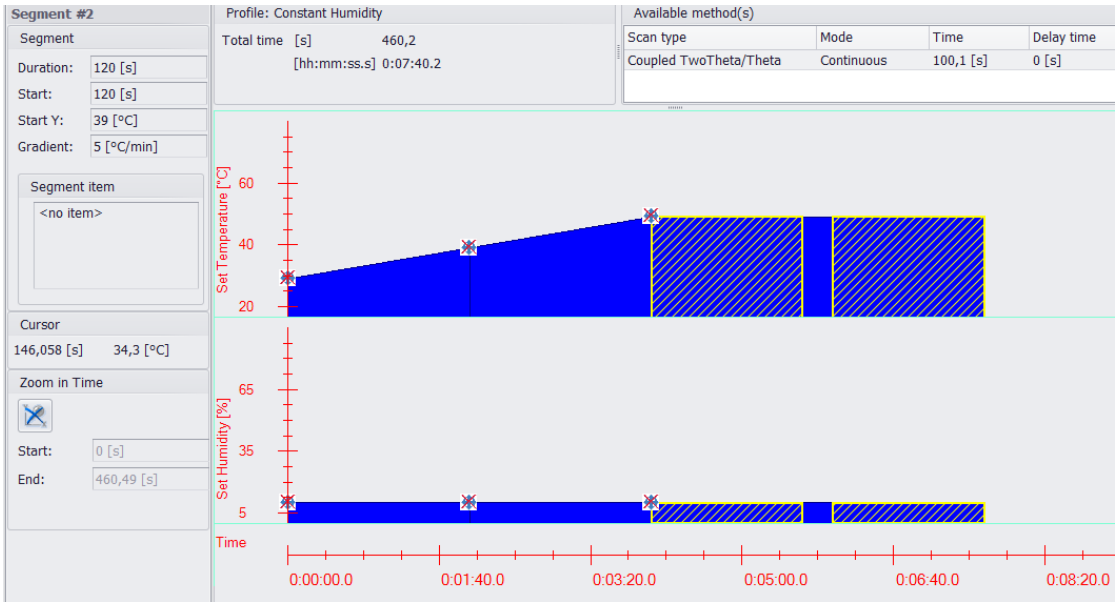


Figure 2.10: Graphical editor

2.1.3.4 Table and Graphical Editor

2.1.3.4.1 Common Layout

In the upper part of the window, both the table and the **Graphical editor** share the same layout,a toolbar, an overview and a **Measurement method** selection:

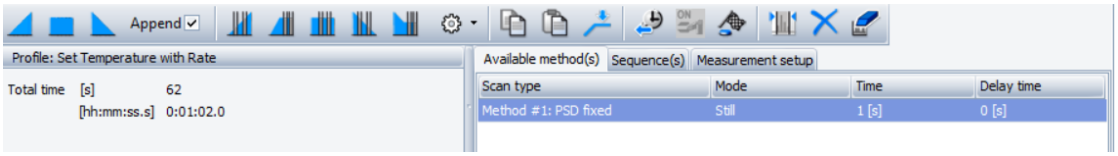


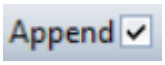
Figure 2.11: Profile editors: common headers

Toolbar

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

It is organized into five groups:

Segment insertion	
	Append/insert an increase of the parameters with maximum speed
	Append/insert a constant segment (no parameter change)
	Append/insert a decrease of the parameters with maximum speed

	Check to append or uncheck to insert a segment
One-click segments	One-click segments append a new segment completely filled with the measurements marked
	Append an increase of the parameters with maximum speed and measurements
	Append a “step” consisting of two segments: a maximum increase and a constant segment with measurements
	Append a constant segment and measurements
	Append a decrease of the parameters with maximum speed and measurements
	Append a “step” consisting of two segments: a maximum decrease and a constant segment with measurements
	Settings for One-click segments: Additional delay: specify an additional delay time used between two subsequent measurements Duration of the constant segment: Adjust here the default duration Optimize one-click measurements “rapid Non-ambient”: during the measurement it is possible to execute a single scan repeated on a one-click segment. The scan must be a still (no drives moved) and it must not have any delays defined. This option affects the whole profile.
Segment modifications	
	Copy the marked segments (together with their segment items)
	Paste the marked or copied segments before the currently marked segment
	Transform the current segment into a constant one
Segment items group	
	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
Profile group	
	Optimize the whole profile in time. This operation tries to minimize the duration of the profile
	Delete either the marked segment or the marked segment item(s) like delay, measurement etc.
	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

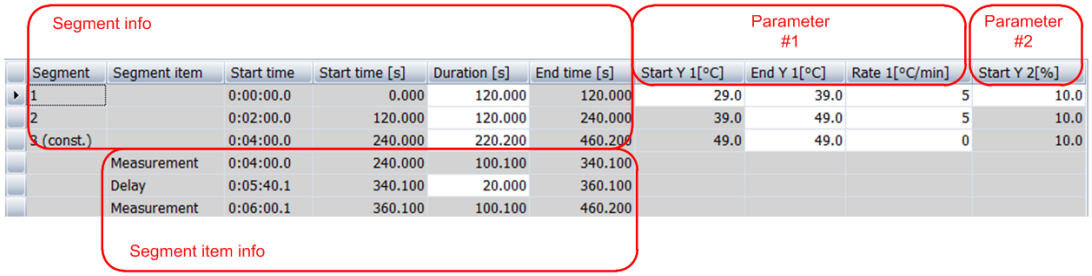
The overview summarizes the current profile.

Available Methods / Sequence(s) / Measurement Setup

To the right, the first tab list the available methods. Instead of using method(s) to insert or append it is also possible to use a sequence or even a measurement setup.

2.1.3.4.2 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).



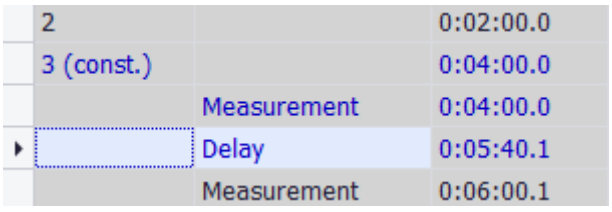
Segment	Segment item	Start time	Start time [s]	Duration [s]	End time [s]	Start Y 1[°C]	End Y 1[°C]	Rate 1[°C/min]	Start Y 2[%]
1		0:00:00.0	0.000	120.000	120.000	29.0	39.0	5	10.0
2		0:02:00.0	120.000	120.000	240.000	39.0	49.0	5	10.0
3 (const.)		0:04:00.0	240.000	220.200	460.200	49.0	49.0	0	10.0
	Measurement	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				

Current Segment:

In the table editor the current segment is the one with

Marking segments:

1. 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:



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

2.1.3.5 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 START JOBS plugin (and restarting the profile as a whole).

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

Press the 

button on the toolbar to add sample position segment item:

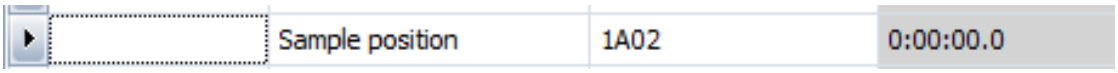
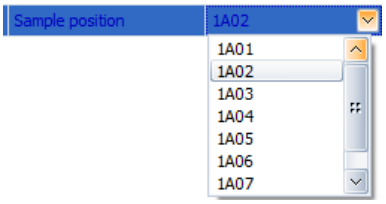


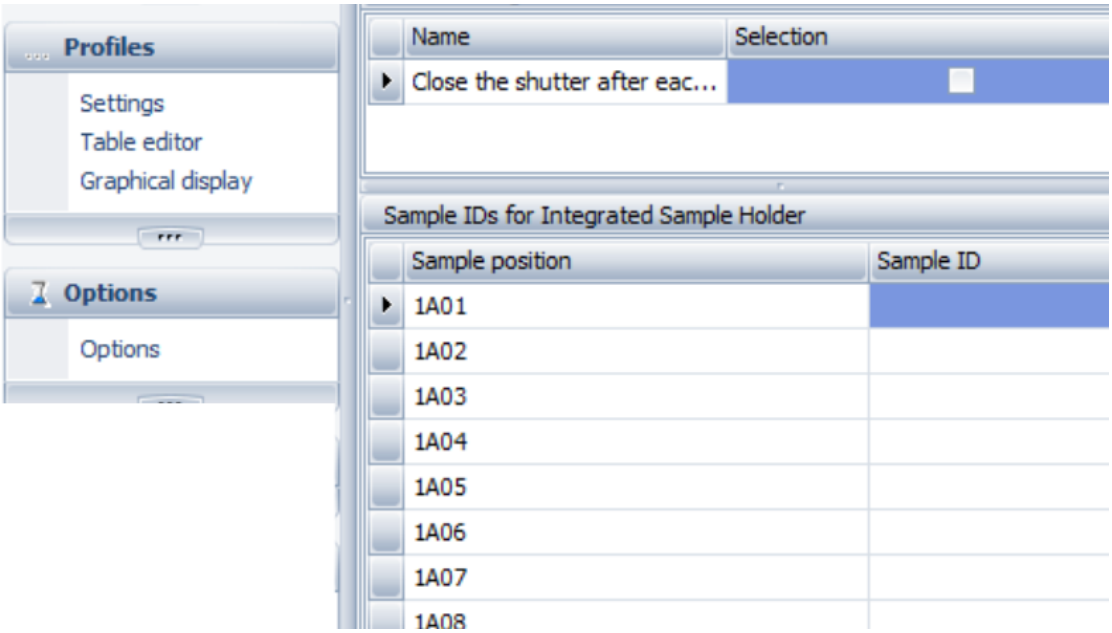
Figure 2.12: The sample position can then be selected from the available positions listed in the combo box:



2.1.3.5.1 Assigning names to a sample position

While the START JOBS plugin allows names to be assigned to the sample positions for single jobs it is also possible to assign them in WIZARD and store them within the BSML.

1. Choose the options module:

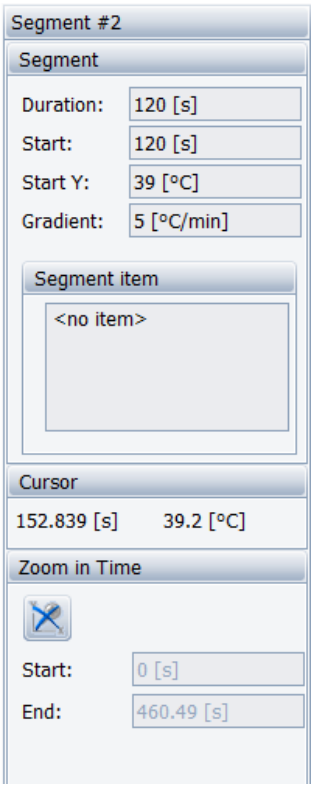


2.1.3.5.2 Graphical Editor

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

Note: Using the toolbar described above, almost all actions (for instance, one-click segments) can be carried out here, too.

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.

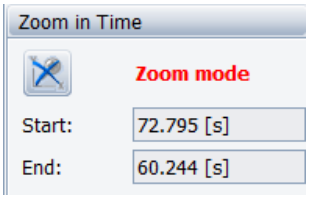


In the upper part the segment duration, start values and gradient are displayed. If the mouse cursor hits a segment item this information is displayed, too.

2.1.3.5.2.1 Zooming

It is possible to zoom the profile in time.

1. Press the left mouse button and move the cursor to the left: the zoom fields in the lower part of the panel are updated:



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

2. 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.

2.1.4 XY Positions

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

Figure 2.13: WIZARD XY positions module

2.1.4.1 XY Positions Form

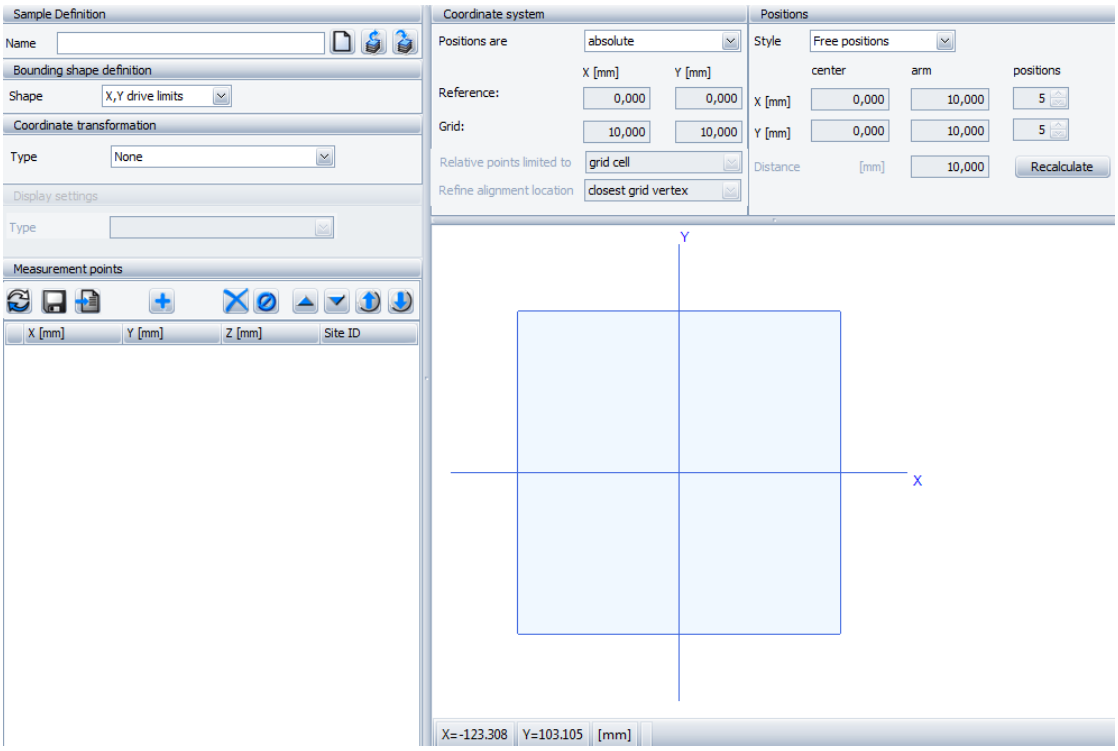


Figure 2.14: XY positions display

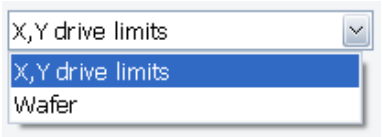
2.1.4.1.1 Sample Definition

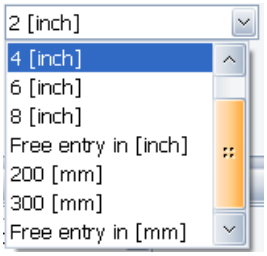
- Allows to save and load sample definitions to and from the database.

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.

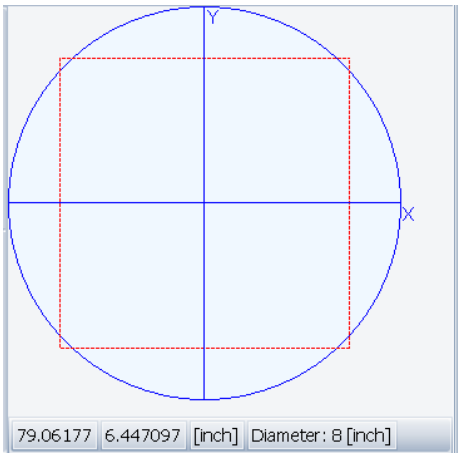
2.1.4.1.2 Bounding Shape Definition

- 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: 

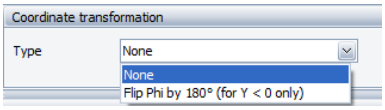
The X,Y positions display changes accordingly:



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

2.1.4.1.3 Coordinate Transformations:

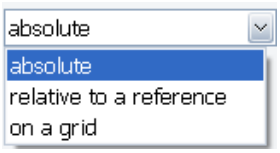
Coordinate transformations are applied during the measurement (they do not affect the graphics display to the right). The availability of the transformations depends on the stage used. : **Flip Phi by 180° (for Y<0 only)**



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

2.1.4.1.4 Coordinate System: Absolute and Relative Coordinates

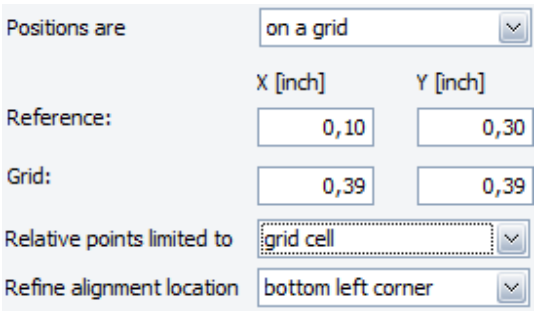
Three coordinate systems are available:



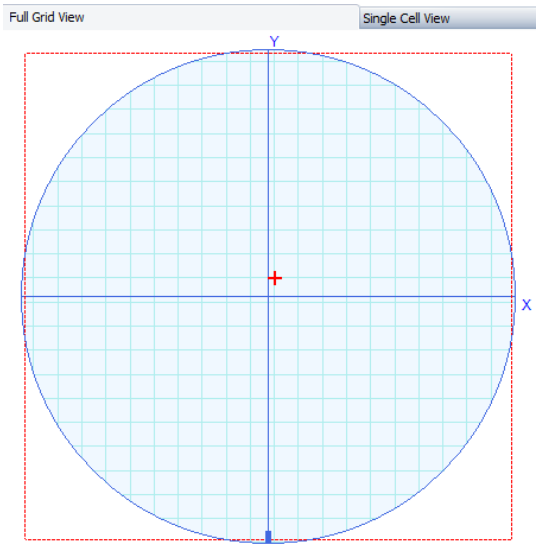
absolute	is the default. All points are defined as absolute positions of the x and y axes.
relative to a reference	defines an offset position. All points are defined as positions relative to the offset position. This offset position may be changed by the measurement script.
on a grid	defines a set of 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:

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



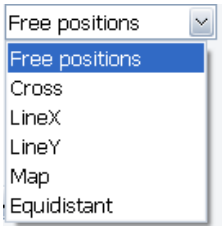
➨ The graphics display changes accordingly:



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

2.1.4.1.5 Positions

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

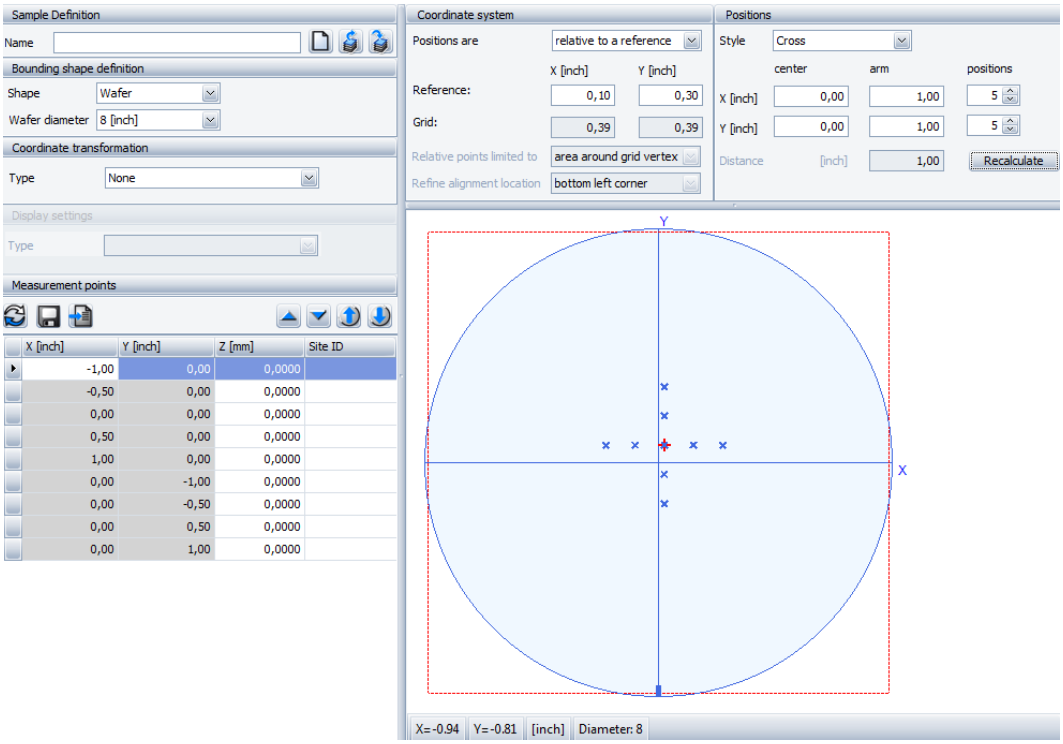


Free positions	the user can enter X and Y positions in the table (add button) or on the graphic display (double click)
Cross	defines an X,Y cross
LineX, LineY	defines a line in either X or Y with an offset in the other coordinate
Map	a rectangular map
Equidistant:	an almost equal distribution over the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

1. 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

1. Choose the positions relative to a reference and select the **Cross style**.
2. 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.

