SENTECH

SpectraRay/4

Software Manual

SpectraRay/4

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SPECTRARAY Software Manual

Covers also the SE 400adv Simulation Software

The Advanced SpectraRay software is a powerful software package designed for simulating, fitting and measuring data of spectroscopic ellipsometers (UV, NIR, and IR), single wavelength ellipsometers and for processing data of reflection and transmission measurements.

Note: A subset of SpectraRay is used for the laser ellipsometer SE 400adv as the package called “Simulation” software. In the text any section related to limits or specific functions of this package uses the term “SE 400adv Simulation” to mark specific content.

Further recommended literature:

R. M. A. Azzam, N. M. Bashara
“Ellipsometry and polarized light”
North Holland New York 1989
ISBN 0 444 870164

A. Röseler
“Infrared Spectroscopic Ellipsometry”
Akademie Verlag Berlin 1990
ISBN 3-05-500623-2

Content

1 SpectraRay Upgrade Information

The software for operating spectroscopic ellipsometers built by SENTECH Instruments is SpectraRay. The software is on the market for nearly 25 years. For many years the features for measuring spectra and modeling were the main features of a software package for optical metrology. Within the past years the situation changed significantly. Some years ago spectroscopic ellipsometers were used mainly in research by scientists who need to control and understand the ellipsometry as a method to the detail. While ellipsometry has been grown to a well-known and accepted method, the typical users can be now operators and engineers in production lines as well as researchers in universities. Now we have two typical user groups.

The first group mainly uses an ellipsometer to repeat measurements with a minimum of effort. These operators only use an ellipsometer as a "tool" without the time to dive into method. For them "time is money" and they need only a "measurement" button and want the software to hide the complexity of ellipsometry and run everything automatically until the final results are displayed. There are usually several operators only putting samples onto the machine and pressing "measure" and a few engineers trained to do limited diagnostics and for setting up the recipes. For this group of users, the execution is in the foreground and changes to recipes are not in the foreground. SENTECH Instruments designed a recipe module as one of the core features of SpectraRay.

While many applications of ellipsometry can be run in recipe mode, there is the second group of users in research which study and develop the new materials. Since researchers need to dive into every detail of the method, they seldom want the software just to run a recipe. Since the properties of material and layer stack are often unknown, they need a step by step method from measurement via modeling to fitting and reporting. SpectraRay/4 assists this mode of operation much better than previous versions by a workflow oriented software interface. The new mayor release introduces this workflow guide and offers a whole bunch of functions to the user in every step. The new design offers the tools needed in each step in a user friendly manner and hides tools needed in later steps of operation. Typical researchers iterate between measurements, modeling and fitting until material descriptions are found by applying standard dielectric functions and methods to put materials onto each other to form a layer stack describing their samples. Advanced modeling requires often understanding the physics behind the software and method.

The SpectraRay/4 software addresses the operators, engineers and the researches as well. It includes both the recipe module and the SE-Advanced module for workflow oriented mode of operation. For SpectraRay/4 a new insitu mode was developed for handling time dependent measurements.

For experienced users of SpectraRay the following gives an overview of the changes introduced by this upgrade. There are numerous changes beside these main features and careful reading the manual is strongly recommended to discover the full power of the new version.

- **New integrated insitu module:** The capability to setup and run time dependent measurements using spectroscopic ellipsometry is now an integral part of SpectraRay.
- **Faster operation:** For the time dependent measurements also the measurement time was reduced.
- **Updated anisotropy module:** The anisotropy option allows the measurement of anisotropic samples.
- **Easier file access:** An explorer style tree view now offers experiments as well as material, model and data files. The Drag and drop supported is further extended. So you can simply drag a material or data out of an experiment file of the windows explorer and drop it in the software. This supersedes the old material and data lists within main screen.
- **Full backward compatibility for files**: You may load any old experiment, model, material or data file. Saving into old file versions is supported allowing cross version operation.

SpectraRay/4 is delivered either as full package or as a light version. The following tables explain the differences and options.

2 Installation manual

2.1 Software setup

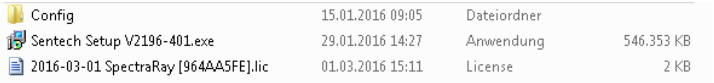
SpectraRay is shipped on a flash memory which serves as installation medium and hardware dongle for licensing purpose. When you receive your SpectraRay package you should receive a flash memory as shown below. For the flash memory an USB port of your computer is used. You must have a free USB port which can be used for the installation and while SpectraRay is running.

Fig. 2-1 SpectraRay flash memory

The flash memory has a serial number on the backside, which is required for any service call regarding your software.

Fig. 2-2 Serial number on flash memory

The software setup is located on the flash memory. If you open the sticks root folder with the explorer you should see the following files and folders:



The setup can be started by simply running the executable “SpectraRay Setup Vyyy-xxx.exe” (where yyy is a version number and xxx is an installation number). There is also a license file (*.lic) which must be available while the software is running and must be on the shipped flash memory. Do not lose the stick and do not delete the license file.

There is a folder “Config” on the stick which contains at least the file “install.config.xml” describing the functions to be installed. Do not delete or change this file because it is related to your measurement tool hardware. Within “Config” there may be also other files related to your specific hardware (calibration data, customer spe-

cific changes, recipe files,…). Do not change these files, never copy the setup alone and install the software always by running the setup from the stick.

Now let us walk through the installation process. After you start the setup, the startup screen appears.

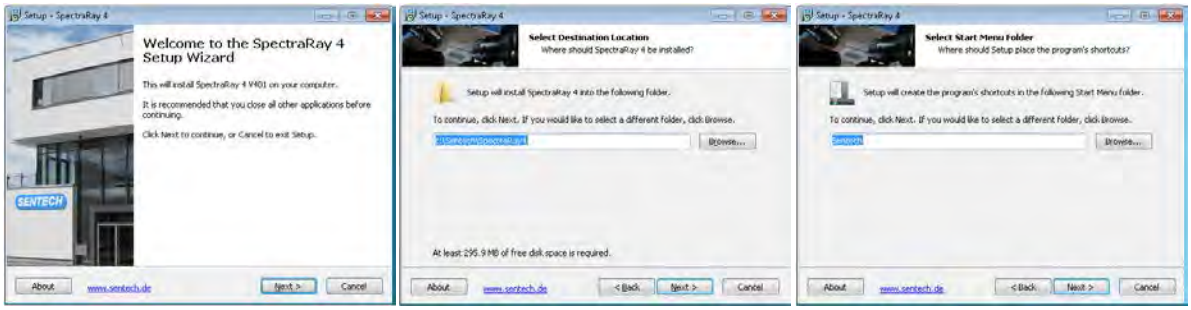


Fig. 2-3 Installation setup

You have to click on next to proceed to the selection of the destination folder and of the startup menu folder. It is strongly recommended to install SpectraRay always into the folder “C:\SENTECH\SpectraRay4”[1].

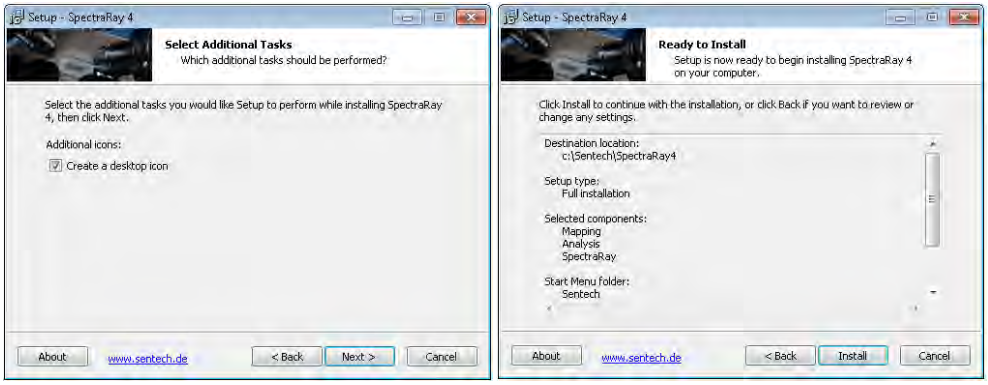


Fig. 2-4 Installation setup

If you go ahead you have a selection for the desktop icon and the quick launch icon. While the desktop icon is available on all operating systems, the quick launch icon is not available on Windows 7[2].