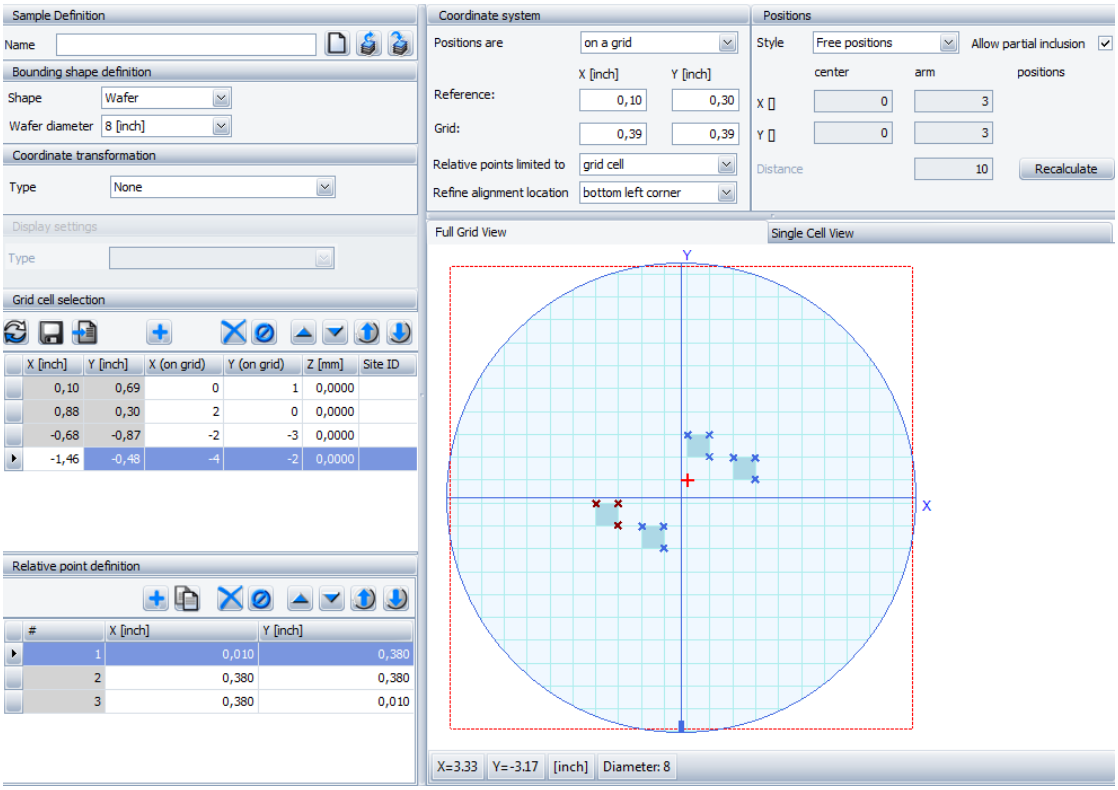


Hint: If the style is set back to free positions it is possible to add or delete single points from the cross.

Example: Free positions on a grid

1. 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.
2. Double click on the grid to select grid cells.
3. 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.

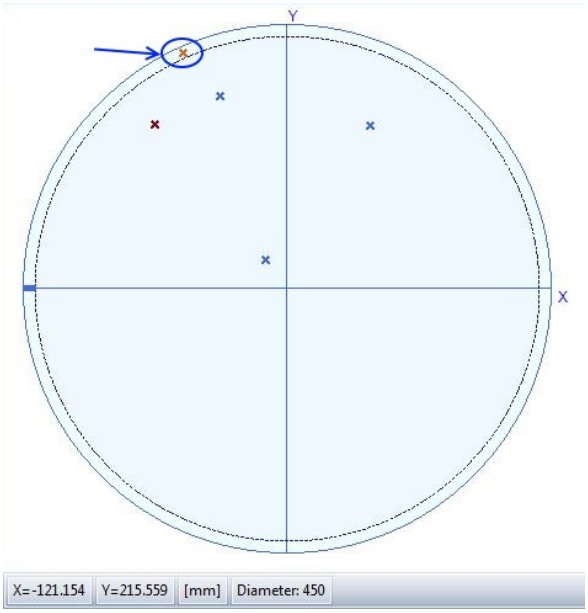
Please note that no measurement is possible unless at least one grid cell and at least one relative point are defined.



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.

2.1.4.2 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.



2.1.4.3 Refine Alignment Form

The form allows defining an alignment.

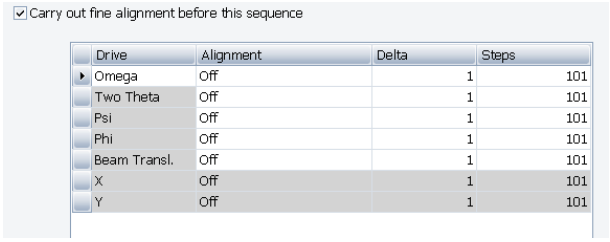


Figure 2.15: Refine alignment form

1. 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:

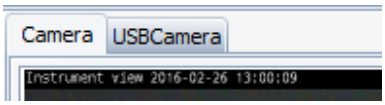
Off	No alignment done
Required	The drive will receive an alignment
Required (fine)	The drive will receive a fine alignment
Done	No alignment has been performed and the drive is considered aligned.

Note

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

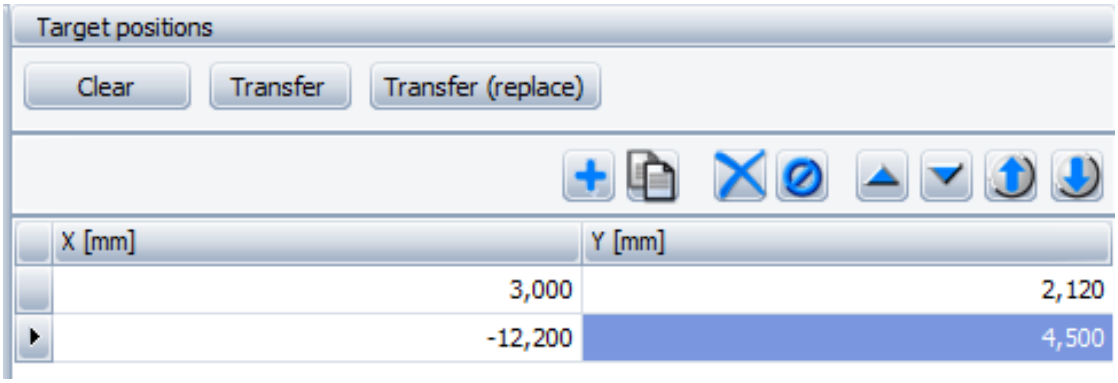
2.1.4.4 Camera

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



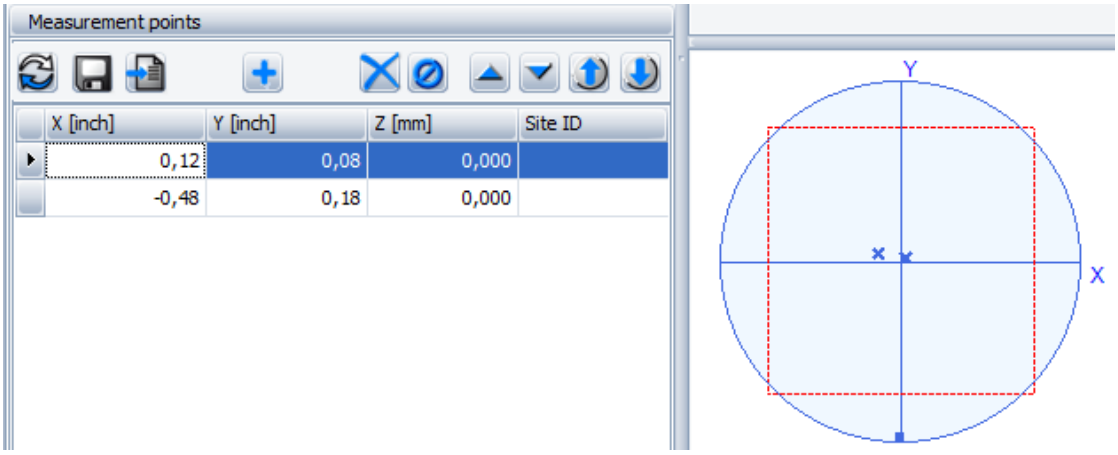
The camera control itself is described in detail in the *MEASUREMENT CENTER User Manual*.

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:

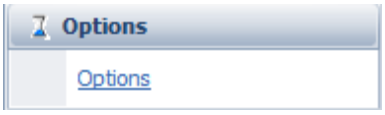


Note

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

2.1.5 Options

The **Options** 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:

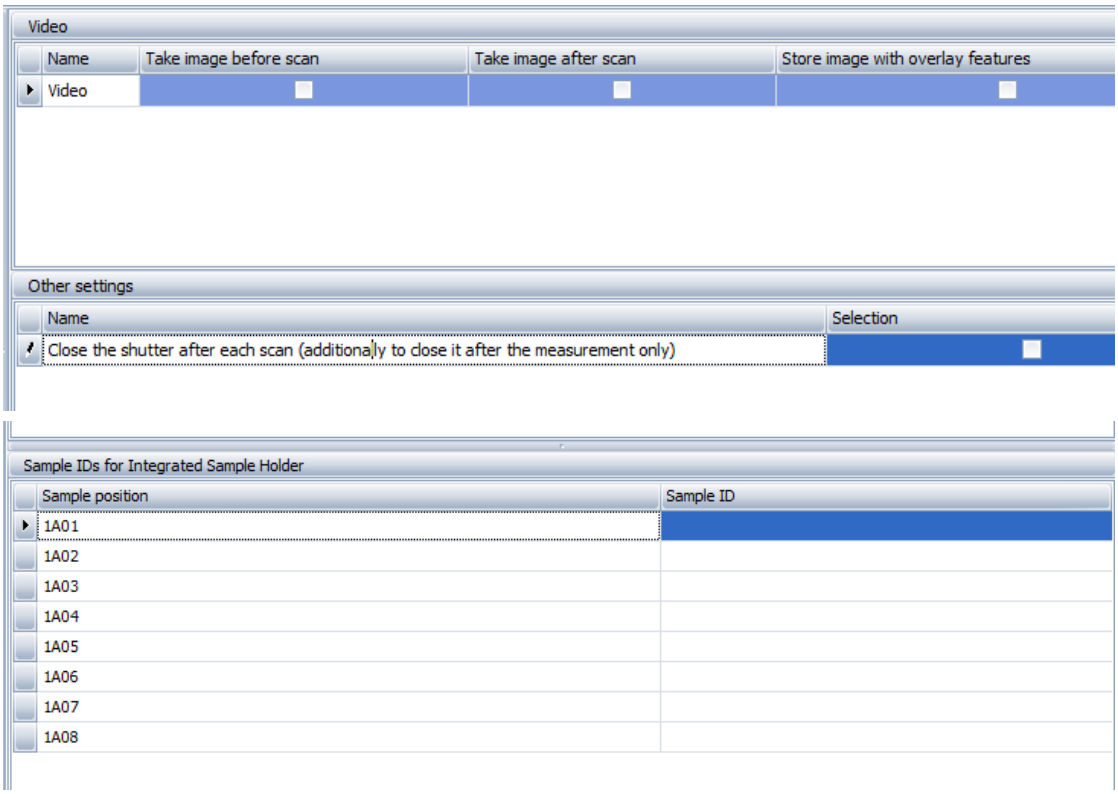


Figure 2.16: Options module

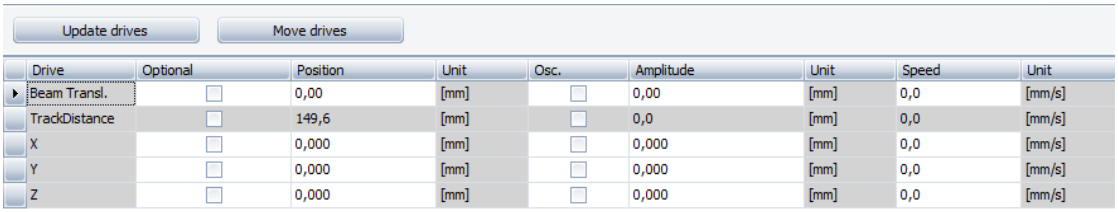
Each video system can take an image just before the scan starts and after the scan finished. The images are stored as JPEG files.

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. For chambers with an internal sample changer one may define sample names for the each sample position, see section *Assigning names to a sample position [▶ 32]*.

2.1.6 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.



Drive	Optional	Position	Unit	Osc.	Amplitude	Unit	Speed	Unit
Beam Transl.	☐	0,00	[mm]	☐	0,00	[mm]	0,0	[mm/s]
TrackDistance	☐	149,6	[mm]	☐	0,0	[mm]	0,0	[mm/s]
X	☐	0,000	[mm]	☐	0,000	[mm]	0,0	[mm/s]
Y	☐	0,000	[mm]	☐	0,000	[mm]	0,0	[mm/s]
Z	☐	0,000	[mm]	☐	0,000	[mm]	0,0	[mm/s]

Figure 2.17: Fig. 20: Fixed drives form

1. Press Update drives to update the default drive positions with the current positions on the instrument.
2. Press Move drives 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.

2.1.7 Summary

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

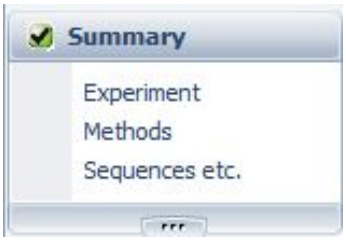


Figure 2.18: Summary module

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, profiles etc.).

2.1.7.1 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*.

2.2 Application specific modules

2.2.1 SAXS

The SAXS experiment template allows defining SAXS measurements on a N8 HORIZON system with a 2D detector. Optionally, a VÅNTEC-1 may be mounted to allow for WAXS measurements. It consists of the following modules:

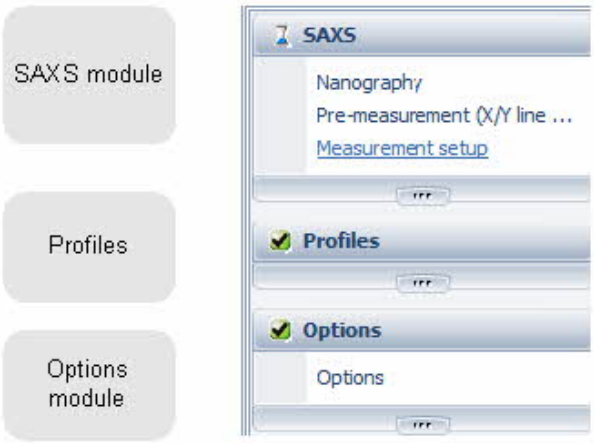


Figure 2.19: SAXS modules

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

Table 2.1: Available measurement setups in SAXS

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

Type	SAXS measurement setup		Detector involved
		Glassy carbon	VÅNTEC-500 in 0D mode

2.2.1.1 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.

2.2.1.1.1 Nanography Map

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

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

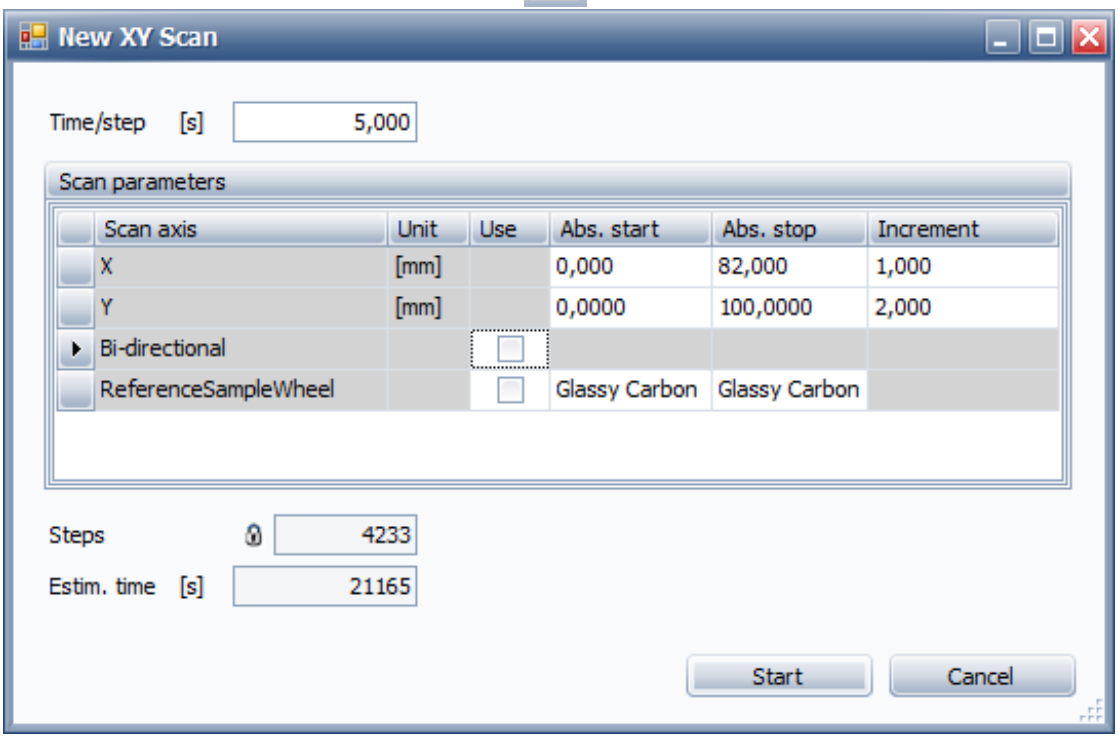
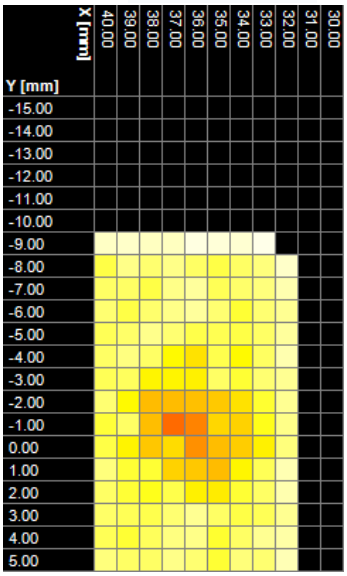


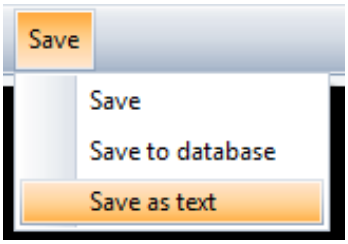
Figure 2.20: SAXS Nanography setup dialog

2. Here, the ranges in X and Y can be entered.
3. 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).
4. It is also possible to measure each X, Y position twice with two different settings of the sample wheel:
5. If done with the parameter setup,

6. press Start to directly start the measurement.



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



8. **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.

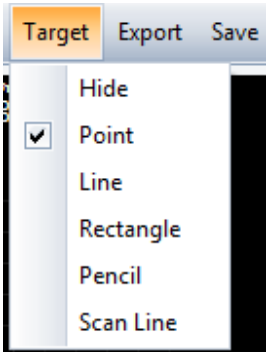
Note

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

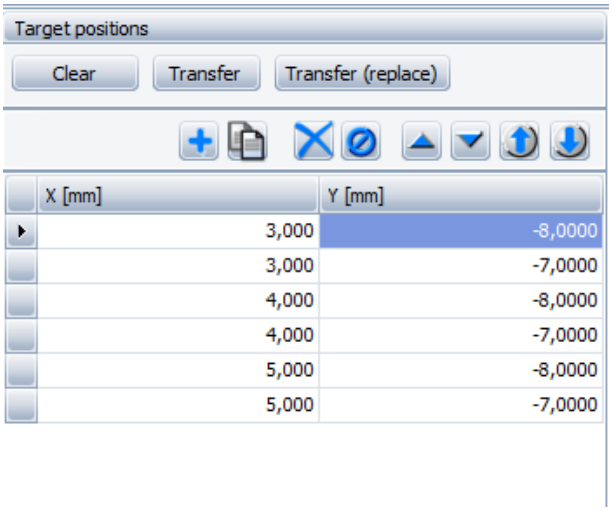
2.2.1.1.1.1 Transfer of Positions

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

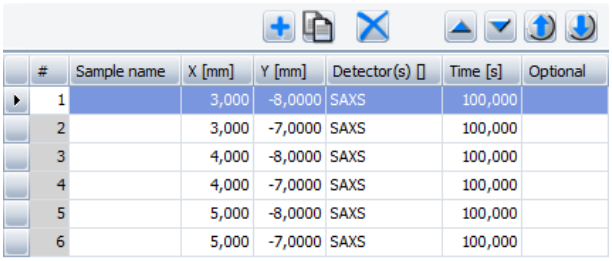
First, select how to select positions using the **Target** menu:



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



1. The actions to select (point, line, rectangle,…) can be combined. The table allows to delete or move X, Y positions using the standard buttons.
2. To transfer them to sample measurements press Transfer or Transfer (replace).
   - ➨ Using the first button will add new positions to the table of sample measurements, the second one will replace all existing X, Y positions.
3. You can see the positions transferred if you click on **Measurement setup** in the module:

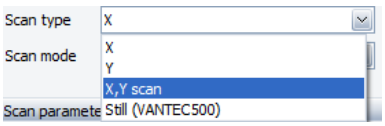


4. Here, you can proceed as described in *Sample Measurements [▶ 47]*.

2.2.1.1.2 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:

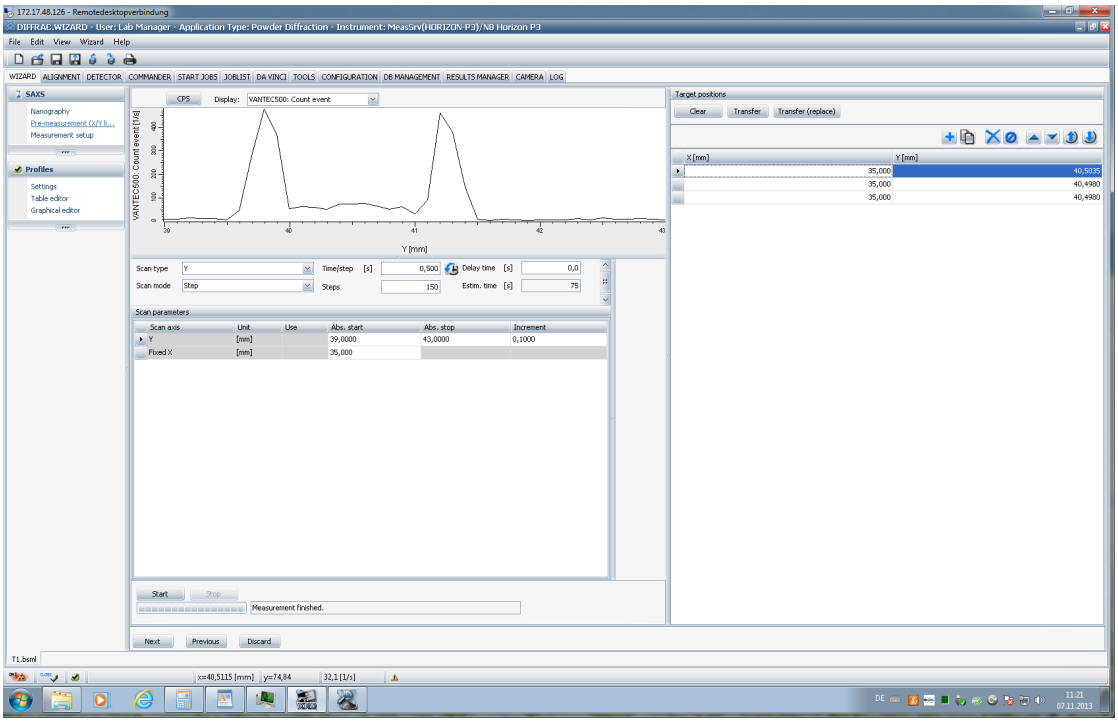


1. Then, define the **Drive** parameters.

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:



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

2.2.1.2 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.

2.2.1.2.1 Definition of a Sample Measurement

Each row in the table creates a sample measurement:

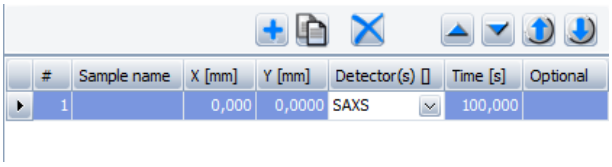


Figure 2.21: SAXS sample measurement table

Table Entries for Sample Measurements

#	The ordinal number of the sample measurement.
Sample name	An optional name of the sample
X	X coordinate
Y	Y coordinate
Detectors	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

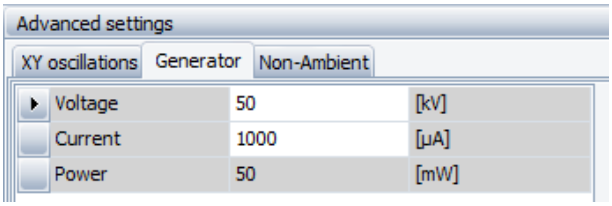
Time	The exposure time
Optional	Indicators for optional measurements: T: transmission Bgrd: background T(Bgrd): Transmission of background

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

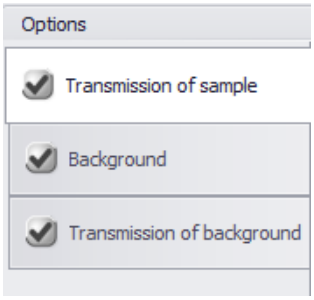
To the top right, it is possible to set **X and Y oscillations**, **Generator** parameters and **Non-ambient** parameters (if a non-ambient chamber was mounted):



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

2.2.1.3 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.

2.2.1.3.1 Transmission of sample

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

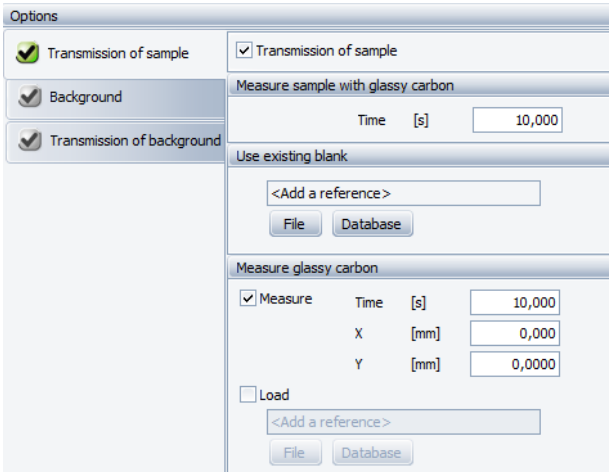


Figure 2.22: SAXS optional measurements

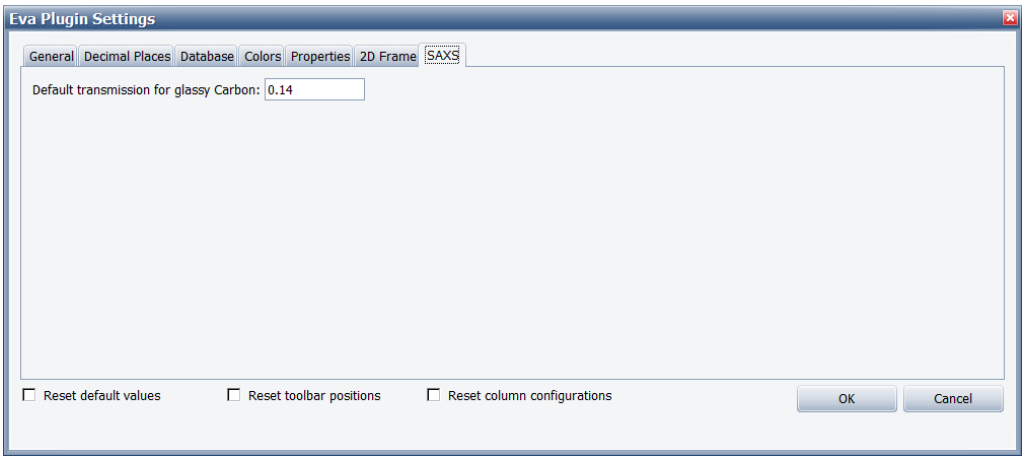
The determination of the transmission of the sample requires three measurements:

Measure the sample with glassy carbon	I_{S+GC}	only the time can be defined here.
Reference an existing blank measurement	I_{BG}	see section *Define a Reference to Existing Measurements [▶ 51]*
Measure the glassy carbon	I_{GC}	This can be measured with a specific X,Y position or a previous measurement can be referenced

The frame intensities of these measurements are saved in the result file and the evaluation software is then able to calculate the transmission of the sample using:

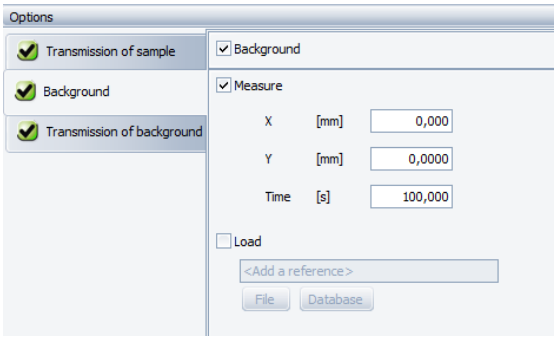
$$\tau_S = \frac{I_{S+GC} - \tau_{GC}\, I_S}{I_{GC} - \tau_{GC}\, I_{BG}}$$

τ_{GC} stands for the transmission of the glassy carbon. The typical value is 0.14 and can be defined in the evaluation software DIFFRAC.SAXS.



2.2.1.3.2 Background

The background may be measured or a previous measurement can be loaded (How to load one, please see section *Define a Reference to Existing Measurements [▶ 51]*.

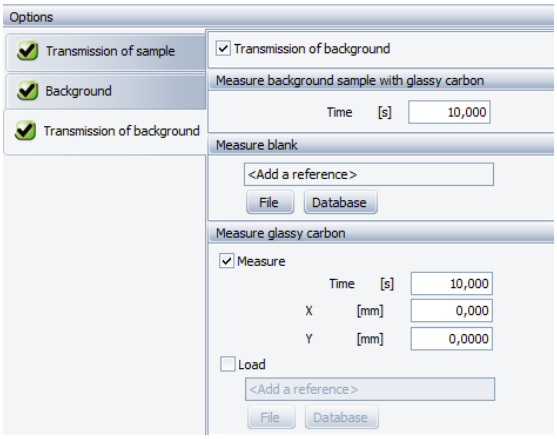


2.2.1.3.3 Transmission of Background

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

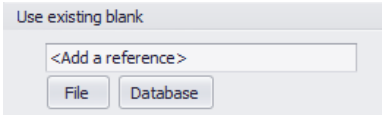
Note

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



2.2.1.3.4 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:



1. Measurement references can come from the database or from a file on disk.
2. Press one of the buttons and the browser dialog opens:

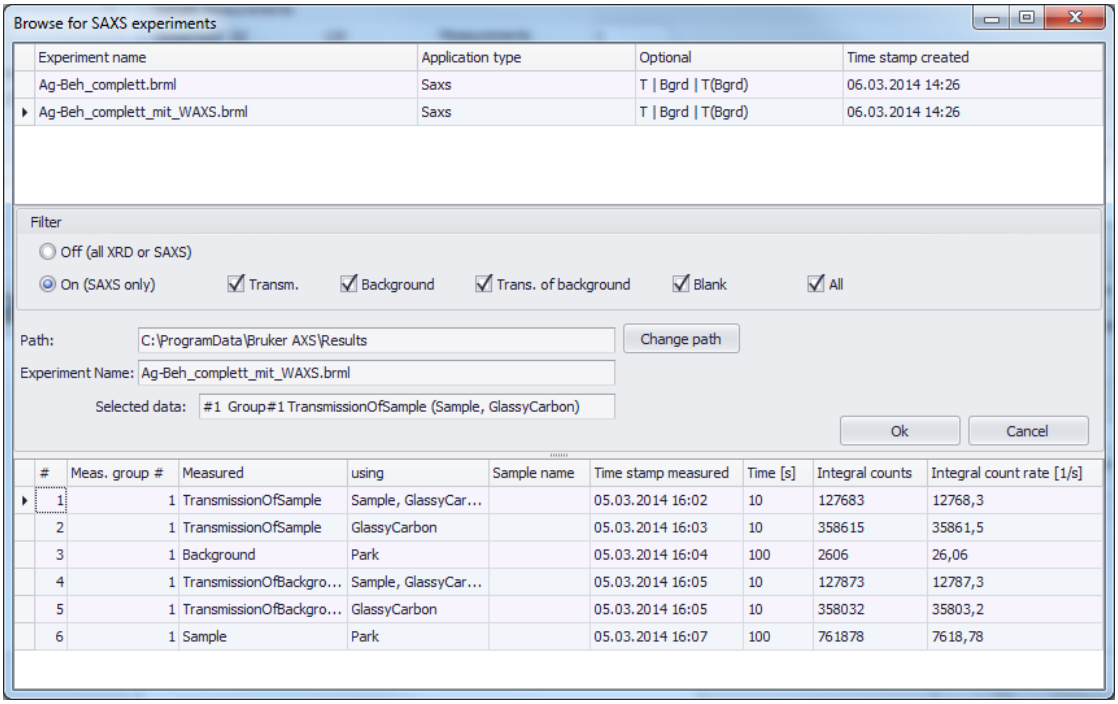


Figure 2.23: SAXS BRML browser

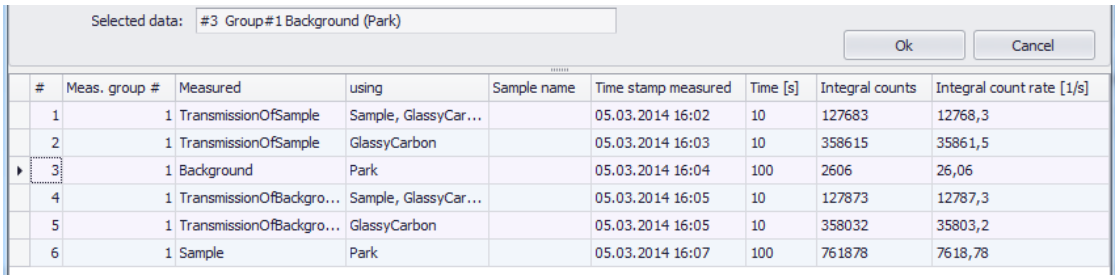
Note that you can use the filter options to restrict the search.

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.



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.

2.2.1.4 Profiles

The profiles module is present if, for instance, a Non-ambient chamber is installed. See the description in *Profiles [▶ 20]*. In SAXS, the complete measurement setup can be put on a profile.

2.2.1.5 Options

Options are described in *Options [▶ 41]*.

2.2.2 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.

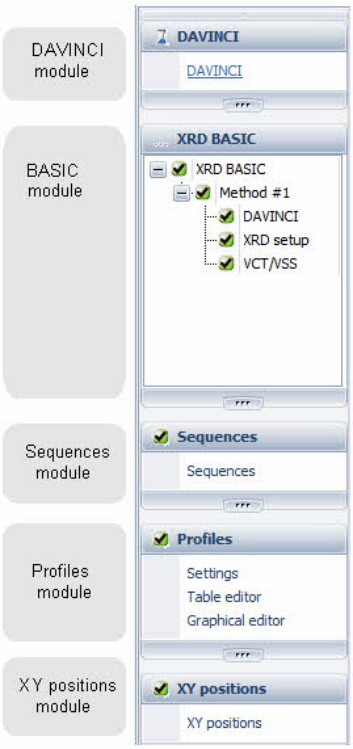
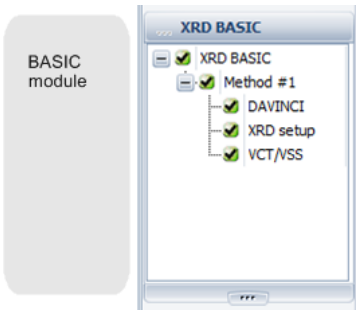


Figure 2.24: XRD modules

2.2.2.1 DAVINCI Module

For this module, see the description i section *DAVINCI [▶ 14]*.

2.2.2.2 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.

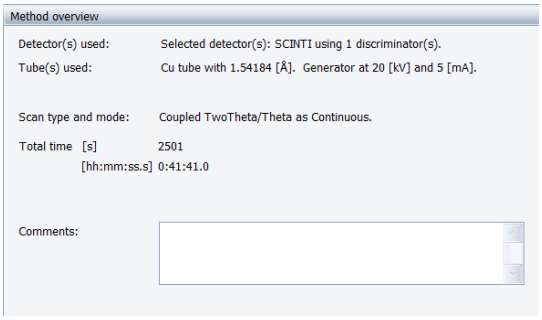
2.2.2.2.1 XRD Basic

This view describes the measurement:

Figure 2.25: 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**.

2.2.2.2.2 Method



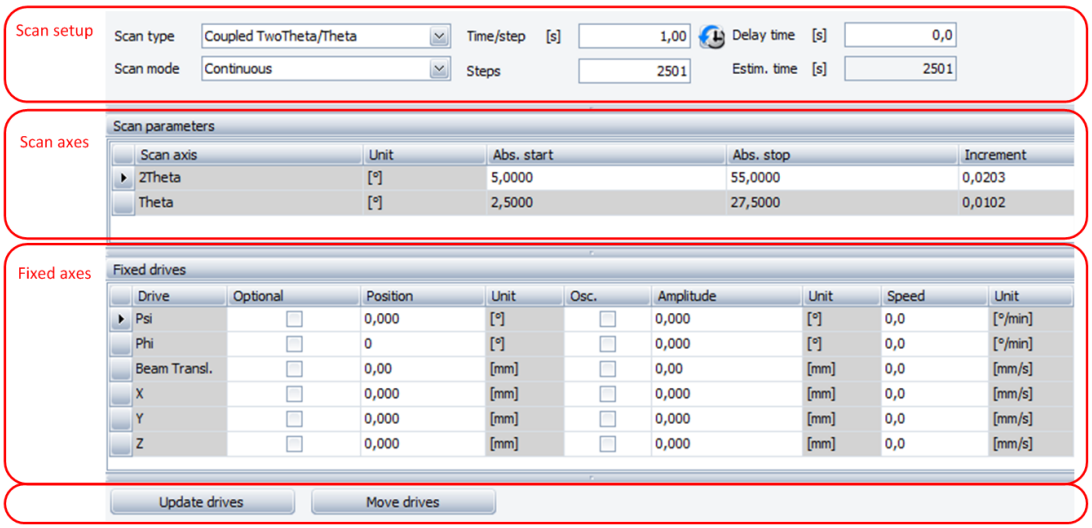
2.2.2.2.2.1 DAVINCI

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.

2.2.2.2.2.2 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 in section *XRD [▶ 52]* for an overview on available **Scan types**.



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 Drive

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 Update drives to transfer the current instrument drive positions to the Positions column in the table, or Move drives 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.

2.2.2.2.2.3 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.

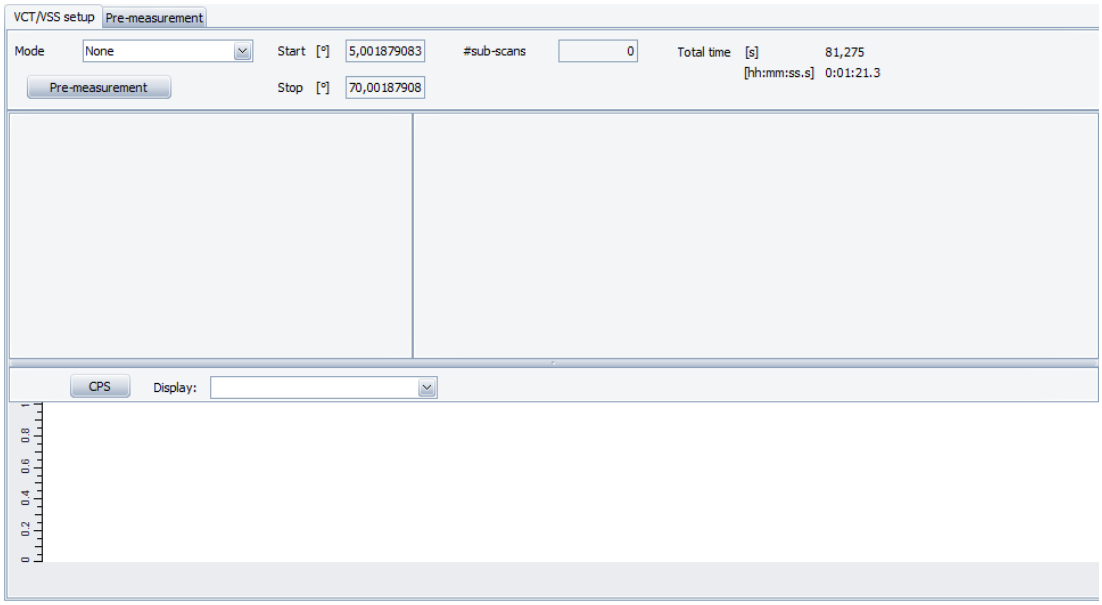


Figure 2.26: VCT/VSS setup

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-sans (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.