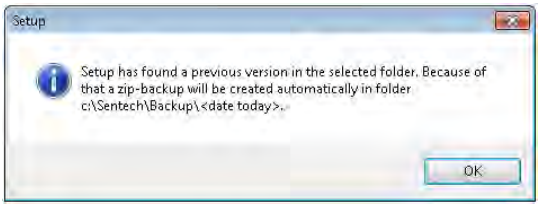


Fig. 2-5-2-6 Message box

[1] Newer operating systems as Windows 7 or Windows Vista limit the write access in folfers liken “c:\Program Files”. This is related to the so called User Account Control (UAC). SpectraRay needs the write access for configuration files and storage of user data. This simplifies having a complete backup by simply copying this folder. If SpectraRay would follow the Windows scheme, the program data and data for each individual user would be spread across multiple folders making change management difficult. Therefore it is strongly recommended to install the software to the folder "c:\SENTECH\SpectraRay4".

[2] The quick launch bar is hidden in Windows 7 and you will not see the added icon until you tweak Windows 7 to show the bar. There are instructions available on the internet, which help to re-enable the quick launch bar.

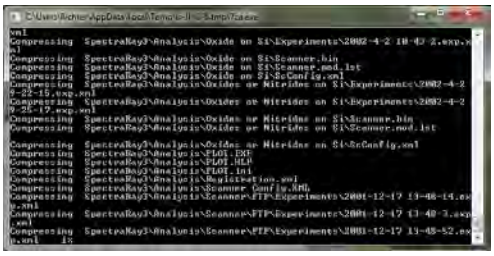


Fig. 2-7 Command window during installation

When you click on “Install” the setup starts copying files. The first check is, whether there is a SpectraRay4-Software already installed in the target folder. In such case you get the message shown above and a backup of the files prior to the installation is created. You should wait until this is finished: Do not try to close the command window shown above, it creates your backup. Depending on your operating system and hardware there may run several child setups (as .NET on Win XP SP2). Finally you get the SpectraRay4 icon on the desktop.

Fig. 2-8 SpectraRay desktop icon

Before closing the setup, you may decide to additionally install some utilities which are helpful when working with many files.

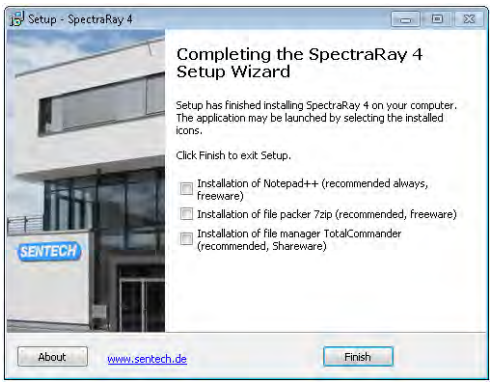


Fig. 2-9 Completing installation

When SpectraRay finishes, it has added some exceptions to the Firewall allowing internal network communication between SpectraRay’s own components. There is no connection to the internet required or used. The only network communication goes to the controller which is usually shipped with SENTECH Instruments metrology devices.

Requirements:

- Windows XP SP2 or later (example Windows Vista or Windows 7)
  - 32 or 64 Bit operating system version for secondary licenses
  - all metrology tools are delivered with 32 Bit operating systems
- 2 GB RAM
- Video 1280x1024 Pixels (or larger)
- USB Port (hardware may require additional ports, this is for the dongle)
- 100 Mbit Network port (for connecting to ellipsometer device)

Important note: ***The USB stick must be attached while SpectraRay is running since it also serves as hardware dongle.***

3 Application frame

The SpectraRay software is started by double clicking the SpectraRay icon on the desktop  .

3.1 Appearance of the application frame

The main application frame window is shown in Fig. 3-1. It consists of the following visible items:

- Title and system menu
- Main menu
- Icon bar
- Main screen

The items in the application frame window can be operated in the usual way offered by Windows programs. The visible buttons and the menu entries can be operated by clicking with the mouse.

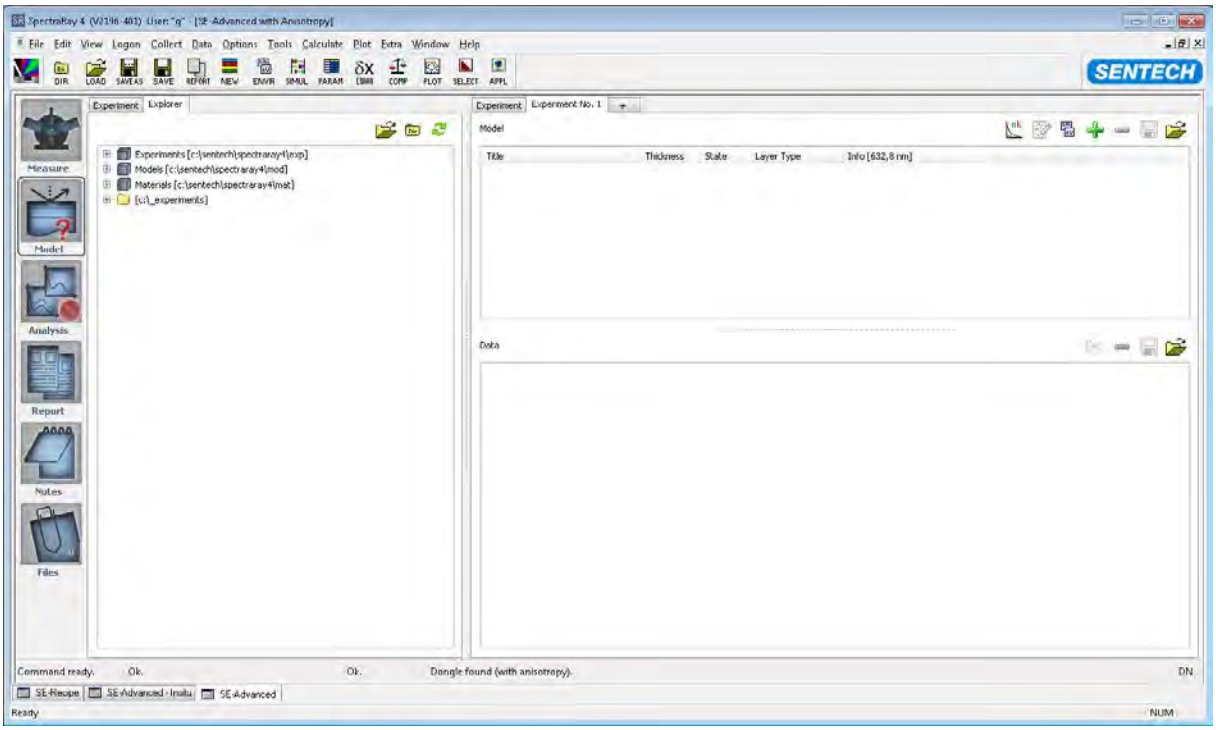


Fig. 3-1 Application frame with start view

3.1.1 Title and system menu

The main application frame has the title “SpectraRay/4”. This frame is the common software basis for all the different measurement tools of Sentech’s product family. This integration of different measurement tools into one common frame has many internal and external advantages such as common data libraries, common calculation routines and similar handling by the user.
The icon in the top left corner can be clicked to show the left system menu with entries for minimizing and closing the window.
The system menu in the top right corner of the frame shown in Fig. 3-2 is used to minimize the frame window, to restore the size of the window to normal and to exit the frame (X button). To exit you can also use the menu “File\Exit”, or <Alt>F4.