- If you change one or both parameters you have to press Apply.
- For a scan from 2Theta = 5° to 70°, you may receive the following:

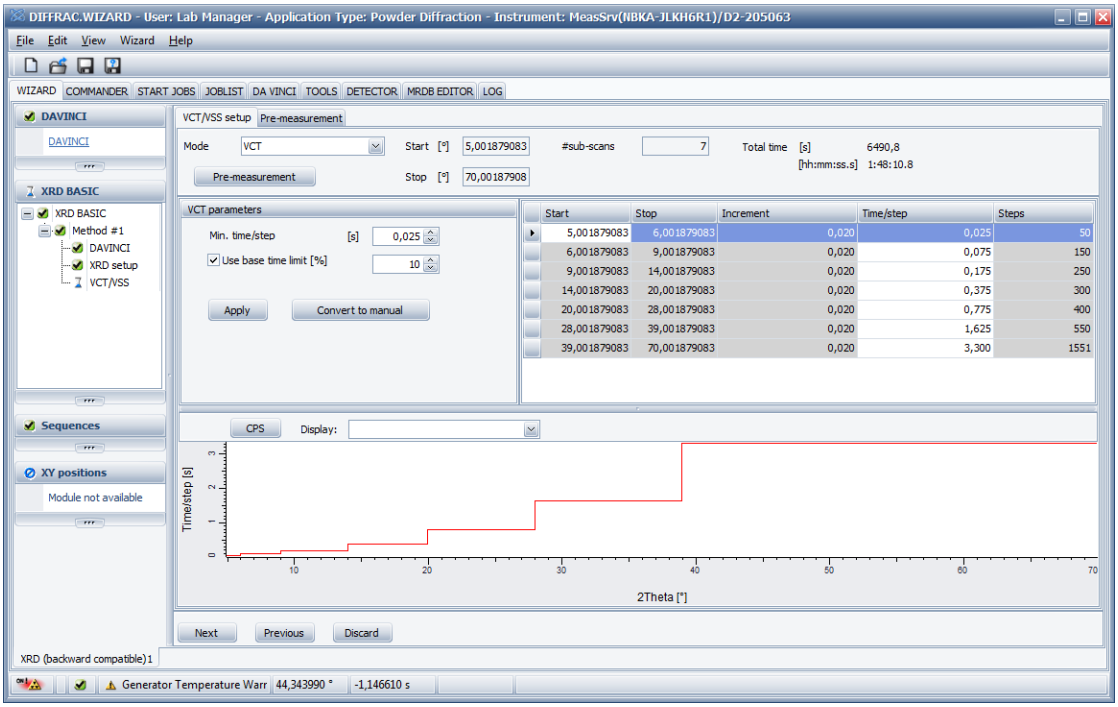


Figure 2.27: VCT

Manual mode

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

1. Click on Convert to manual.
   ➨ As a result, both **Increment** and **Time/step** can be edited for each sub-scan:

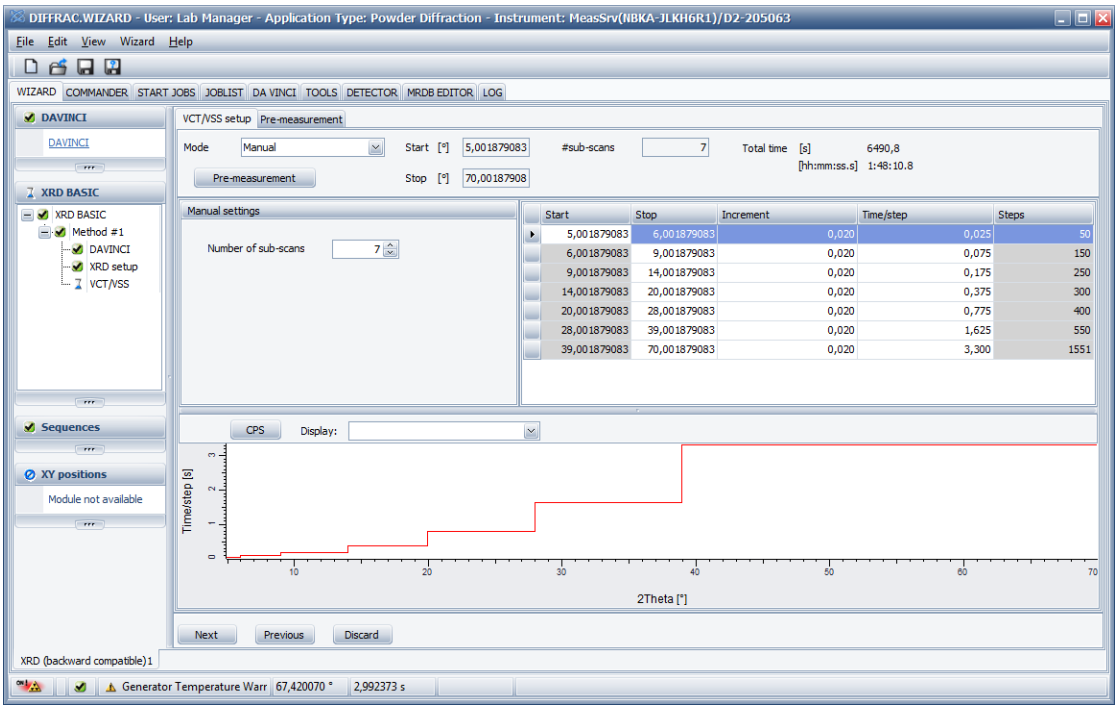
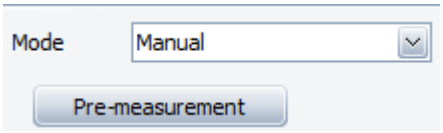


Figure 2.28: Manual VCT/VSS

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:

1. 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.

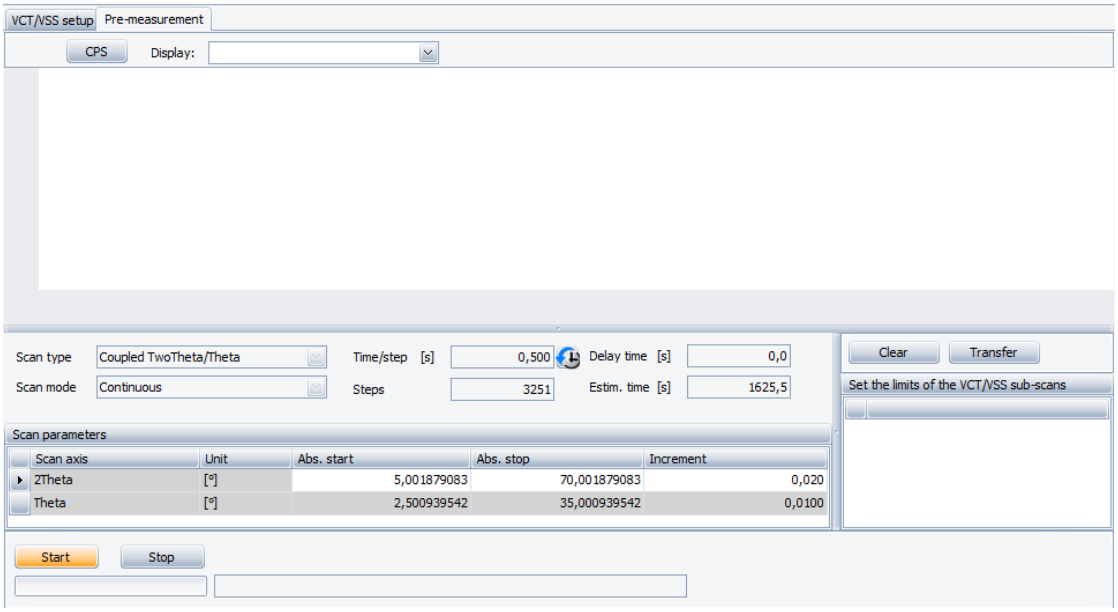
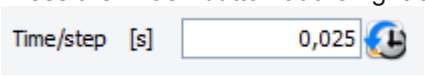


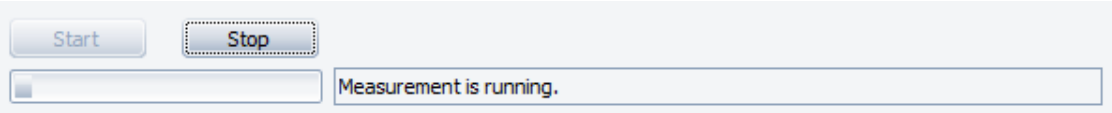
Figure 2.29: VCT/VSS pre-measurement

2. 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).

3. 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.

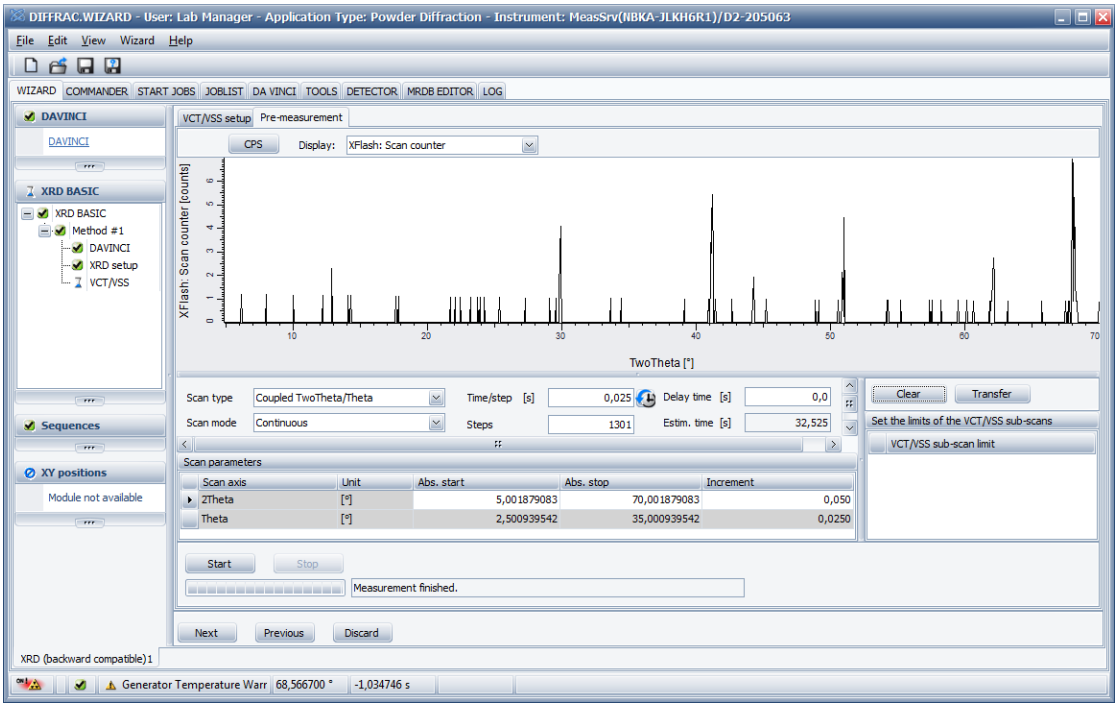
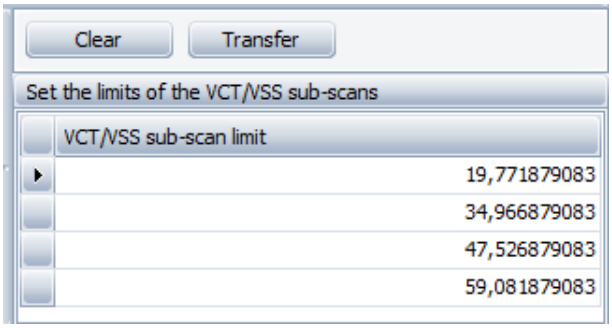


Figure 2.30: VCT/VSS pre-measurement executed

4. 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:



5. 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 subs-scan.

6. You may now change **Increment** and **Time/step** as usual.

➥ The current scan is also shown in the manual setup:

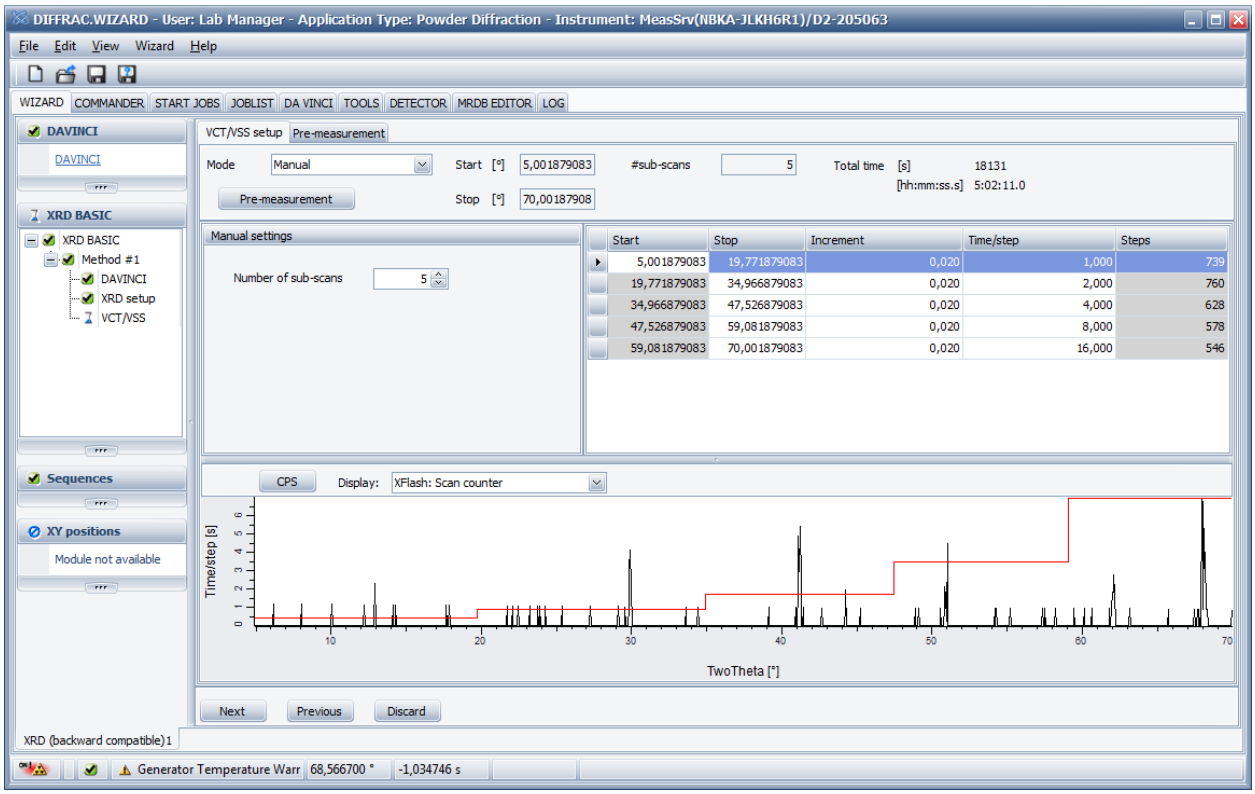


Figure 2.31: Using the pre-measurement to define sub-scans

2.2.3 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.

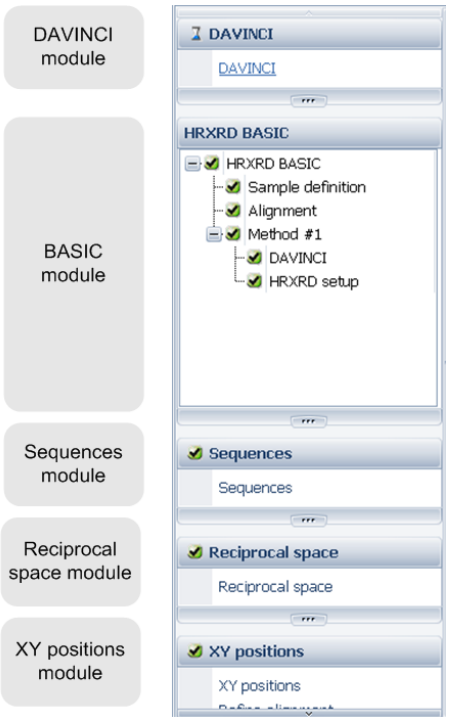
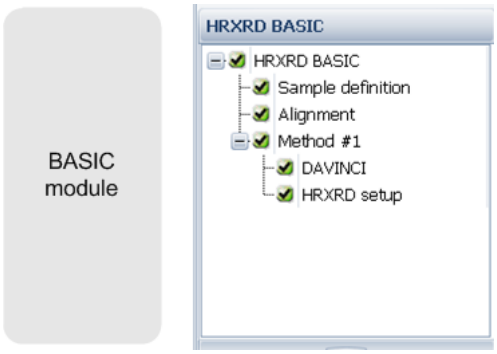


Figure 2.32: Modules in HR-XRD

2.2.3.1 DAVINCI Module

For this module, see the description in section *DAVINCI [▶ 14]*.

2.2.3.2 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.

2.2.3.2.1 HRXRD Basic

This view describes the measurement:

Figure 2.33: 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**.

2.2.3.2.2 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**

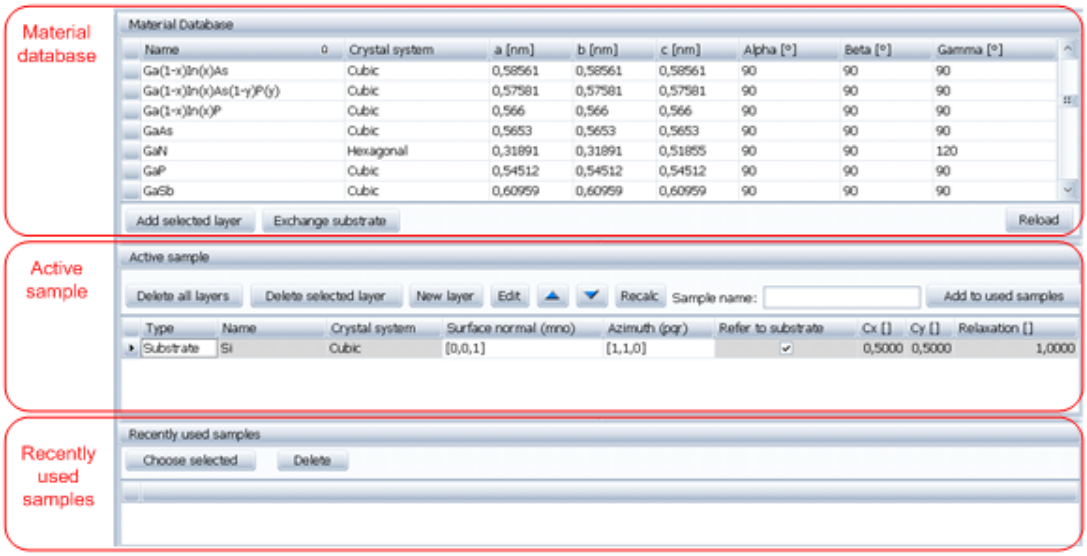


Figure 2.34: Sample definition form

2.2.3.2.2.1 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.

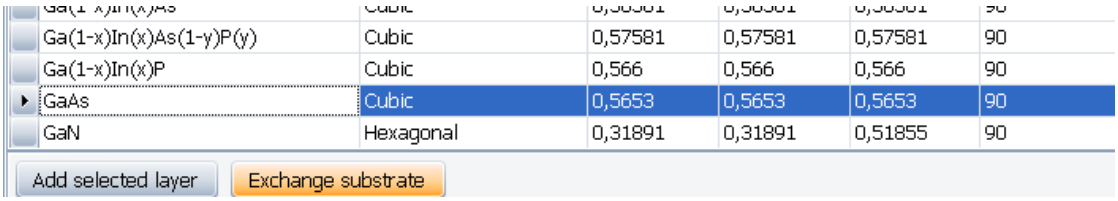
Note

If the content of the material database is changed using the MRDB EDITOR plugin, 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.

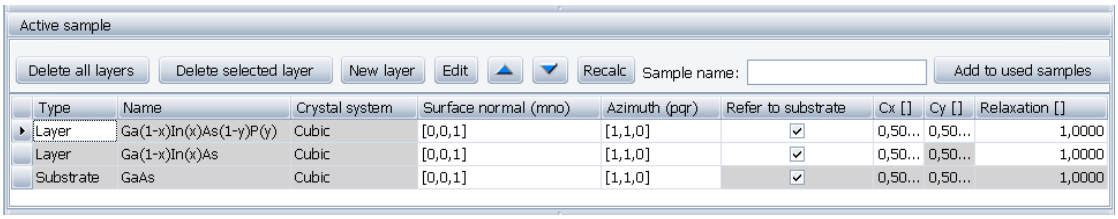
1. Mark **GaAs** in the materials table and press the **Exchange substrate** button:



2. 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.

2.2.3.2.2.2 Active Sample

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



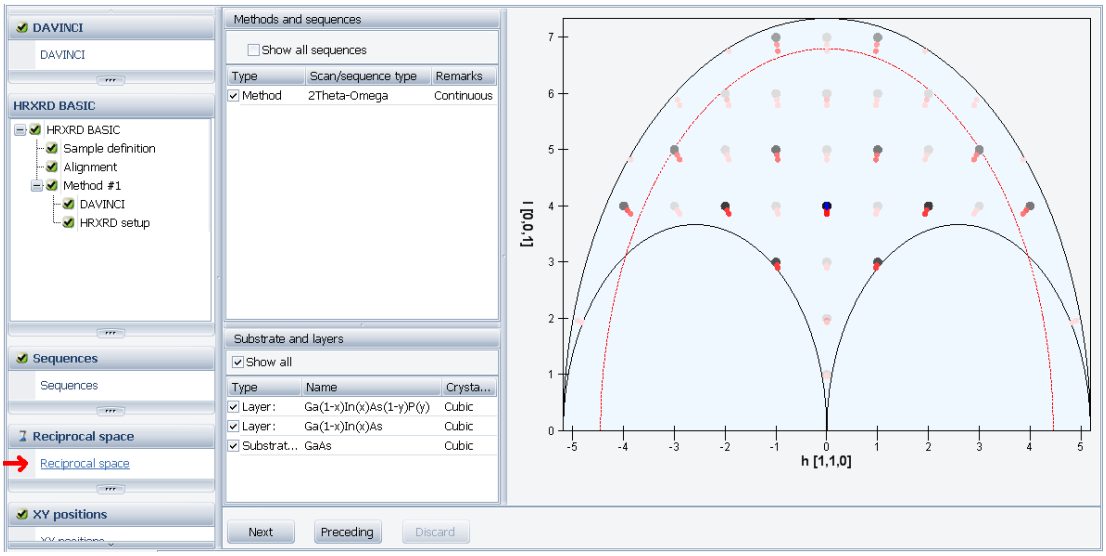
Note

If the sample just defined will be used in other experiments, it can be stored in the database. (see section *Recently used samples [▶ 63]*.

Sample in Reciprocal Space

▶ The sample, which has just been defined using the **Reciprocal space** display can now be controlled.

1. Click on the **Reciprocal space** module. The module itself is described in detail on *Reciprocal Space Module [▶ 67]*.



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

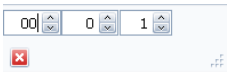
Refer to Substrate

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.

1. Click into the cell to open a small dialog:

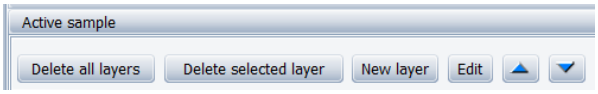


2. and change the values.
3. To close the dialog type **<Esc>** (changes not stored) or **<F4>** (changes stored).
   - ➨ The red button will store the changes.

⇨ 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:



2.2.3.2.2.3 Recently used samples

1. To store the samples created for later usage enter a sample name and
2. 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.