Fig. 3-2 System menu of the frame to minimize, restore the size and quit.

When the frame is running the icon shown in Fig. 3-3 is displayed in the task bar which is usually at the bottom of the Windows screen. Click the icon to restore the size if the window was minimized before.

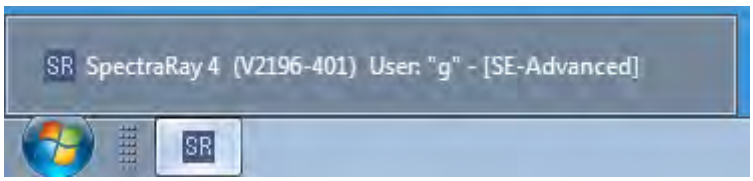


Fig. 3-3: Icon in the Windows task bar for the application frame.

3.1.2 Main menu

The main menu offers entries to all the functions of the modules of the SpectraRay software. The appearance depends on the selected module.

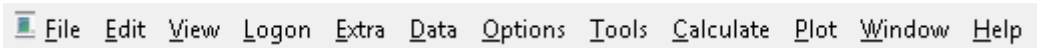


Fig. 3-4-3-5: The main menu of the SE-Advanced-module

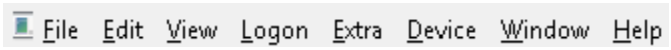


Fig. 3-6 The main menu of the SE-Recipe-module

3.1.3 Icon bar

The icon bar gives fast access by instructive icons to the most often used functions of the frame. The appearance depends on the selected module.

Fig. 3-7: The icon bar of the SE-Recipe-module consisting of the icons for often used functions

Fig. 3-8 The icon bar of the SE-Advanced-module consisting of the icons for often used functions

Moving the mouse over the icon displays the meaning of the icon.

3.1.4 Main screen

The appearance of the main screens also strongly depends on the selected module.

3.1.5 View menu

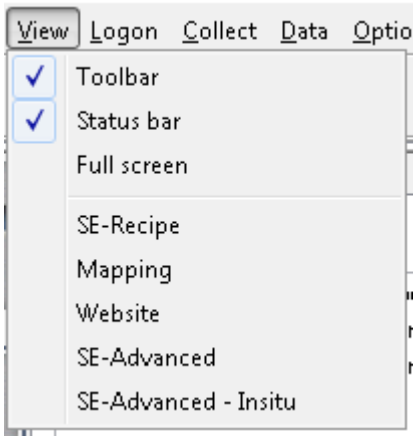


Fig. 3-9 The view menu

The view menu allows configuring the display of the items within the frame window. The toolbar and the status bar can be shown or hidden.
The menu also offers the navigation to the available modules. These are the main screen for the SE-Recipe, the SE-Advanced, the FTPadvanced, mapping and a copy of SENTECH's website.

3.2 User management

Click “Logon/User Administration” to open the following window:

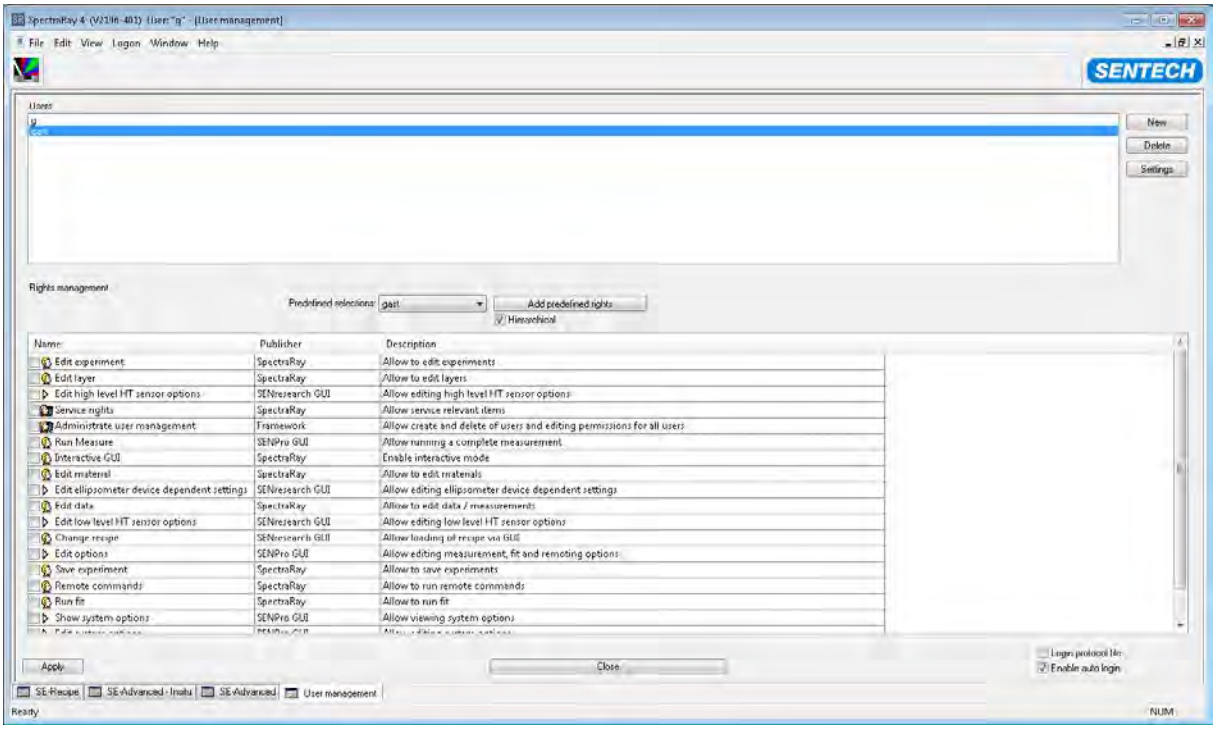


Fig. 3-10: User management view

In this view management of all access rights can be done. It is possible to insert/change and delete users and to assign various rights to single users. Only users with administrative rights can do this.

3.2.1 User administration

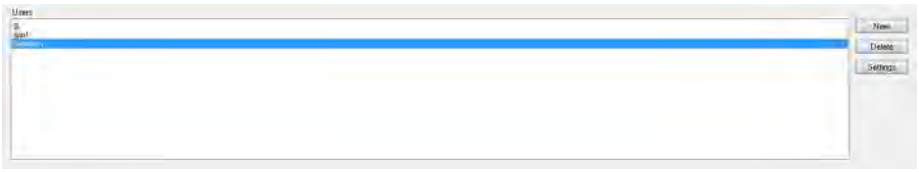


Fig. 3-11: User frame

In the upper frame all existing users are shown. With the button 

a new user can be created.

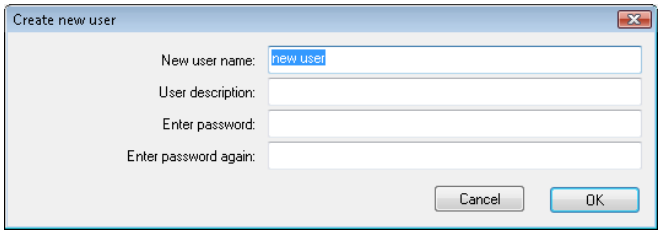


Fig. 3-12: Create new user

With the button 

an existing user can be deleted.

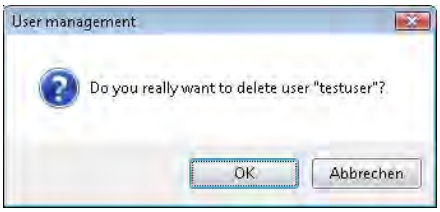


Fig. 3-13: Delete a user

With the button Settings an existing user can be modified.

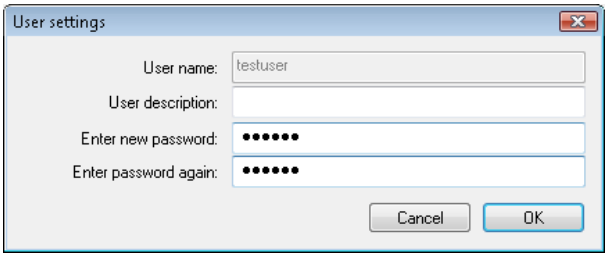


Fig. 3-14-3-15: Modify a user

3.2.2 Rights administration

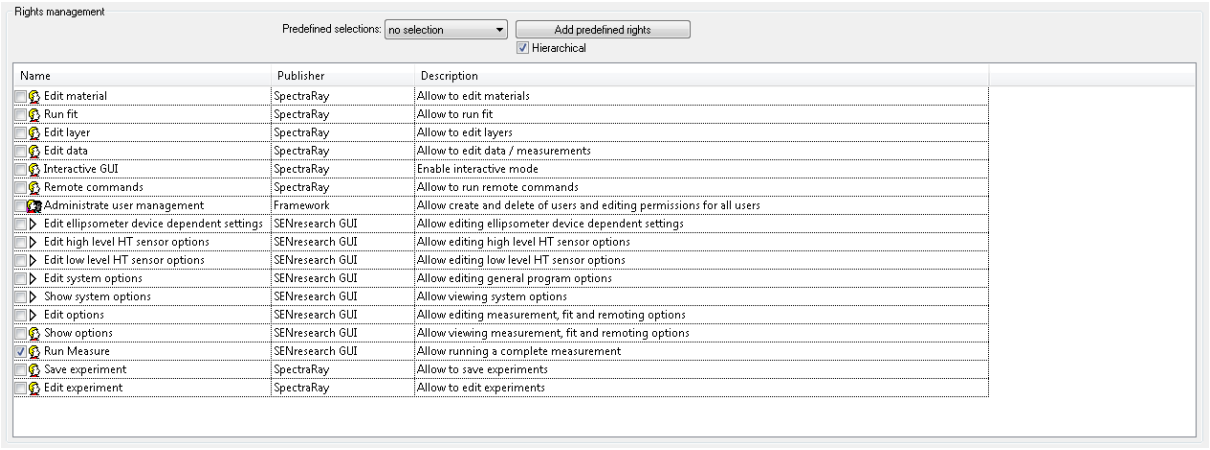
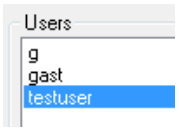


Fig. 3-16: Rights frame

With these settings existing rights can be assigned to users. To change rights of a user, this user must be selected in the upper frame.



Currently assigned rights are checked in the lower frame. Now single rights can be select or unselect to change rights of the selected user. All rights have a category and it is possible to add all rights of a category to a user with one step. To do this select wanted category from the list box and click the button

.

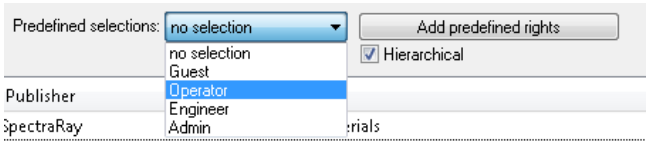


Fig. 3-17: Predefined right selections

Now all rights of this category are added to the selected user.

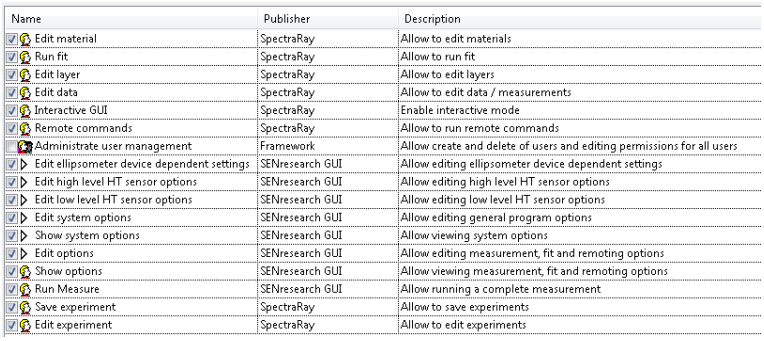


Fig. 3-18: Modified user rights

By clicking the button 

all changes are applied immediately without restart of the software.

4 SE-Recipe-module

In this chapter the appearance and the handling of the SE-Recipe-module will be described.

4.1 Main menu

The main menu offers entries to all the functions of the SE-Recipe-module.

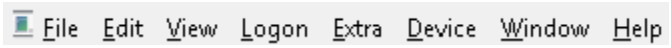


Fig. 4-1 The main menu of the SE-Recipe-module

4.1.1 File menu

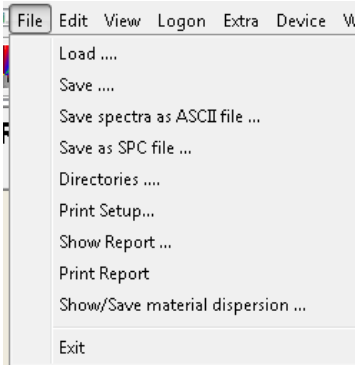


Fig. 4-2 The file menus of the different modules

The file menu allows loading and saving applications and experiments. It also allows setting up the properties of the printer and to preview and print reports.

4.1.2 Edit menu

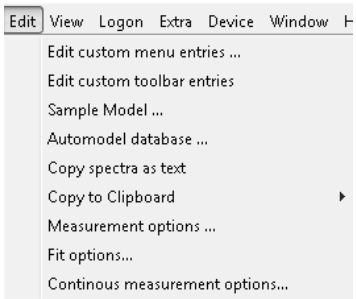


Fig. 4-3 The edit menu

To get a description for the menus please go to the according section:

- Edit custom menu entries ... (Appendix J)
- Edit custom toolbar entries ... (Appendix K)
- Sample Model… (sec. 4.5.8.1., p. 50)
- AutoModel database… (sec. 4.5.9., p.59)
- Copy spectra as text (copies spectra data to clipboard)
- Copy to Clipboard (submenus allow copying of various data to clipboard)
- Measurement options… (sec. 4.5.2., p. 38)

- Fit options… (sec. 4.5.3., p. 40)
- Continuous measurement options… (sec. 4.5.5., p. 42)

4.1.3 View menu

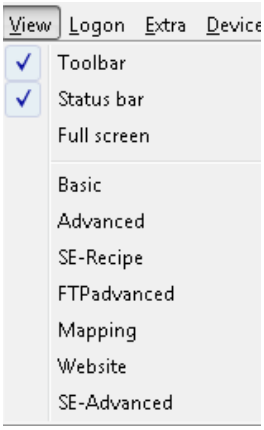


Fig. 4-4 The view menu

The view menu allows configuring the display of the items within the frame window. The toolbar and the status bar can be shown or hidden. This results in the typical appearance of the frame as shown in Fig. 4-5.