2.2.3.2.3 Alignment

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

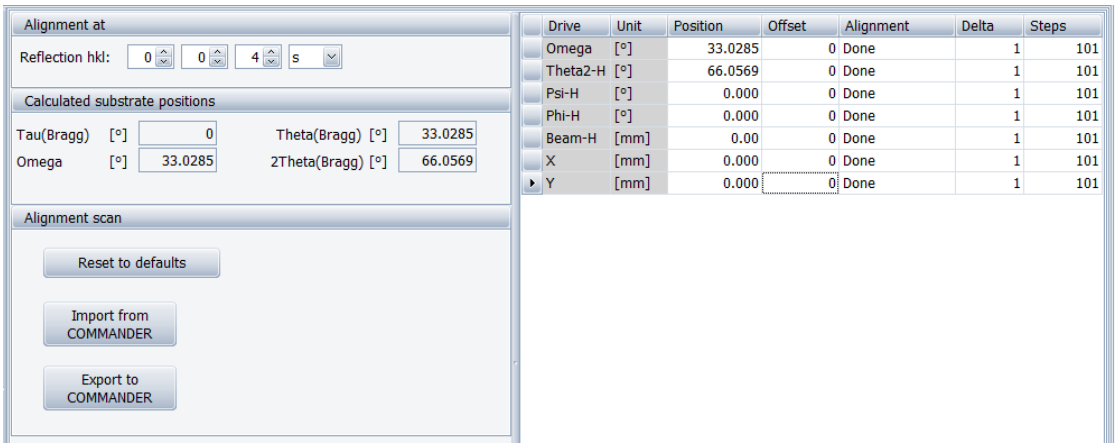
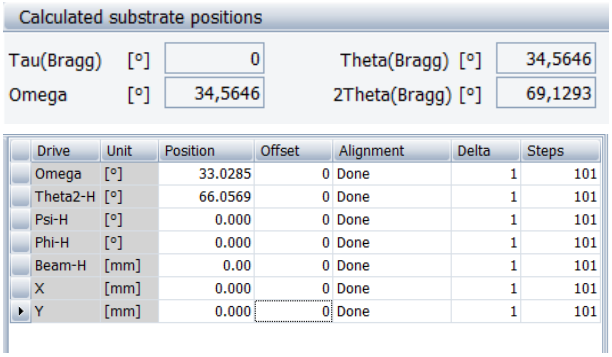


Figure 2.35: Sample alignment form

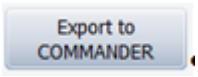
If the reflection is modified at the upper left

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

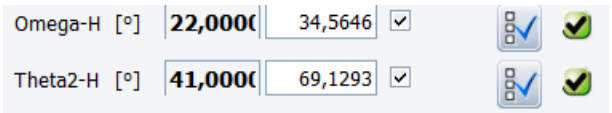


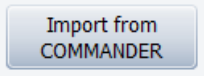
2.2.3.2.3.1 Exchanging Positions between WIZARD and COMMANDER

If the reflection has been chosen, the theoretical sample positions can be transferred to the COMMANDER plugin:

1. Use 

2. Then, switch to the COMMANDER plugin:



3. The drives can be moved or the **Alignment** scans can be performed.
4. After locating the positions, use ***T*ransmit drive positions** from the COMMANDER menu and
5. click 

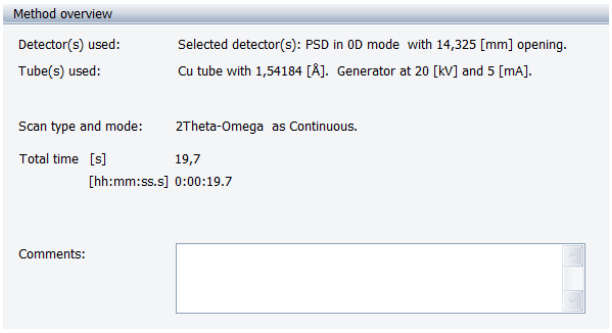
in the WIZARD for the chosen experiment to be updated.

⇨ 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

2.2.3.2.4 Method

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



It is possible to enter method specific comments.

2.2.3.2.4.1 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.

2.2.3.2.4.2 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 in section *High resolution XRD [▶ 102]* 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 HRXRD, the **Scan axes** are relative. This means that the scan coordinates refer to the aligned reflection.

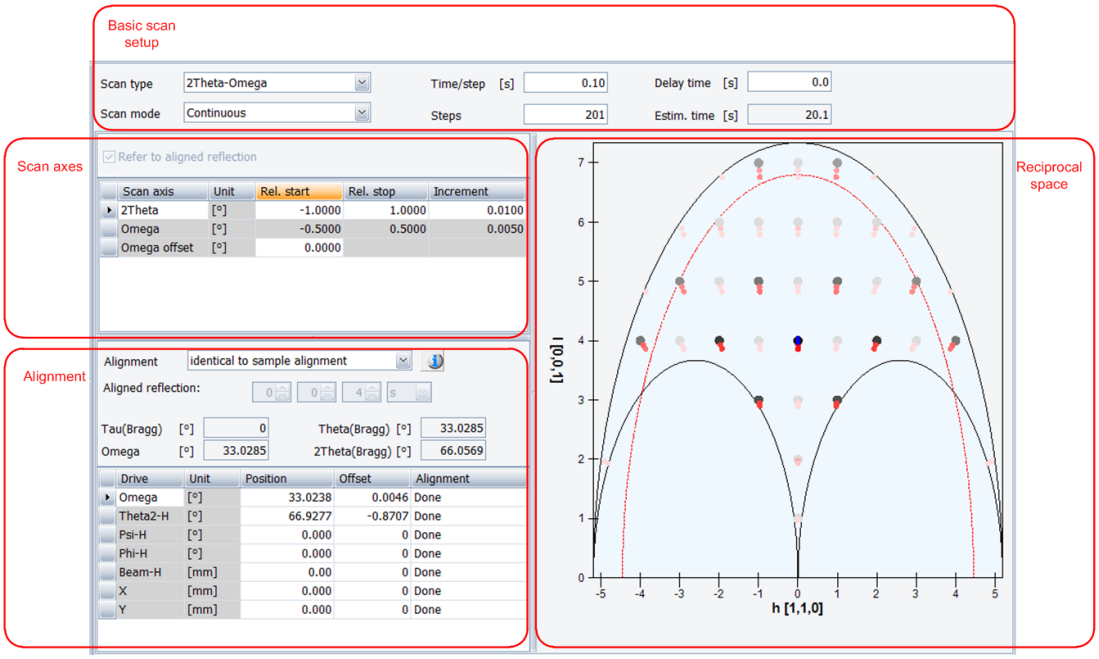
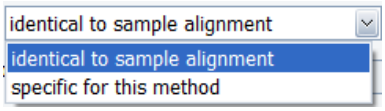


Figure 2.36: HRXRD scan setup

Alignment

The alignment is identical to the alignment defined by default. However, it may be switched to a method specific alignment. This renders the aligned reflection different for each single method. (see section *Alignment [▶ 63]*)



Reciprocal Space

The lower right panel shows the current scan in reciprocal space. For further information see the description in *Reciprocal Space Module [▶ 67]*

2.2.3.3 Sequences in HRXRD

HR-XRD provides several special sequences. For an introduction to the sequences module, see section *Sequences [▶ 17]*.

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.

2.2.3.4 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.

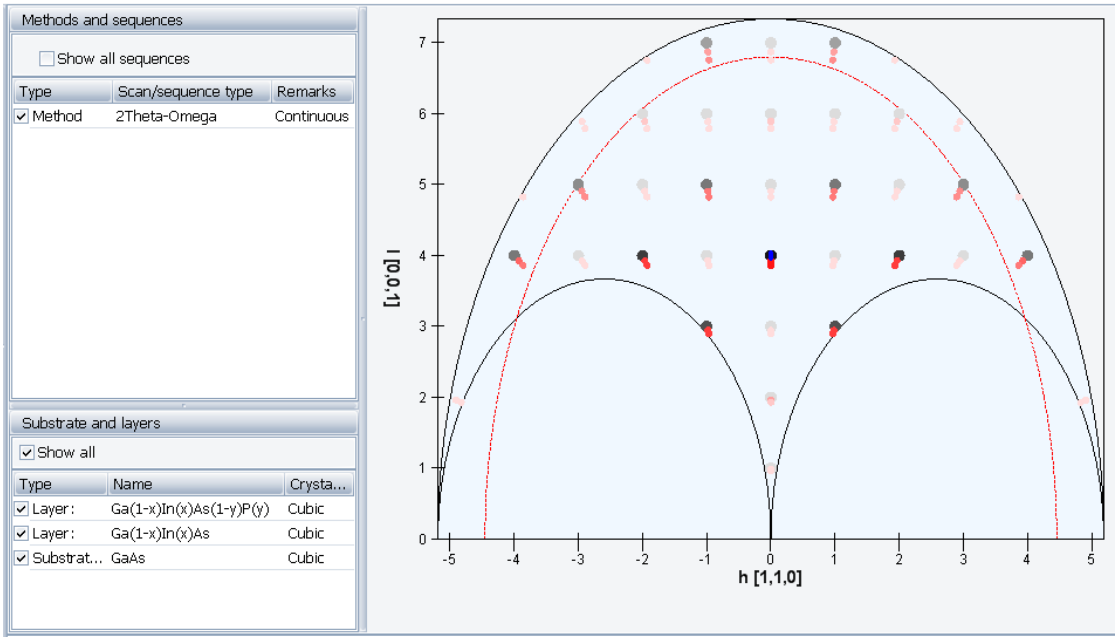


Figure 2.37: Reciprocal space display

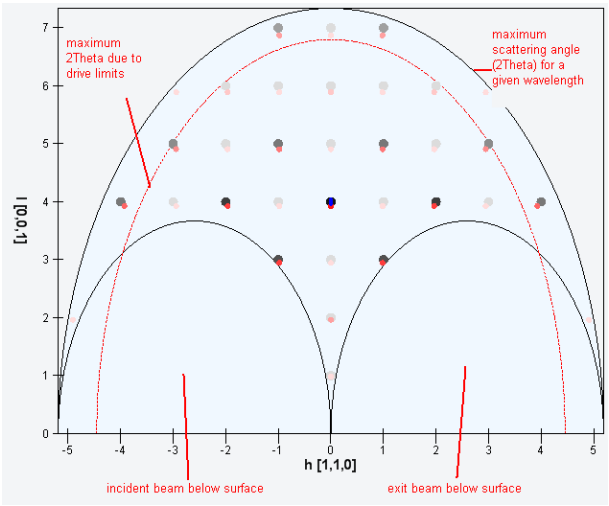


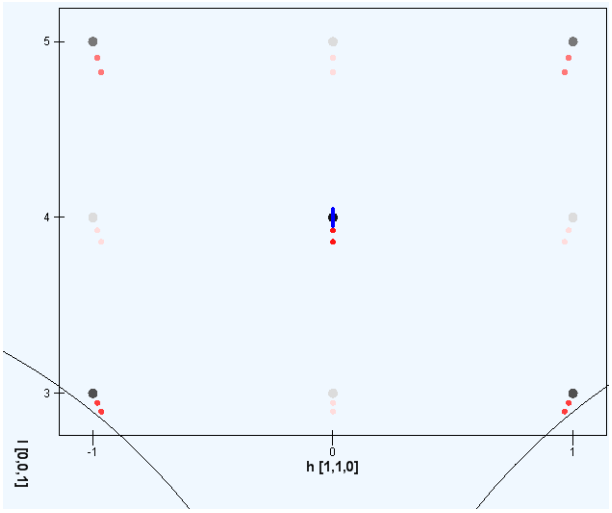
Figure 2.38: Reciprocal space limits

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.

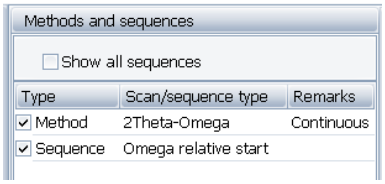
The user can zoom into the display.

1. Click on the left mouse button. Move the mouse and release it:



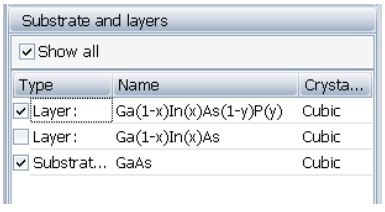
Select Sequences for Display

- 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.



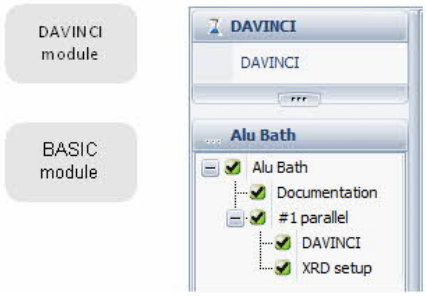
2.2.3.5 XY Positions Module

For this module, see the description in section *Profiles [▶ 20]*.

2.2.4 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).



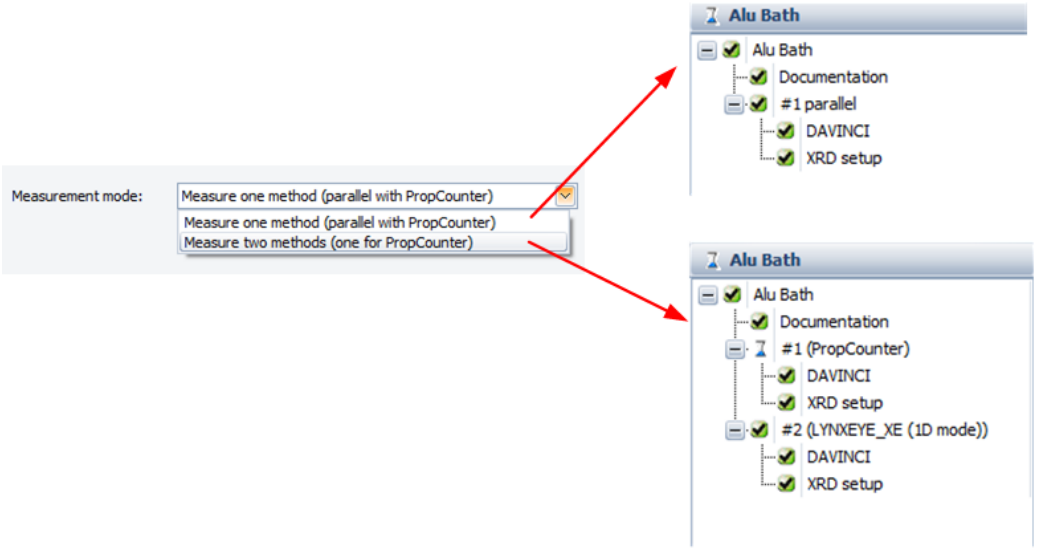
2.2.4.1 DAVINCI module

For this module, see the description in *DAVINCI [▶ 14]*.

2.2.4.2 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 [▶ 53]*.

2.2.4.3 Options

Options are described in *Options [▶ 41]*.

2.2.5 Stress

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

Figure 2.39: 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.

2.2.5.1 DAVINCI module

For this module, see the description *DAVINCI [▶ 14]*.

2.2.5.2 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.

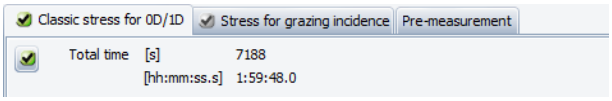
Depending on the Stress application and the detectors used for the measurement setup different setups can be chosen:

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

2.2.5.2.1 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 found below *Overview: Available Measurement Setups in Stress [▶ 72]*.



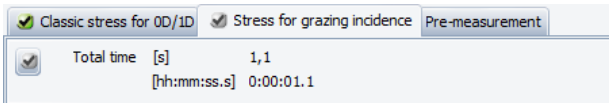
Each measurement setup is shown on a single tab. In addition, there may be a pre-measurement tab (if supported by the detector).

Note

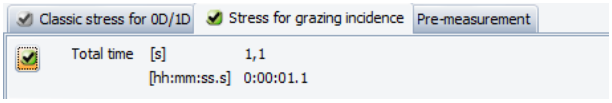
Only one measurement setup can be active at a time. The active setup is indicated in the tab header with a green check mark. To activate a measurement setup, select the corresponding tab and press the select button.

2.2.5.2.1.1 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:



1. 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.



2.2.5.2.1.2 Overview: Available Measurement Setups in Stress

Table 2.2: Available measurement setups in Stress

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

2.2.5.2.2 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.

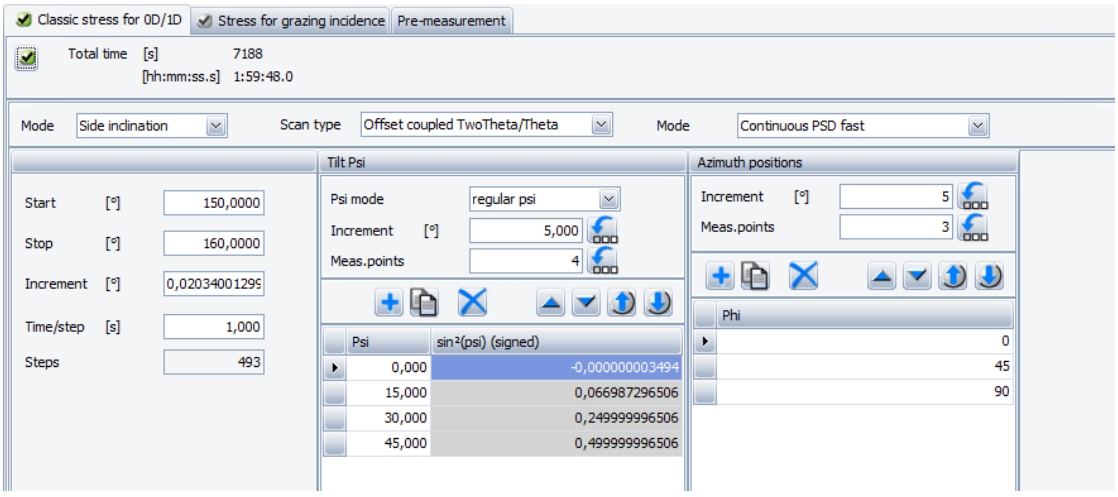
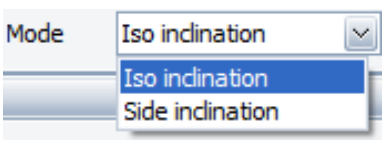


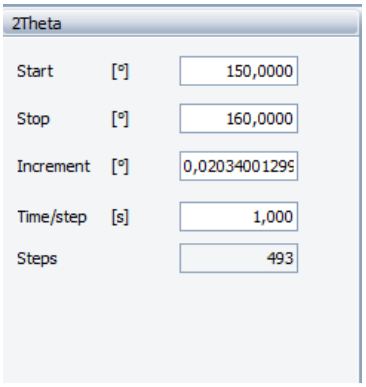
Figure 2.40: Classic Stress

1. In **Classic Stress** you have to choose between **Iso inclination** (also called **Omega mode**) and **Side inclination** (also called **Psi mode**):



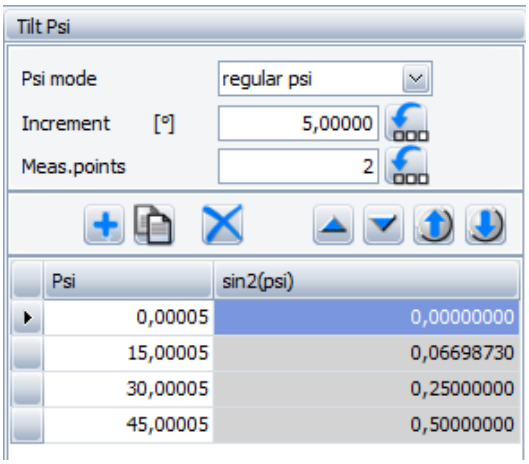
➨ The **Scan type** is fixed to an **Offset coupled TwoTheta/Theta scan**. The **Scan modes** available depend on the detector chosen. In our example a 1D detector was selected. Therefore, only a **Continuous PSD fast** scan is possible. 0D detectors may allow choosing between a **Step** and a **Continuous**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

2. 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:



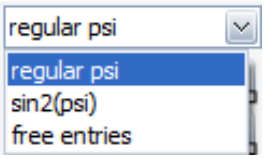
2.2.5.2.2.1 Tilt psi

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



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:



1. In the **regular psi** scheme, you enter **Psi** values in the left column, the **sin2(psi)** are calculated.
2. In the **sin2(psi)** scheme, you enter values between 0 and 1 in the right column and the **Psi** are calculated.
3. Using the scheme free entries, you can enter values in both columns.
4. Furthermore, using the **regular psi** and the **sin2(psi)** scheme, you can enter an increment or the number of measurement points. Then, press the button  :

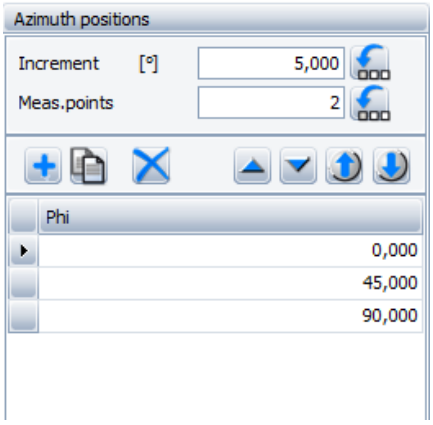
➨ this takes the first and the last **Psi** (or **sin2(psi)**) value from the table and calculates all others in this range.

5. 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

2.2.5.2.2.2 Azimuth Positions

1. Finally, enter the **Azimuth** (or **Phi**) **positions** in the right most panel:



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

2.2.5.2.2.3 Pre-measurement for Classic Stress

If you are not sure about the sample it is possible to carry out a pre-measurement.