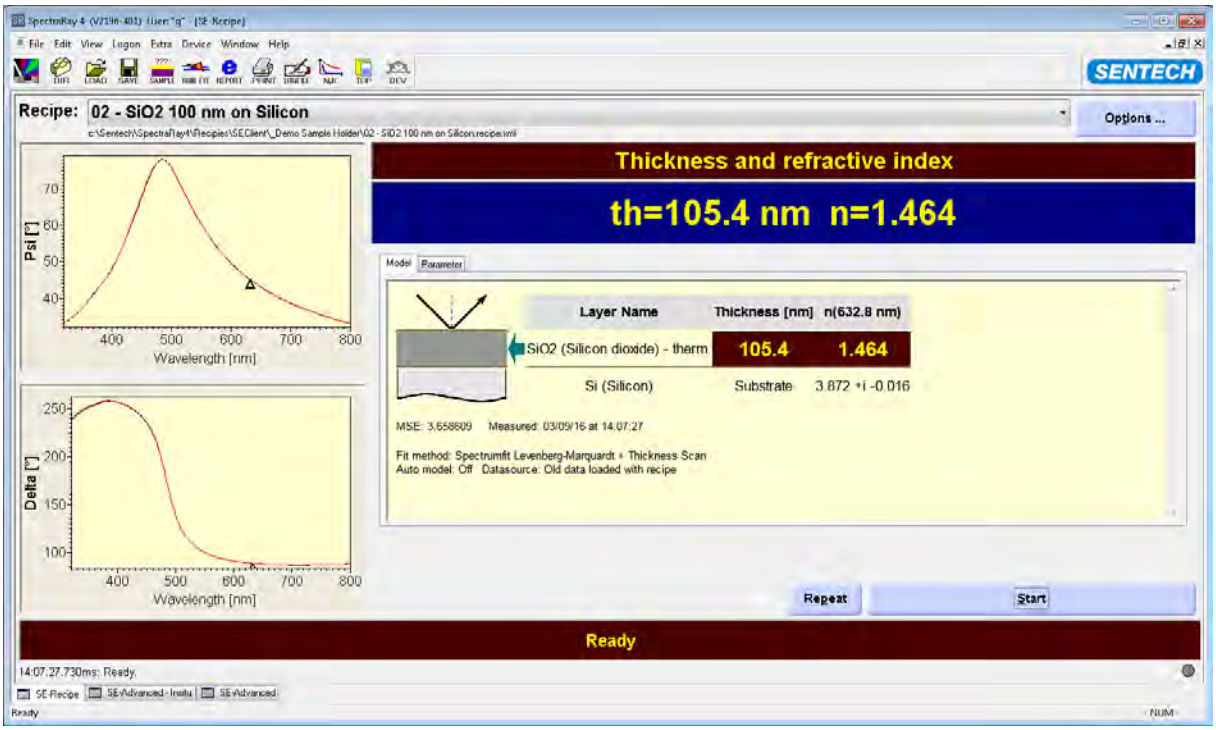


Fig. 4-5: Typical appearance of the frame window with the main user screen for SE-Recipe

Choosing the “Advanced” item means that the GUI is switched in a view state, where a user can modify some model parameters in a quick way and can see some more detailed results in the parameter view. Choosing the “Basic” item means that the GUI is switched in a view state, where no modification of the model is possible in the main screen and only main results are shown.
The menu also offers the navigation to the available modules. These are the main screen for the SE-Recipe, the SE-Advanced, the FTPadvanced, mapping and a copy of SENTECH’s website.

4.1.4 Logon menu

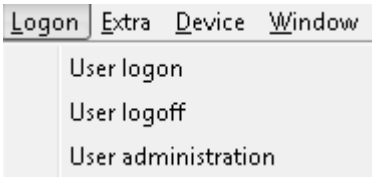


Fig. 4-6 The logon menu

This menu allows a change of current user login and an access to user management view.

4.1.5 Extra menu

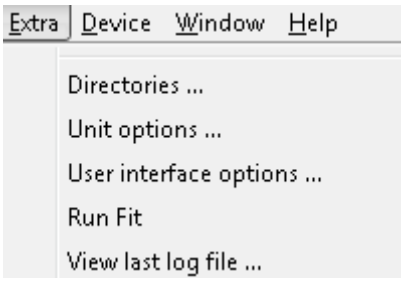


Fig. 4-7 The extra menu

The Extra menu gives access to all settings which are necessary to define a measurement with the selected module or to handle the results.

4.1.5.1 Directories …

In the directories tab one may set default directories for recipes, loading and saving of files.

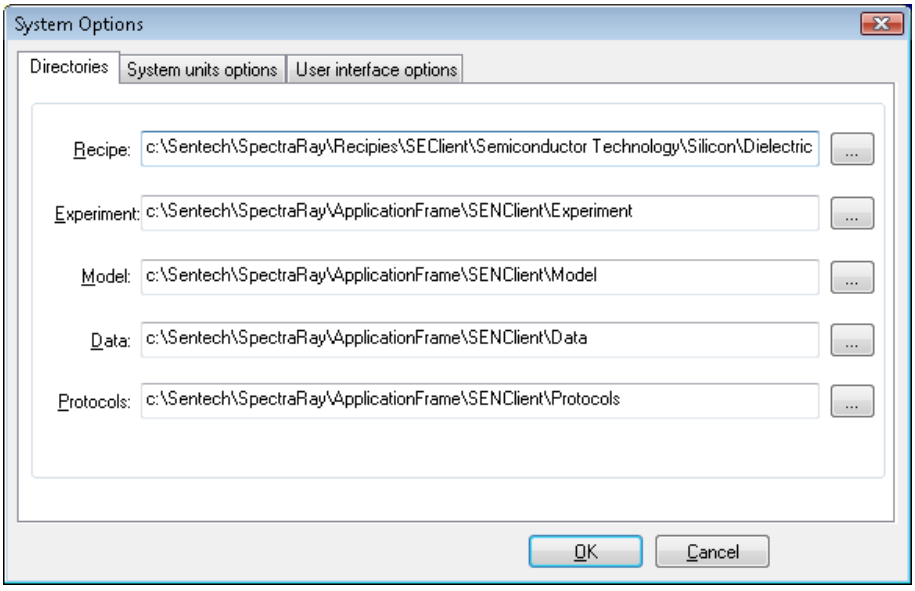


Fig. 4-8: The directories tab

Clicking on the three dots on the right of e.g. the recipe directory line opens a window like the following. Here you may select a folder for this directory.

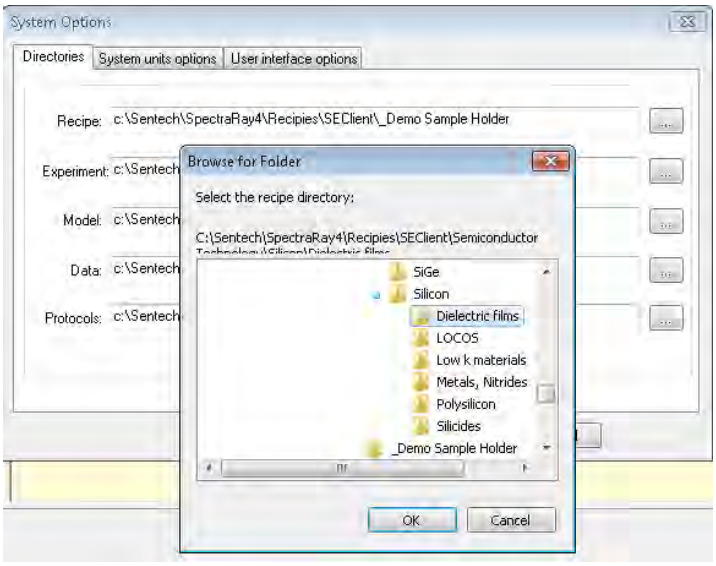


Fig. 4-9 Browsing for a recipe directory folder

4.1.5.2 Unit options … (System units options)

Clicking on “Unit options” reveals the following window:

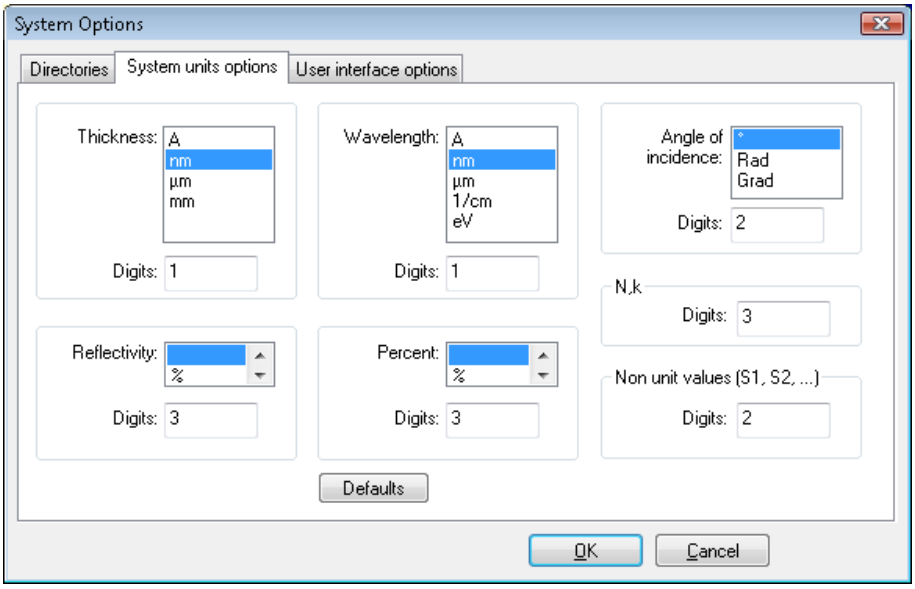


Fig. 4-10: System unit options

Here one can choose the units for the display of various measurement result types. It does not influence the data.

4.1.5.3 User interface options

The user interface options tab allows setting some properties of the graphical user interface (GUI).

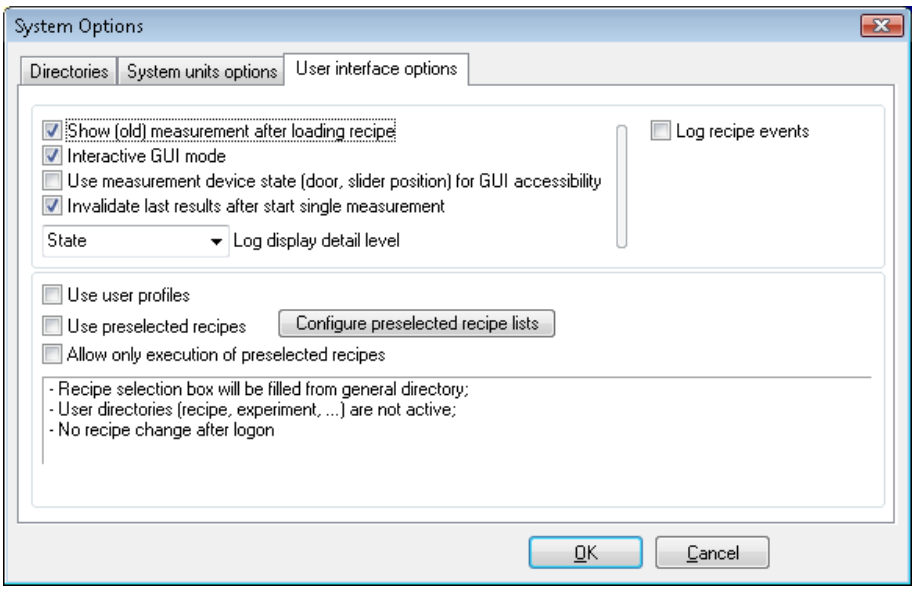
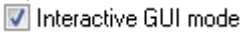


Fig. 4-11: The user interface options tab

If checked, the measurement data from a former measurement will be displayed after loading a recipe (if available).



If checked, the GUI is switched in a view state, where a user can modify some model parameters in a quick way and can see some more detailed results in the parameter view.

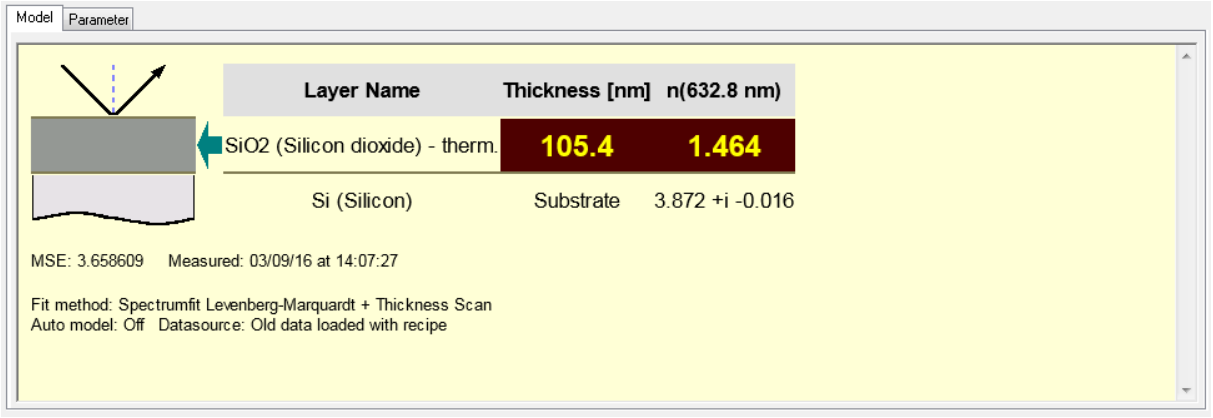


Fig. 4-12: Register tabs for advanced settings

If not selected, the GUI is switched in a view state, where no modification of the model is possible in the main screen and only main results are shown.

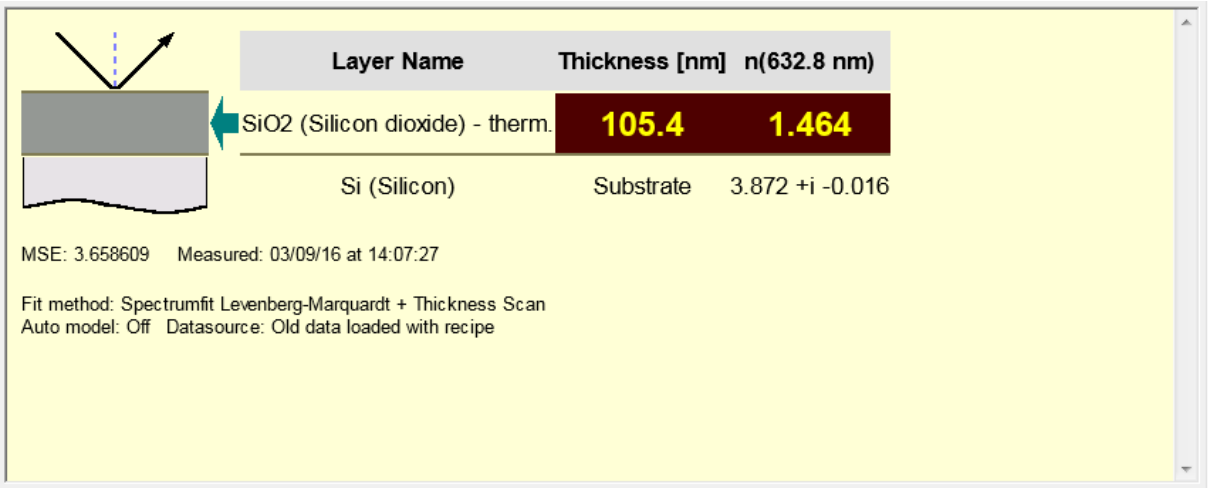
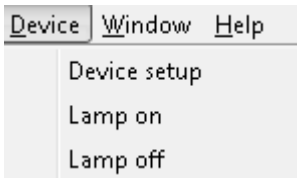


Fig. 4-13: No register tabs for simple operability

If checked, the accessibility of the software depends on the state of the measurement device (e.g.: if door is open, you can't start a measurement).