1. To do so, mark the **Psi** and **Phi** entry you want to measure with a click on the row.
2. Then, change to the tab **Pre-measurement**:

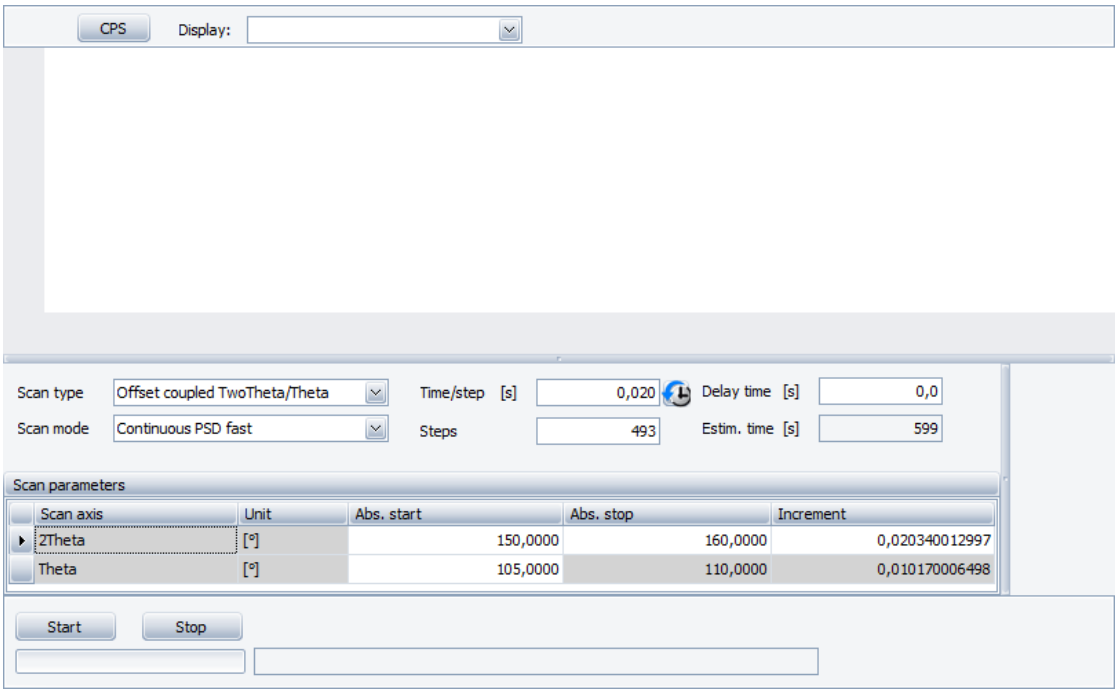
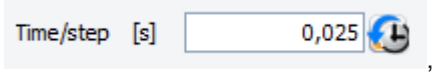
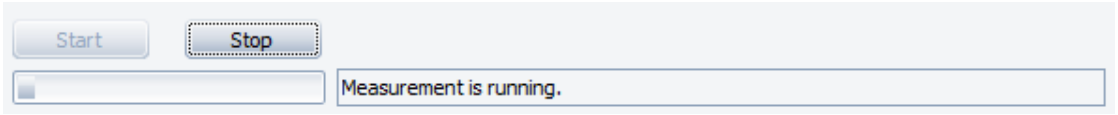


Figure 2.41: Stress pre-measurement

3. You may choose between different **Scan types** and change **Scan parameters.**
4. To get the fastest possible scan time press the **Clock** button at the right of the **Time/step** field 

, (it is calculated from the current scan axis increment, the scan mode and the fastest possible detector readout).
5. 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.

2.2.5.2.3 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.

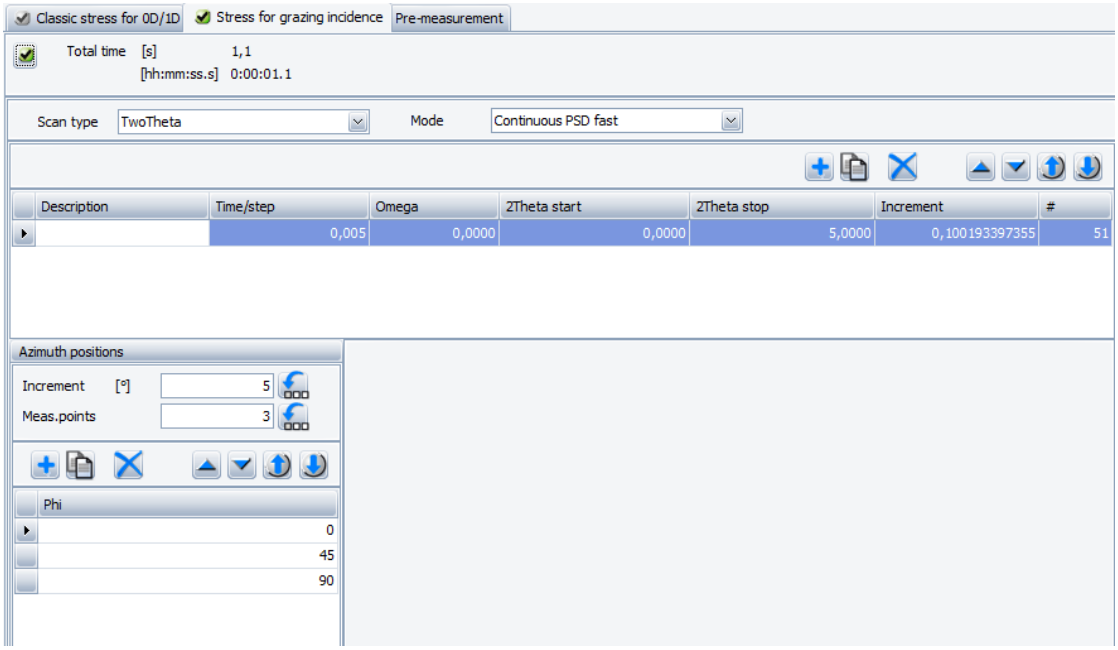
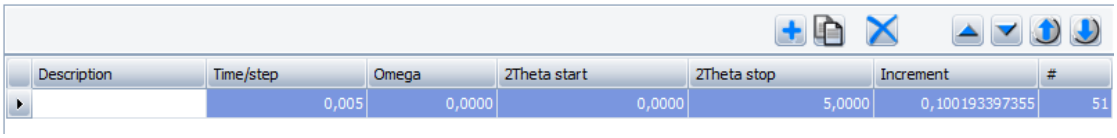


Figure 2.42: Stress for grazing incidence

2.2.5.2.3.1 Reflections

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



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

2.2.5.2.3.2 Azimuth positions

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

2.2.5.2.3.3 Pre-measurement for Grazing incidence Stress

If you are not sure about the sample it is possible to carry out a pre-measurement.

1. To do so, mark the **Phi** entry you want to measure with a click on the row.
2. 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.

2.2.5.2.4 Stress Measurement Setup: Stress 2D Side Mode

A **Stress setup for 2D detectors** is similar to the **Pole figure setup** used for **Texture**, see *Measurement setup: Reflection Texture 2D [▶ 90]*.

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.

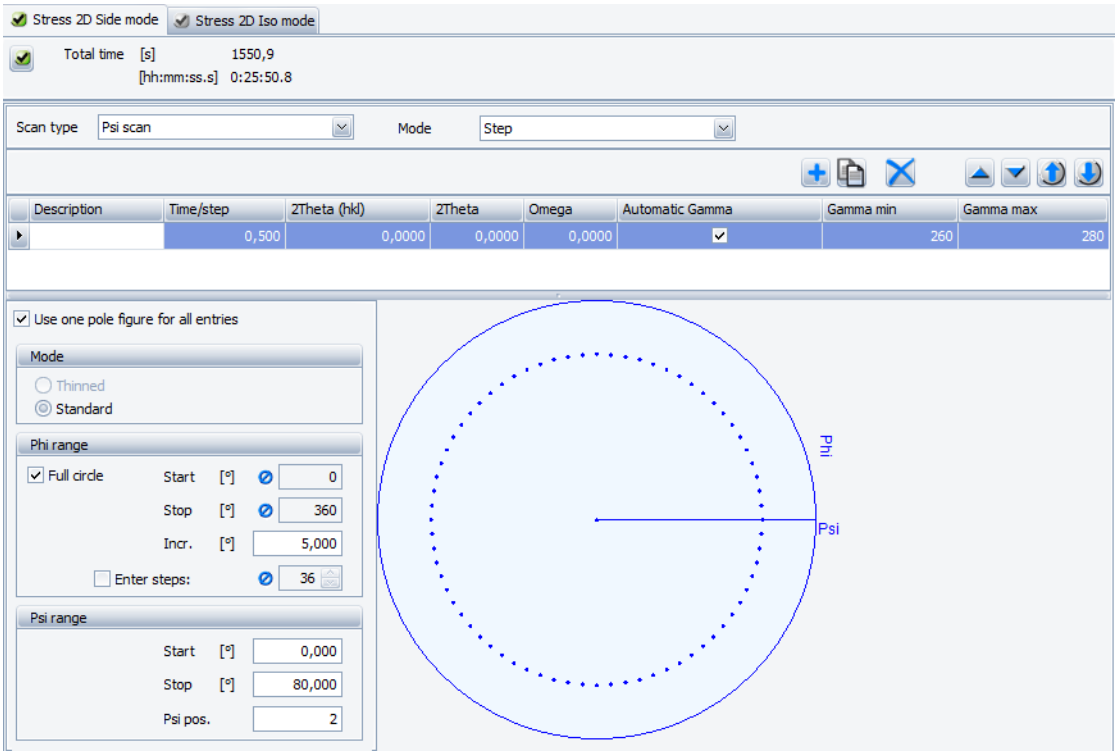


Figure 2.43: Stress 2D Side mode

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

2.2.5.2.4.1 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.

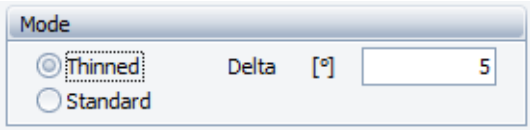
2.2.5.2.4.2 Reflections

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

Description	This can be any text.
Time/step	This is the time spent per orientation (please see the note below).
2Theta (hkl)	Theoretical 2Theta of the reflection. If modified, the value for Omega will be calculated to the half of 2Theta.
2Theta	2Theta where to position the detector center.
Omega	Enter an Omega value here if the half of 2Theta is not wanted.
Automatic Gamma	Check the box to use automatic Gamma calculation. If unchecked the Gamma min and max in the next columns are used. See the description in *2D Scheme Planning and the Pole Figure Display [▶ 79]*
Gamma min	Here, enter a value for the Gamma min.
Gamma max	Here, enter a value for the Gamma max.

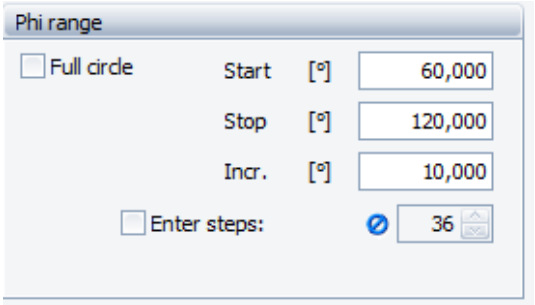
2.2.5.2.4.3 Pole Figure

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

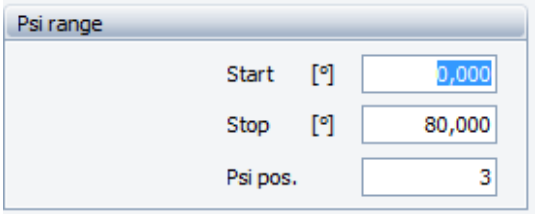


▶ It is possible to use either a full **Phi** circle or to define a **Phi** sector:

1. 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**:



2. The **Psi** range can be set with **Start**, **Stop** and the number of **Psi positions**:



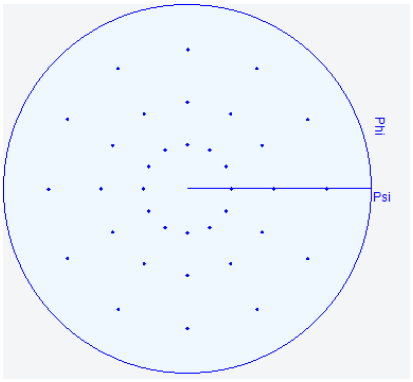
2.2.5.2.5 2D Scheme Planning and the Pole Figure Display

Note

While 2D scheme planning is described here for Stress 2D side mode it is available for all measurement setups using the pole figure display, e.g. Stress 2D Iso mode and Texture 2D.

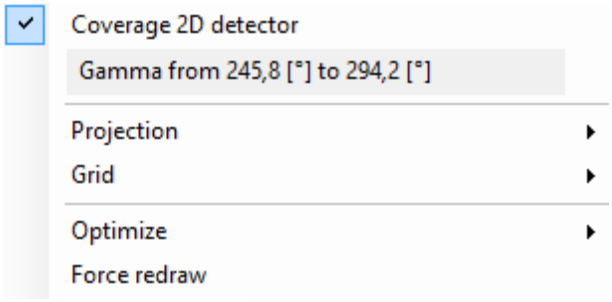
2.2.5.2.5.1 The Pole Figure Display and its Options

This display shows the coverage of the measurements in the Phi-Psi space. It is also the key access for the 2D scheme planning and other measurement optimizations. It provides several options in the context menu discussed next.

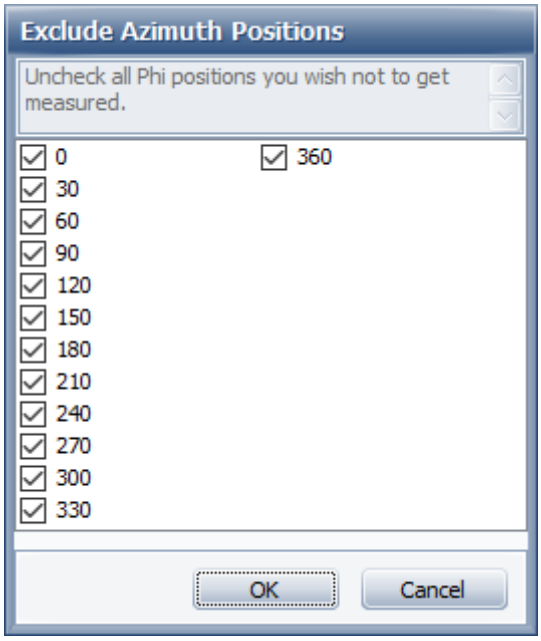


Pole Figure Display Context Menu

1. To open this menu use a click with the right mouse button while the mouse cursor stays over the pole figure.



Coverage 2D detector	Check to show the Gamma range at each position (either automatically calculated or manually entered).This is described in the section Scheme Planning below.
Gamma from .. to …	Shows the currently used Gamma min and max.
Projection	The projection may be chosen between **Stereographic, Orthographic** and **Equal area**.
Grid	Check whether to show a Phi grid (each 30°) or a Psi grid (each 10°).
Optimize	Different options are available here to exclude (Phi, Psi) points in the pole figure which may be redundant due to symmetry.
Select azimuth positions	A dialog opens to choose azimuth positions:

	
Measurement at Psi=0°	Choose whether to make a single measurement Phi=0° or to measure all azimuth values.
Force redraw	Click to force a redraw of the display

2.2.5.2.5.2 2D Scheme Planning

Introduction

Already in snap shot mode (still scan without any drive movements), 2D detectors provide a large angular coverage often covering several (hkl) reflections in one image. If a 0D or 1D detector is used a similar coverage has to be achieved with scans including drive movements.

The image attained with a 2D detector covers 2Theta and a certain Gamma range (Gamma denotes the angle around the axis of the diffraction cone) which depends on detector geometry, sample distance and the 2Theta. For details, please see *Bob B. He, Two-Dimensional X-Ray Diffraction, Wiley 2009*.

To optimize measurement time, one should avoid both “orientation gaps” (due to a too sparse Gamma coverage) and “orientation overlaps” (due to a too narrow Gamma range).

The WIZARD **Pole Figure Display** facilitates the measurement planning by displaying the covered **Psi/Phi** range of the detector. The corresponding Gamma range of the detector for a specified (hkl)-reflection can be obtained in three ways:

- Automatic calculation depending on detector geometry, sample distance and 2Theta(hkl)
- Manually entered values
- Transfer of values from a measurement carried out with COMMANDER.

All three options are described in the sections below.

Note on Gamma: all Gamma values shown (or entered) in the WIZARD are absolute values. We follow the convention in *Two-Dimensional X-Ray Diffraction* cited above, so the calibrated center of a 2D detector is at Gamma =270°. Here, one can also find the formulas used for the calculations.

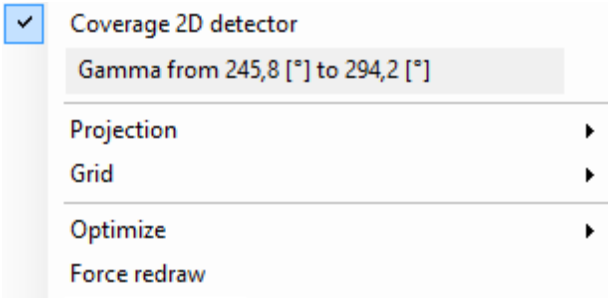
Automatic Gamma Calculation

The gamma range is calculated depending on the **2Theta (hkl)**, the **2Theta p**osition of the detector center, and *Omega* as entered in the table together with the detector sample distance and the detector geometry. The detector geometry takes into account

- a circular detector (like the VANTEC-500) which will diminish the possible gamma range when **2Theta (hkl)**, and the **2Theta center** position differ
- a rectangular detector (like the EIGER2) where a ROI (region of interest) can be defined and may be even asymmetrically opened in Gamma
- Geometric effects due to a flat detector surface and the sample distance

Note: It is assumed that only a part (sector) of the (hkl) reflection is visible, i.e. Gamma is determined by the detector geometry. For the calculation the maximum detector height is used.

To activate automatic Gamma calculation use the context menu of the pole figure display and check **Coverage 2D detector**:



The **Gamma min** and **max** get immediately calculated using the 2Theta (hkl), 2Theta and Omega specified in the table. The values are shown in the next line of the tooltip. The covered **Phi/Psi range** is drawn for each position in the pole figure:

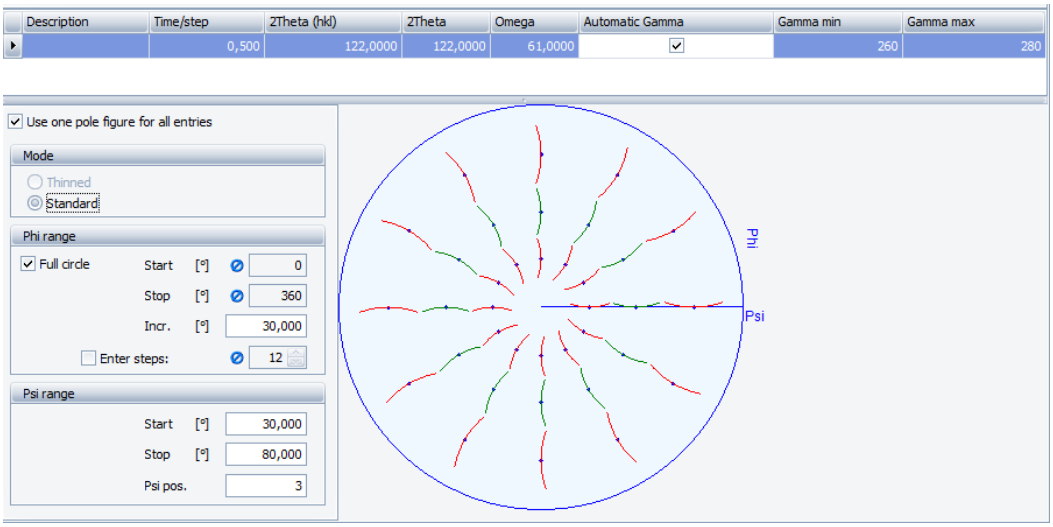
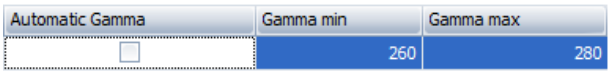


Figure 2.44: 2D Scheme planning

In the example shown, a symmetrically opened detector is used (VANTEC-500). In case of an EIGER2 detector the ROI may be chosen to be asymmetric and **Gamma min** and **max** will be asymmetric, too.

Manual Gamma Values

To enter **Gamma** values manually (for instance determined using another program like DIFFRAC.EVA, DIFFRAC.TEXTURE or DIFFRAC.LEPTOS) the check box in the table must be unchecked:



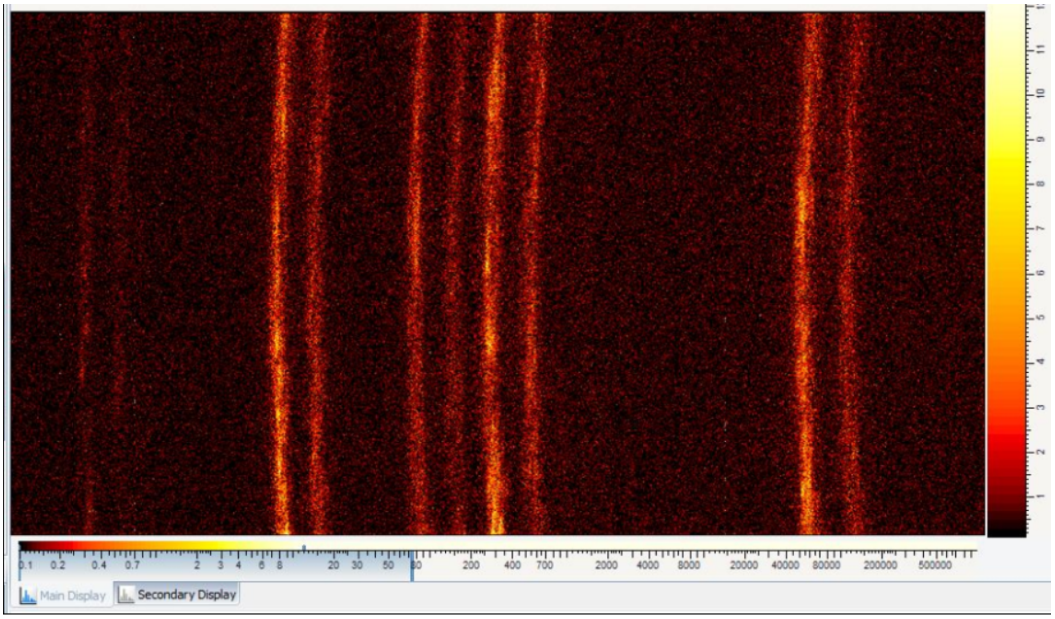
The **Gamma** values entered must be determined from other programs using measurements under identical conditions regarding detector sample distance and 2Theta range.

Using the COMMANDER to Determine Gamma

To use this option, a still scan in COMMANDER at the wished 2Theta position is needed.

COMMANDER plugin

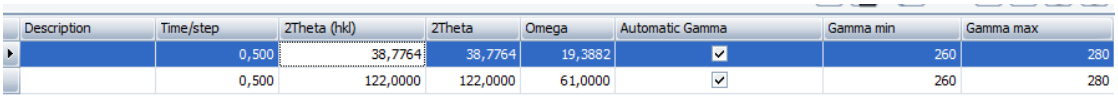
To use this option, make a still scan in COMMANDER:



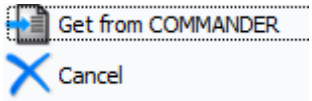
1. Move the mouse cursor to the position whished in the image taken and use the context menu (right mouse button).
   - ➨ It provides **Transmit to WIZARD → Gamma minimum value or Gamma maximum value or 2Theta (hkl)**.
2. Move the mouse cursor in the image taken accordingly to determine all values whished and choose the corresponding **Transmit to WIZARD** operation.

WIZARD plugin

1. Switch to the WIZARD plugin:
2. If you wish to set **2Theta (hkl)**: move the mouse cursor over the cell you want to change



3. and use context menu:



4. Select **Get from COMMANDER** and the **2Theta (hkl)** value will be copied.
5. Repeat this (if wished) for **Gamma min** and **Gamma max**.

Note: it is not necessary to transmit all three values. For instance, one may transmit only **Gamma min** or **Gamma max**. In the case you press **Get from COMMANDER** for a value not yet transmitted an error is shown in the status bar.

2.2.5.2.6 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.

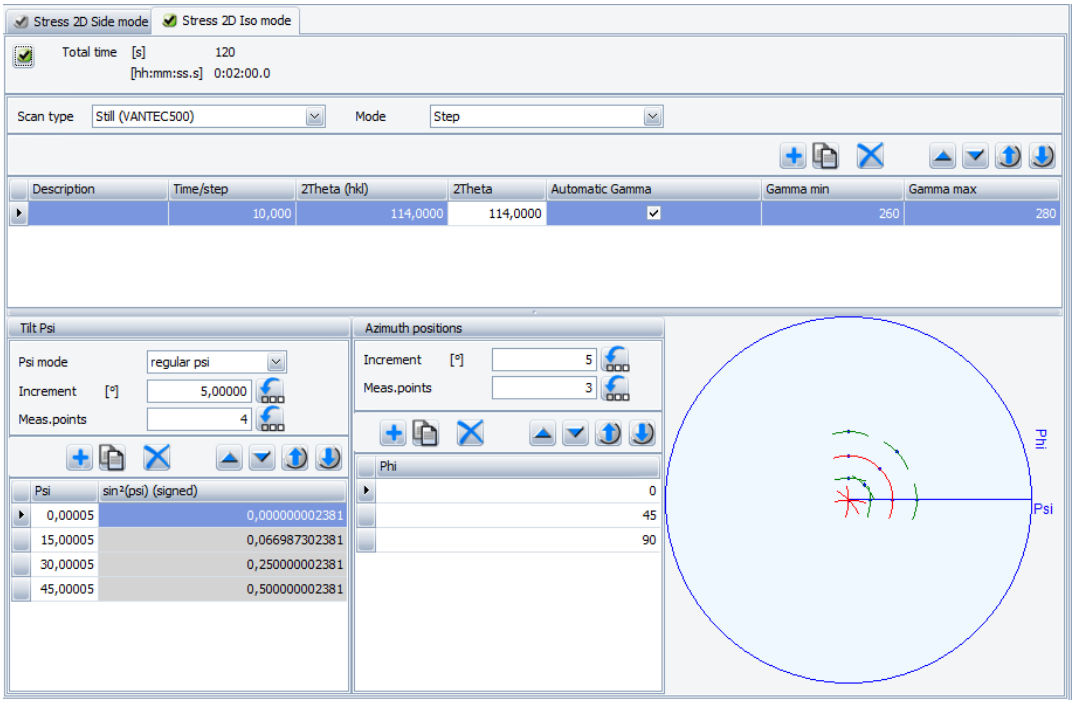


Figure 2.45: Stress 2D Iso mode (with Coverage 2D Detector enabled)

2.2.5.2.6.1 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, **2Theta (hkl)**. The use of **Gamma i**s described above, see *2D Scheme Planning and the Pole Figure Display [▶ 79]*.

2.2.5.2.6.2 Tilt Psi

The **Psi** table is described in *Stress Measurement Setup: Classic Stress for 0D/1D [▶ 72]*.

For each Psi in the table, omega is calculated from: **Omega = 2Thetahkl / 2 + Psi**.

Note that Psi must follow the condition: **|Psi| > 2Thetahkl / 2**.

2.2.5.2.6.3 Azimuth Positions

Finally, enter the azimuth (or Phi) positions in the right most panel as described in *Stress Measurement Setup: Classic Stress for 0D/1D [▶ 72]*.

2.2.5.2.6.4 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 [▶ 41]*.

2.2.5.3 XY Positions Module

For this module, see the description in section *Profiles [▶ 20]*.

2.2.6 TEXTURE

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

Figure 2.46: 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.

2.2.6.1 DAVINCI Module

For this module, see the description in *DAVINCI [▶ 14]*.

2.2.6.2 TEXTURE BASIC Module

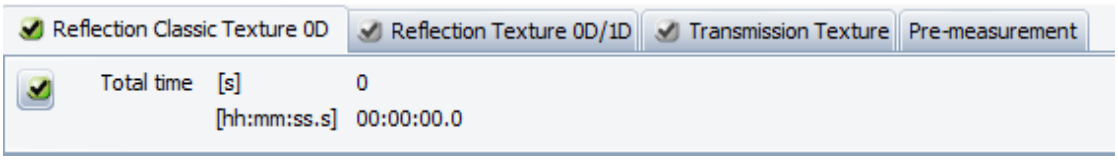
The basic module has two module items. The first item defines the **Pole figure** and the schemes. The second item **Drives** is used to modify the settings for all drives independent on the texture measurement itself.

2.2.6.2.1 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.

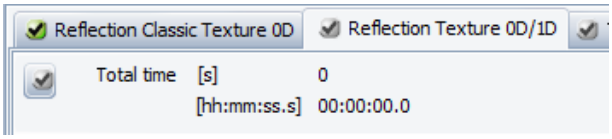
Note

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.

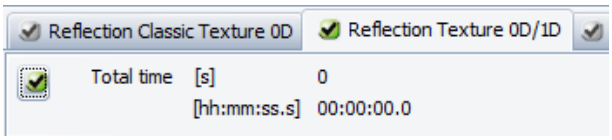
2.2.6.2.1.1 Example: Activate a Measurement Setup

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

1. 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.



2.2.6.2.1.2 Overview: Available Measurement Setups in Texture

Table 2.3: Available measurement setups in Texture

Chosen detector	Texture measurement setup	Possible scan type(s)	Remarks
0D detector or 1D detector/ Pilatus in 0D 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
1D 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°
2D detector	Reflection Texture 2D	Phi scan	

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.

2.2.6.2.2 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:

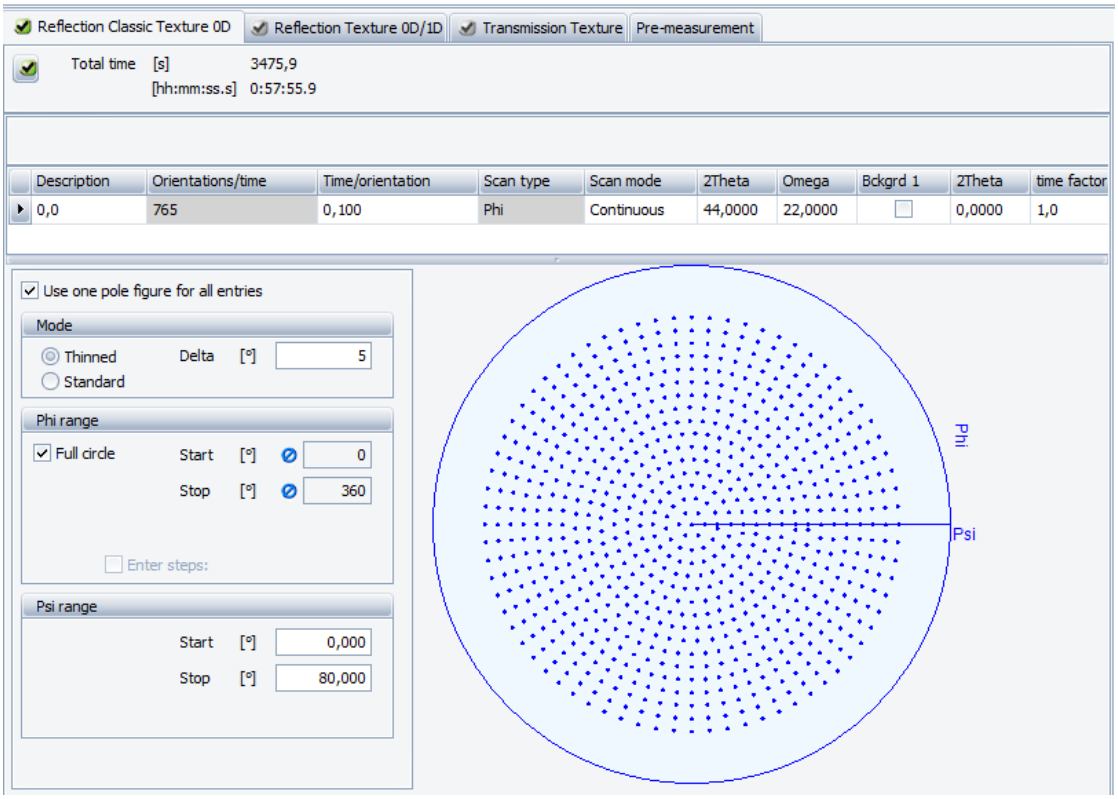


Figure 2.47: Classic Texture 0D

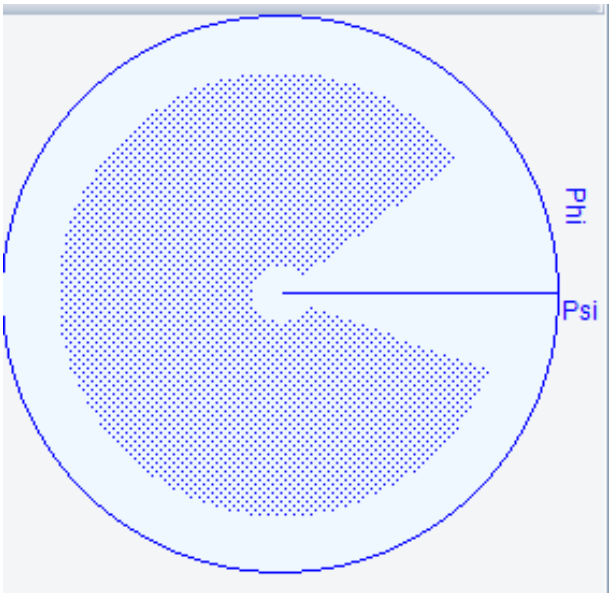
Note

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

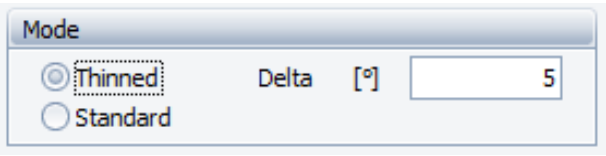
Note

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:



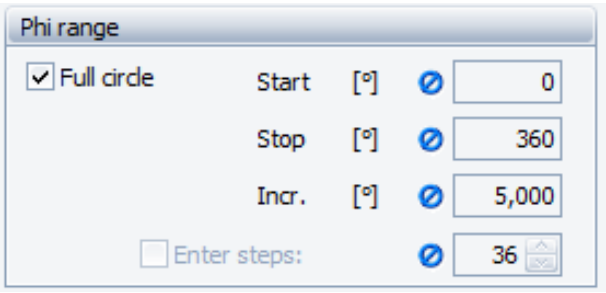
The coverage of the **Phi-Psi** space can be defined in various ways:



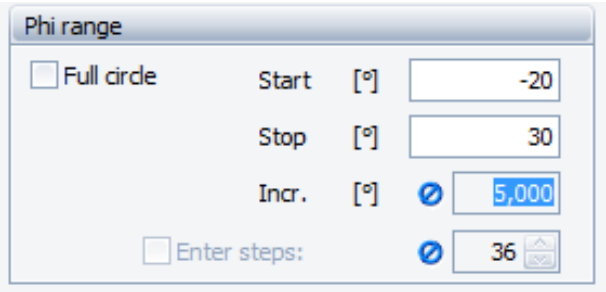
Thinned mode: the orientations are equally distributed, as shown in the figure above.

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

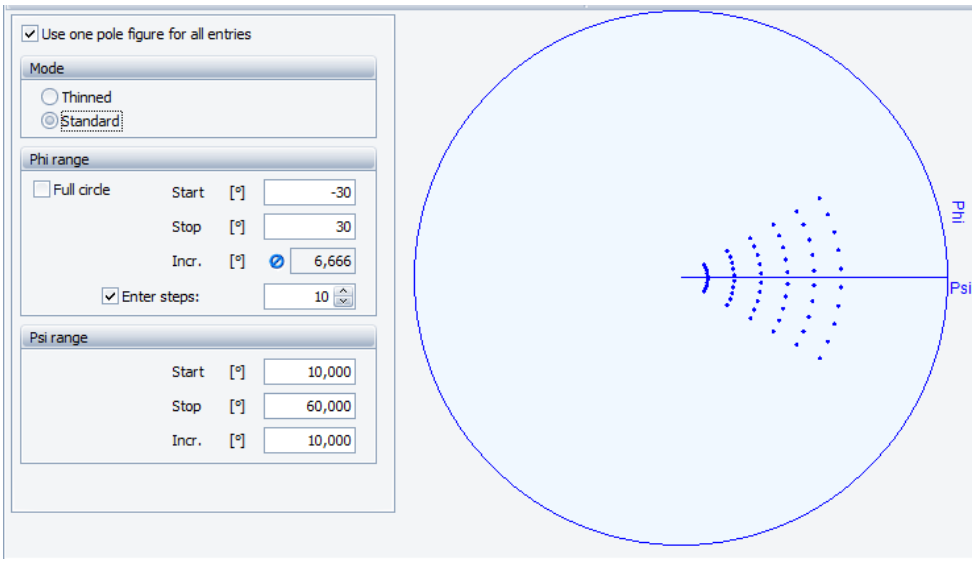


or may define a sector only by un-checking the **Full circle** check box.



Furthermore, Psi can be restricted.

The example shows a **Phi sector** in standard mode:



2.2.6.2.2.1 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.

2.2.6.2.3 Measurement Setup: Reflection Classic Texture 0D

This measurement setup is only available if either a 0D detector is configured and selected in the DAVINCI. A 0D detector can be a scintillation counter or solid state detector. 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.

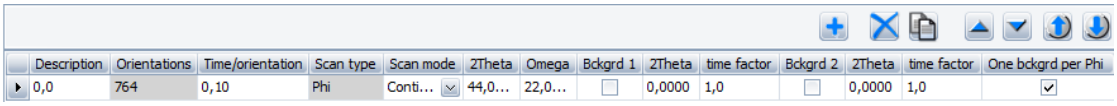


Table Entries in Reflection Classic Texture 0D

Description	This can be any text.
Orientations	The number of orientations as calculated from the pole figure
Time/orientation	This is the time spent per orientation (please see the note below).
Scan type	In the classic setup this is fixed to a Phi scan.
2Theta	Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
Omega	Enter an Omega value here if the half of 2Theta is not wanted.
Background 1 or 2:	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.
One background per Phi	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

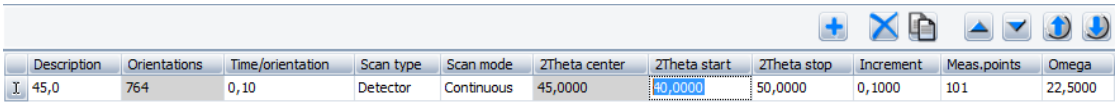
The toolbar at the top of the table can be used to modify the number of schemes:

	
	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

2.2.6.2.4 Measurement Setup: Reflection Texture 0D/1D

This measurement setup is only available if either a 0D detector or a PSD in 1D 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 in *TEXTURE Measurement Setups [▶ 84]*.



Description	Orientations	Time/orientation	Scan type	Scan mode	2Theta center	2Theta start	2Theta stop	Increment	Meas.points	Omega
45,0	764	0,10	Detector	Continuous	45,0000	43,0000	50,0000	0,1000	101	22,5000

Table entries in Reflection Texture 0D/1D

Description	This can be any text.
Orientations	The number of orientations as calculated from the pole figure
Time/orientation	This is the time spent per orientation (please see the note below).
Scan type	Depending on the detector chosen, different scan types can be chosen, see overview in *TEXTURE [▶ 84]*.
Scan mode	Depending on the detector and scan type different modes are allowed

2Theta center	Read only for moving scans (detector scan, offset coupled TwoTheta/Theta). For still scans (PSD fixed or ThetaF) enter the 2Theta value here.
2Theta start	Read only for still scans. Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
2Theta stop	Read only for still scans. Enter a 2Theta value here. If modified, the value for Omega will be calculated to the half of 2Theta.
Increment	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.
Meas.points	For still scans this is fixed. For moved scans it can be entered instead of the increment which is then recalculated.
Omega	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.

2.2.6.2.5 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:

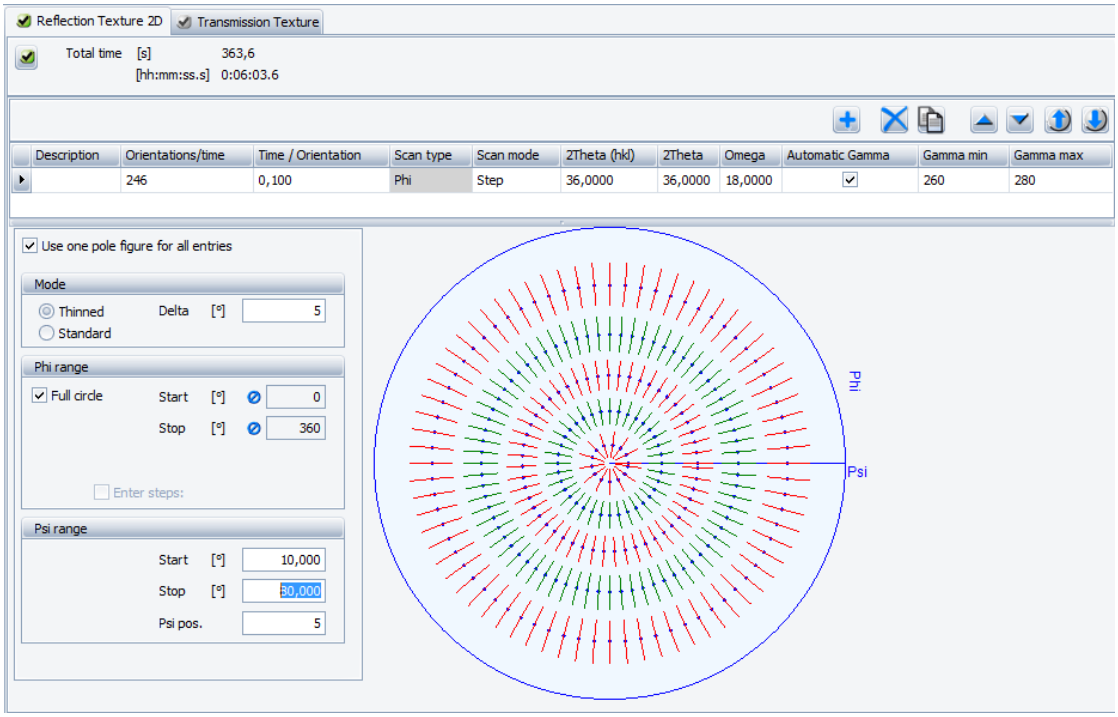


Figure 2.48: Texture 2D setup

Table Entries in Reflection Texture 2D

Description	This can be any text.
Orientations	The number of orientations as calculated from the pole figure
Time/orientation	This is the time spent per orientation (please see the note below).
Scan type	This is fixed to a Phi scan.
Scan mode	Step or continuous run can be chosen
2Theta (hkl)	Theoretical 2Theta of the reflection. If modified, the value for Omega will be calculated to the half of 2Theta.
2Theta	2Theta where to position the detector center.
Omega	This is automatically calculated from the 2Theta. Enter an Omega value here if the half of 2Theta is not wanted.
Automatic Gamma	Check the box to use automatic Gamma calculation. If unchecked the Gamma min and max in the next columns are used. See the description in *2D Scheme Planning and the Pole Figure Display [▶ 79]*.
Gamma min	Here, enter a value for the Gamma min.
Gamma max	Here, enter a value for the Gamma max.