The software shows in the log window some information about the current system state. Here a user can select, in which levels he is interested.

4.1.6 Device menu



The Device menu gives access to the measurement device driver and the probe alignment system. It also gives the user the possibility to switch on/off the Xenon lamp explicitly.

4.1.7 Window menu

The standard window menu allows arranging the windows with the functions "Cascade", "Tile\Horizontal", "Tile\Vertical" and "Arrange Icons". At the bottom of the submenu list the active windows are shown and one of them can be made active, that means it gets the input focus.

4.1.8 Help menu

The help menu shows the file version of the application frame.

4.2 Icon bar

The icon bar gives fast access by instructive icons to the most often used functions of the frame.
The functions are (from left to right): directories | load data | save data | edit sample model | run fit | create a report for internet explorer for printing | print a report | view logfile | show n, k | add current recipe to preselected list of user | show device setup. Moving the mouse over the icon displays the meaning of the icon.

Fig. 4-14: The toolbar consisting of the icons for often used functions

4.3 Main screen

As shown in Fig. 4-5 the main screen for the SE-Recipe-module consists of the following items which are described below:

- List of available recipes
- Sample model with layer names, thicknesses and refractive indices
- Status message and error message
- Measurement result
- Graphical display
- Button to start measurements (Start)
- A Button (Repeat/Stop) for repeated measurements

4.3.1 List of available recipes

The list of available recipes allows selecting a certain predefined measurement task. The selection of the recipe sets all the settings necessary for the measurement including the sample model, reference model, integration times, spectral range used for evaluation, evaluation method etc. The settings of the previously loaded recipe are overwritten.
It is essential to choose the correct recipe before measuring the sample as it is not possible to measure all samples successfully with the same recipe. The most important part of the recipe is the sample model which has to be chosen correctly for a certain measurement task. Therefore it is useful to predefine recipes for certain types of samples.
Recipes may enable the AutoModel feature. In this case a database is activated and an automatic detection of the model takes place during the evaluation of the measurement result. Then a certain variety of different sample types can be measured with the same recipe.

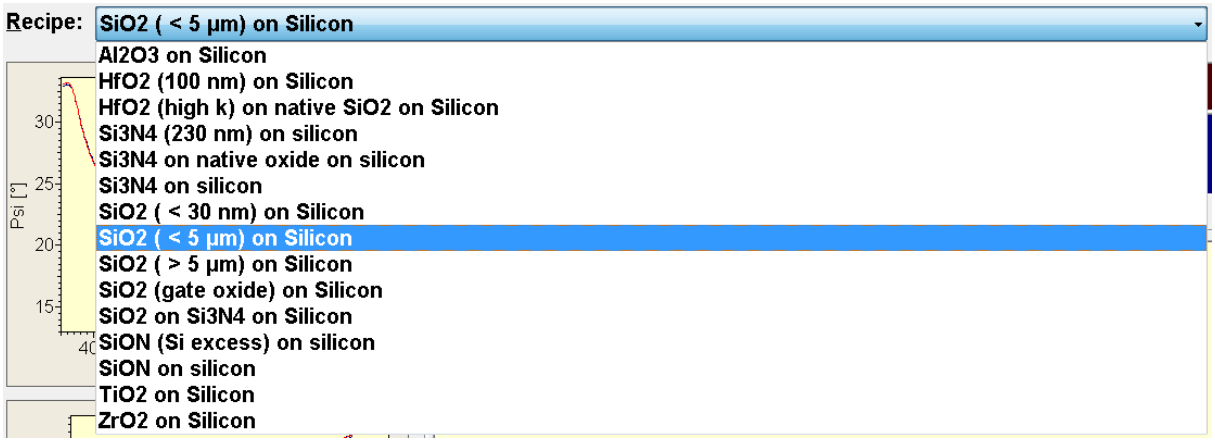


Fig. 4-15: List of available recipes.

4.3.2 Status message and error message

The big status message at the bottom and the smaller error message below the graphical display give information about the state of the measurement device. Moreover the additional help function is displayed in certain cases as shown in Fig. 4-16.

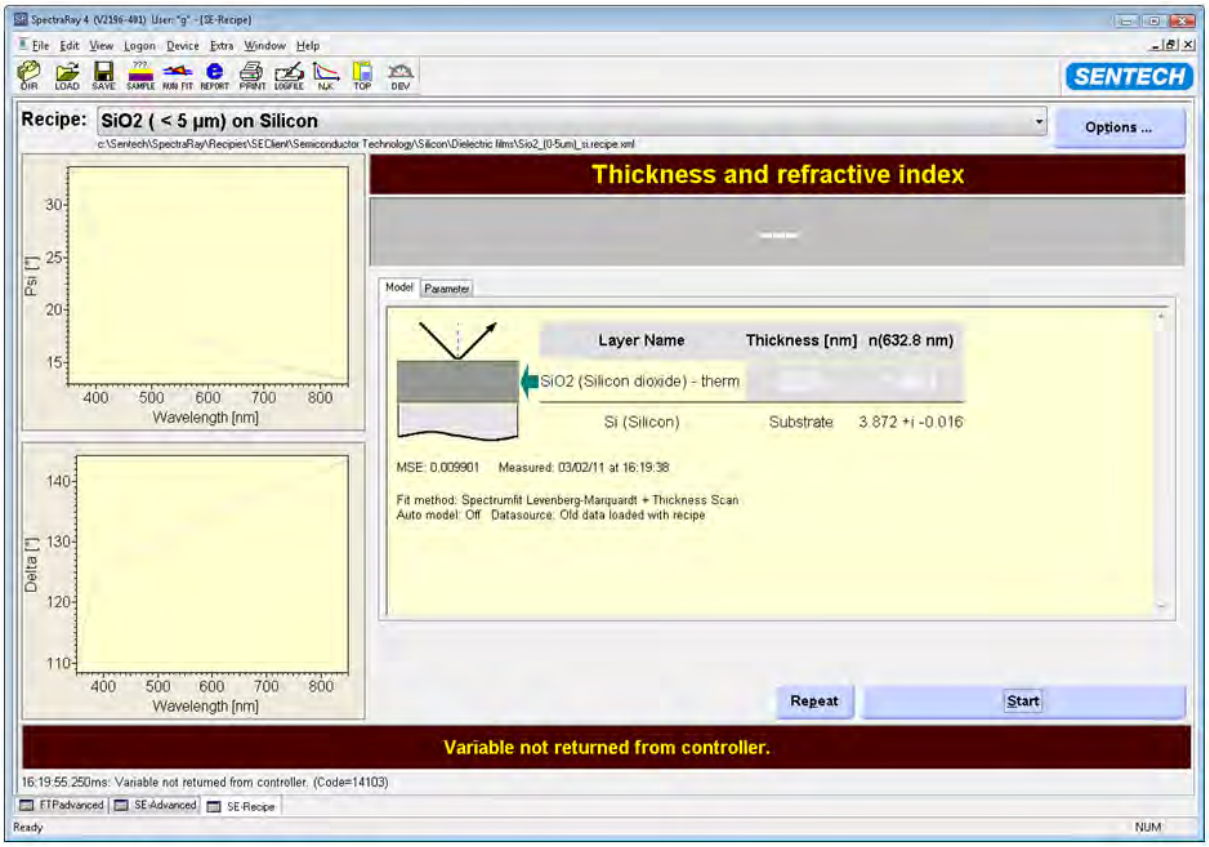


Fig. 4-16: Main screen with information in the model window in case of problems.