2.2.6.2.6 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 [▶ 41]*

2.2.6.3 XY Positions Module

For this module, see the description in *Profiles [▶ 20]*.

2.2.7 TXRF

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

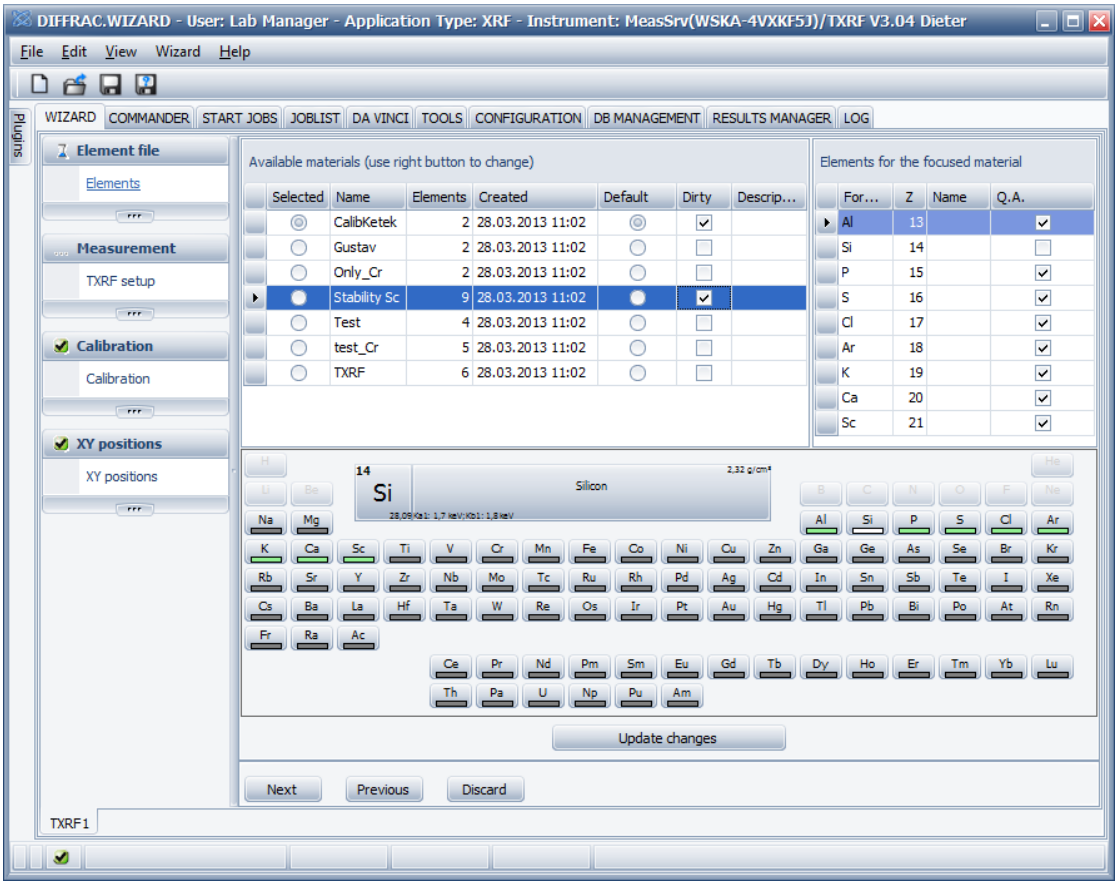


Figure 2.49: TXRF setup

2.2.7.1 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):

- If you load an experiment containing a material that does not exists, 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).
- 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).

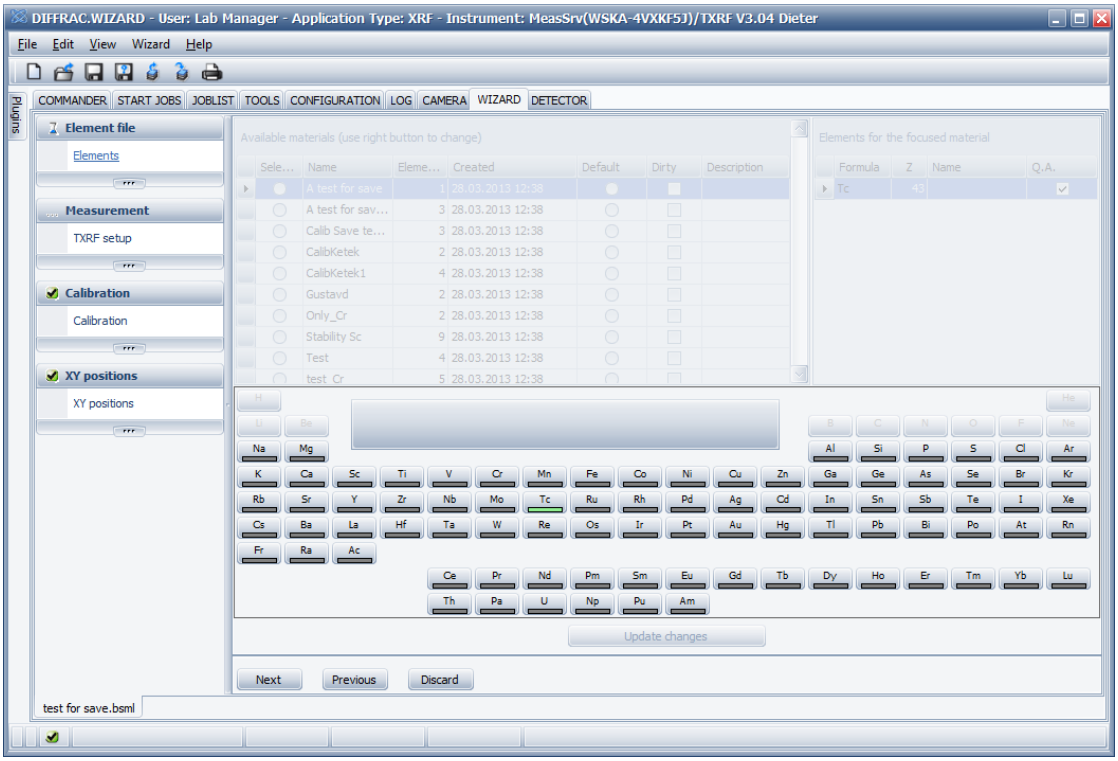


Figure 2.50: Element file dialog if material is different from the one in the database

2.2.7.2 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.

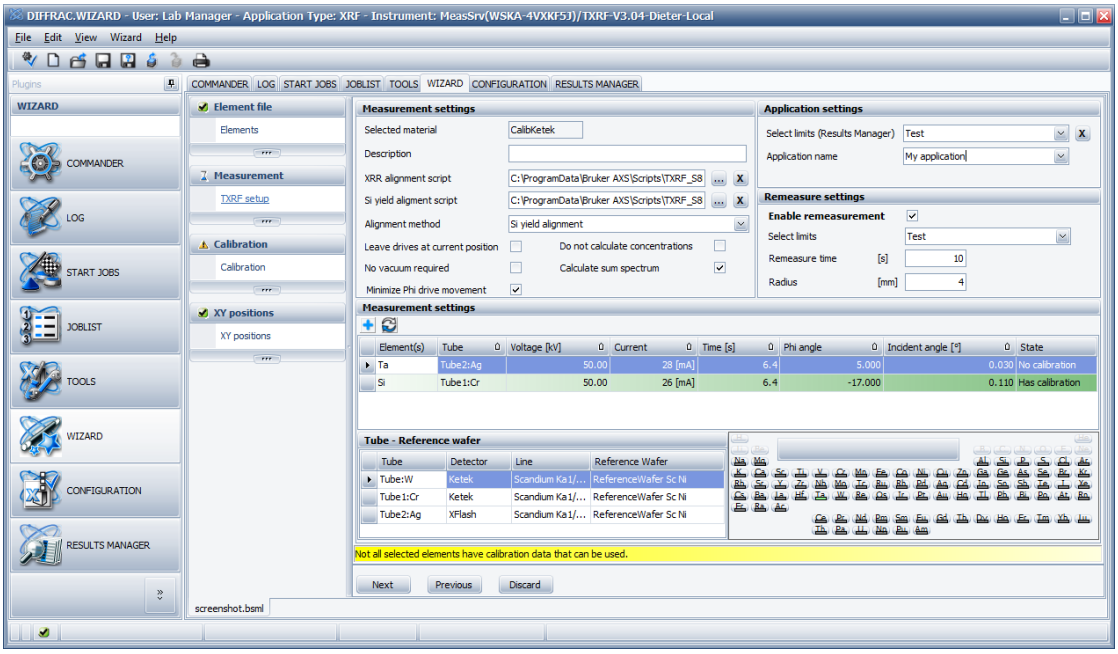


Figure 2.51: TXRF Setup dialog

2.2.7.2.1 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. The 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	Calculate sum spectra
Calculate sum spectraMinimize 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 in the center.

2.2.7.2.2 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.

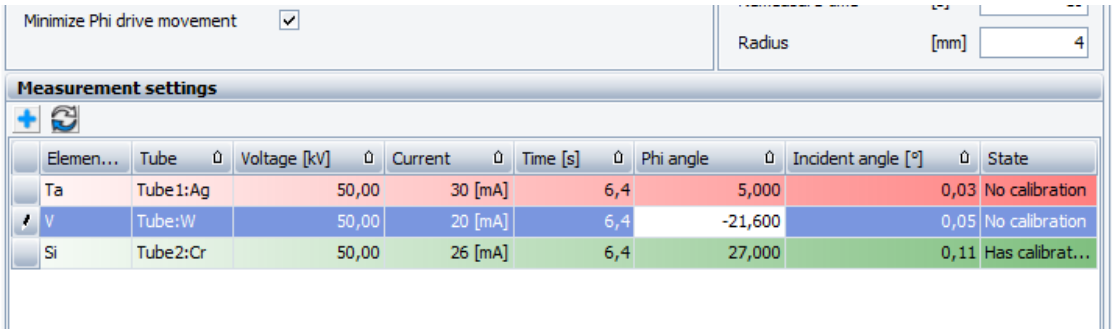


Figure 2.52: TXRF measurement settings

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 angl**e and **Incident angle**. If you change any of these values, an existing calibration cannot be used anymore.

2.2.7.2.3 Tube – Reference Wafer

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

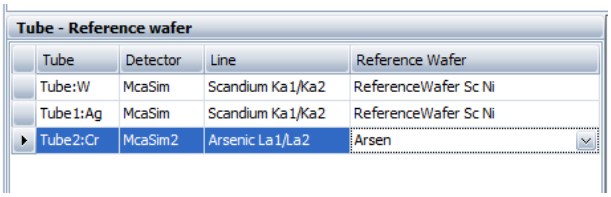


Figure 2.53: Tube - Reference wafer settings

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.

2.2.7.2.4 Application Settings

Measurements are grouped in the RESULTS 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 RESULTS MANAGER) which allows coloring results by warning and error limits (not yet implemented).

2.2.7.2.5 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.

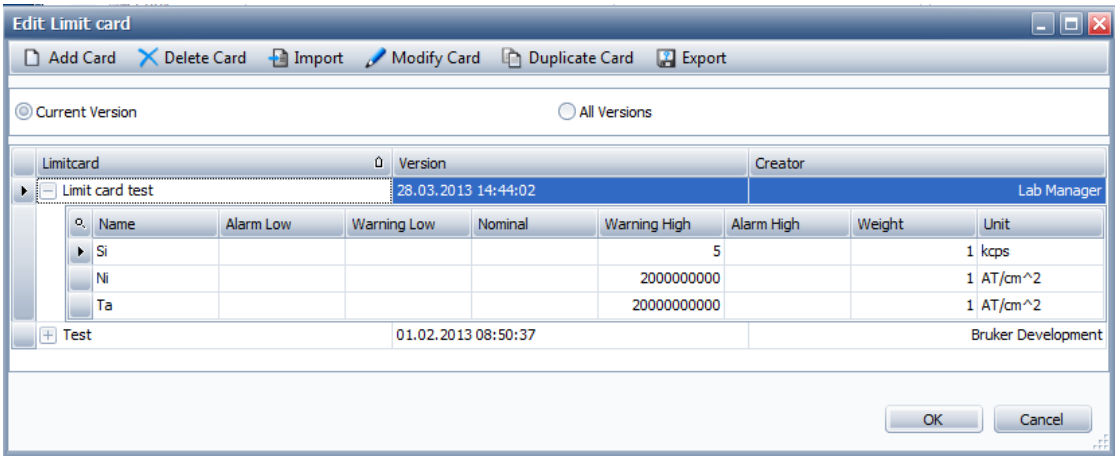


Figure 2.54: Limit card settings

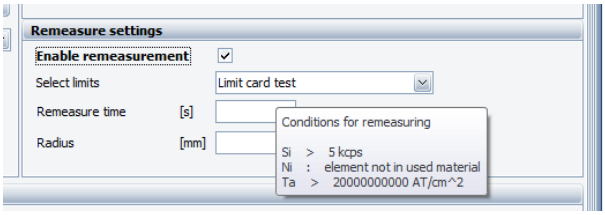


Figure 2.55: Remeasure settings

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.

2.2.7.3 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.

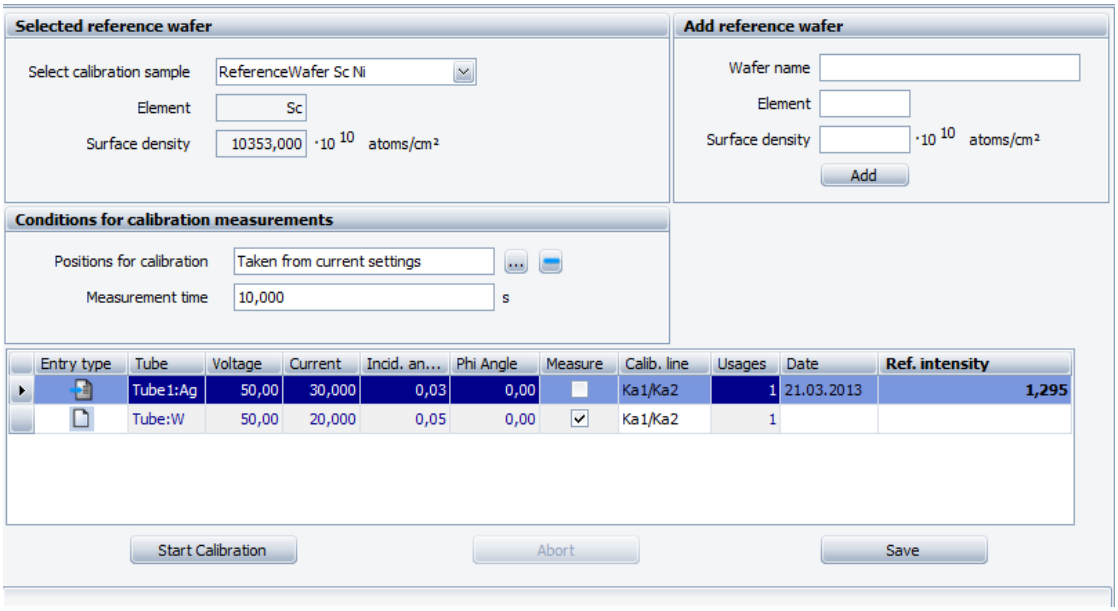


Figure 2.56: Calibration settings

- 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.

3 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).

3.1 Calibration

Table 3.1: Technical scan types

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	

3.2 XRD

Table 3.2: Scan types in XRD

Scan type	Detectors	Scan modes	Remarks
For 0D			
Coupled TwoTheta/Theta	0D detectors or 0D mode of 1D detectors, PILATUS or EIGER	Continuous Step	
	1D detector at 0°	Continuous PSD fast	
	LYNXEYE in 2D mode at 90°	Continuous Step	
Offset coupled TwoTheta/ Theta	0D detectors or 0D mode of 1D detectors, PILATUS or EIGER	Continuous Step	
	1D detector at 0°	Continuous PSD fast	
	LYNXEYE in 2D mode at 90°	Continuous Step	
Rocking	0D detectors or 0D mode of 1D detectors, PILATUS or EIGER	Continuous Step	

Scan type	Detectors	Scan modes	Remarks
Theta	0D detectors or 0D mode of 1D detectors, PILATUS or EIGER	Continuous Step	Theta/Theta goniometer only. Available in COMMANDER only.
TwoTheta	0D detectors or 0D mode of 1D detectors, PILATUS or EIGER	Continuous Step	
	1D detector at 0°	Continuous PSD fast	
	LYNXEYE in 2D mode at 90°	Continuous Step	
For 1D			
Coupled TwoTheta/Theta	EIGER in 2D mode	Continuous Continuous NOUT Continuous VDO 1	
Offset coupled TwoTheta/ Theta		Continuous Continuous NOUT Continuous VDO 1	
Rocking		Continuous Continuous NOUT Continuous VDO 1	
TwoTheta			
Coupled TwoTheta/Theta (VDO) 1, 4	LYNXEYE XE / XE-T 4	Continuous PSD fast, Continuous PSD fast (no overtravel) 3,4,	Scans with variable detector opening (VDO). 1, 4
Offset coupled TwoTheta/ Theta (VDO) 1, 4			
TwoTheta (VDO) 1, 4			
PSD fixed	For 1D detectors	Still	
Still scans	For every detector	Still	
For 2D			
Coupled TwoTheta/Theta	PHOTON	Continuous Continuous Run (Single Frame)	
Offset Coupled TwoTheta/ Theta		Continuous Continuous Run (Single Frame)	
Rocking		Continuous Continuous Run (Single Frame)	
Still		Step (SSD)	
Coupled TwoTheta/Theta	PILATUS	Step	
TwoTheta		Step	

Scan type	Detectors	Scan modes	Remarks
Offset Coupled TwoTheta/ Theta		Step	
Rocking		Step Continuous Run Continuous (exact)	
Still		Step	
Coupled TwoTheta/Theta	VÅNTEC	Step Step (with Count Limit) Cont. Run Continuous (Exact)	
Offset Coupled TwoTheta/ Theta		Step Step (with Count Limit) Cont. Run Continuous (Exact)	
Rocking		Step Step (with Count Limit) Cont. Run Continuous (Exact)	
Still		Step Step (with Count Limit)	
Coupled TwoTheta/Theta	EIGER	Step Continuous Continuous NOUT Continuous VDO 1	
Offset Coupled TwoTheta/ Theta		Step Continuous Continuous NOUT Continuous VDO 1	
Rocking		Step Continuous Continuous NOUT Continuous VDO 1	
TwoTheta		Step Continuous Continuous NOUT Continuous VDO 1	
Still		Step	

Notes:

1	VDO	Variable Detector Opening: For a TwoTheta/Theta scan or a TwoTheta scan the opening of the LYNXEYE XE or XE-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 XE-T hardware sold.

3.3 High resolution XRD

Table 3.3: Scan types in HRXRD

Scan type	Detectors	Scan modes	Remarks
2Theta-Omega	0D detectors or PILATUS / 1D detector in 0D mode	Continuous Step	
	1D detector at 0°	Continuous PSD fast	
Omega-2Theta	0D detectors or PILATUS / 1D detector in 0D mode	Continuous Step	
	1D detector at 0°	Continuous PSD fast rapidRSM 1	
Rocking curve	0D detectors or PILATUS / 1D detector in 0D mode	Continuous Step	
	1D detector at 0°	rapidRSM 1	
TwoTheta	0D detectors or PILATUS /1D detector in 0D mode	Continuous Step	
	1D detector at 0°	Continuous rapidRSM 1	
Reciprocal space	0D detectors or PILATUS / 1D detector in 0D mode	Step	
PSD fixed	For PSDs only	Still	
2Theta-Omega	EIGER 1D	Continuous	
Omega-2Theta		Continuous	
2Theta		Continuous	
Still		Still	
2Theta-Omega	EIGER 2D mode, VANTEC-500	Step	
Omega-2Theta			
2Theta			
Still			
Single axis scans for specific axes	0D detectors or 1D detector in 0D mode or 2D detector	Step	

Notes:

1	rapidRSM	rapidRSM is a special mode for LYNXEYE and VANTEC-1 to execute an almost delay-free reciprocal space map measurement which would be otherwise defined as a sequence.

3.4 Alu Bath

Note: The advanced application type is defined in WIZARD only. These scan types are described *Alu Bath [▶ 69]*

3.5 SAXS

Note: The advanced application type is defined in WIZARD only. These scan types are described in *SAXS [▶ 43]*.

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

Table 3.4: Scan types in COMMANDER for SAXS

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

3.6 SCXRD

Table 3.5: Scan types in COMMANDER for SCXRD

Scan type	Detectors	Scan modes	Remarks
Omega	Photon	Continuous (exact) Continuous Run (single Frame)	
Phi-Psi	Photon	Continuous (exact) Continuous Run (single Frame)	
Omega	VÅNTEC-500	Cont. Run	
Still	VÅNTEC-500	Step Step (with Count Limit)	
Theta-Phi	VÅNTEC-500	Cont. Run	
Phi-Psi	VÅNTEC-500	Cont. Run (single frame)	

3.7 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 [▶ 70]*.

3.8 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 [▶ 84]*.

3.9 XRF

Table 3.6: Scan types in COMMANDER for 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	

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