4.3.3 Measurement result

The big field on the right shows the resulting thickness and optionally n, k (if selected to fit) after a measurement. It shows the values for a selected layer as shown in chapter 4.5.8. Default behavior is to show the topmost thickness that has been measured even if there are more thickness values set as fitted parameter. The thickness parameters can be shown together with the sample model in the sample model window. If no valid measurement is present, the field shows "---". If no fit method is selected, the measurement values at the observation wavelength are shown.

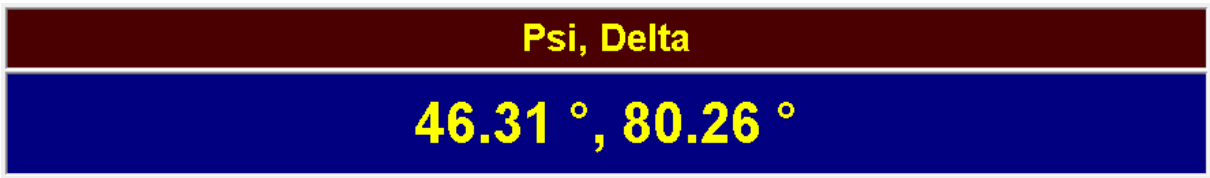


Fig. 4-17: Measurement values at observation wavelength

Clicking on this field allows setting another starting thickness value. It is possible to type in the number in or to press a character on the keyboard of the PC (see table below). Press<Esc> to leave the field without change or the space bar (blank) to accept the new starting value in the field.

Character	a	s	d	f	g	h	j	k
Increment (nm)	-100	-25	-5	-1	+1	+5	+25	+100

Tab. 4-1 Keyboard characters to change the thickness value by the corresponding increment.

4.3.4 Graphical display

The graphical display shows the measured results such as (Ψ, Δ) or (S1, S2) or (S1C, S2C) or (n, k) values for one spectral measurement or thickness variation versus time. It also shows model data for these values.
The graphical display can be changed by mouse actions:

- Zooming in by selection of a rectangle (Move the mouse to one corner, press the left mouse button and keep it pressed until the opposite corner). The zoom can be repeated.
- Auto scale to maximum x- and y-range by a simple click into the yellow area. Use autoscale especially if the measured values are out of the previously defined zoom range.

4.3.4.1 Observation wavelength

It is possible to change the observation wavelength in a quick way. Just right click in one of the left graphical displays. A popup window will be shown.

Fig. 4-18: Changing observation wavelength

In this window you can change the observation wavelength with the slider or manually in the edit field. After closing this window the whole GUI will be updated.

4.3.4.2 Spectrum mode

The graphical display usually shows the measured and fitted values versus wavelength of the light in blue and red color respectively (Fig. 4-5). The display is used for an intuitive check of the measurement by the user: for a good measurement both curves should overlap as good as possible.

If the measured and fitted curves are too far apart the measurement should be checked. Some usual reasons for wrong measurements are:

- Selection of a wrong recipe or wrong recipe settings
- Wrong alignment of the sample

4.3.4.3 Continuous mode

In the continuous mode the graphical display shows the measured thickness and MSE information versus time or single measurement results (see chapter 0).

4.4 Performing measurements

4.4.1 Sample measurement

After selecting a recipe the sample measurement can take place. In the case you do not have an automatic alignment system (e.g. SENDURO®) you have to align your sample first. Then you can start the measurement by clicking on the button “Start” in the main user screen. After the measurement is performed the evaluation takes place and the result is displayed as shown in Fig. 4-19.

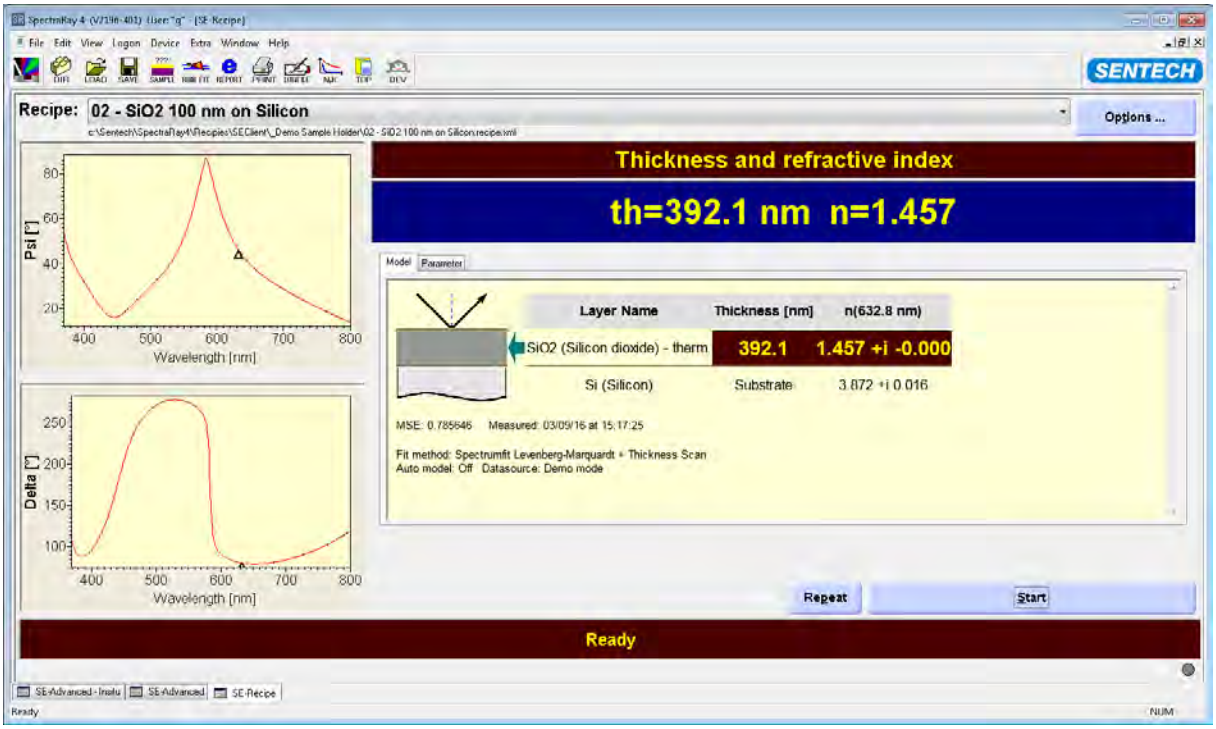


Fig. 4-19 Display of results after a successful measurement.

4.4.2 Repetitive sample measurement

For process control or measurements of stability it is desirable to perform repetitive measurements. The option screen for continuous measurements allows setting up the number of repetitions, the display mode, the logging mode etc.
To perform a repetitive sample measurement click the button “Repeat” and then the button “Start”. Click the button “Stop” which appears instead of the button “Repeat” during the measurement to abort the sequence.
The display for a continuous measurement is shown in Fig. 4-20. The measured thickness is shown in the graphical display versus time (if selected in options\continuous measurement options). In the model window the statistical values are shown in addition to the information for a single measurement:

- Average
- 3 sigma
- Minimum
- Maximum

The display is updated with each measurement, so it is possible to view the process. After the continuous measurement is finished or aborted the message shown in Fig. 4-21-4-22 is displayed. If the result logging is enabled in the option screen for continuous measurements, it is possible to view the result file as shown in Fig. 4-24. Details about the format are explained in the section 4.5.5 about the option screen for continuous measurements.

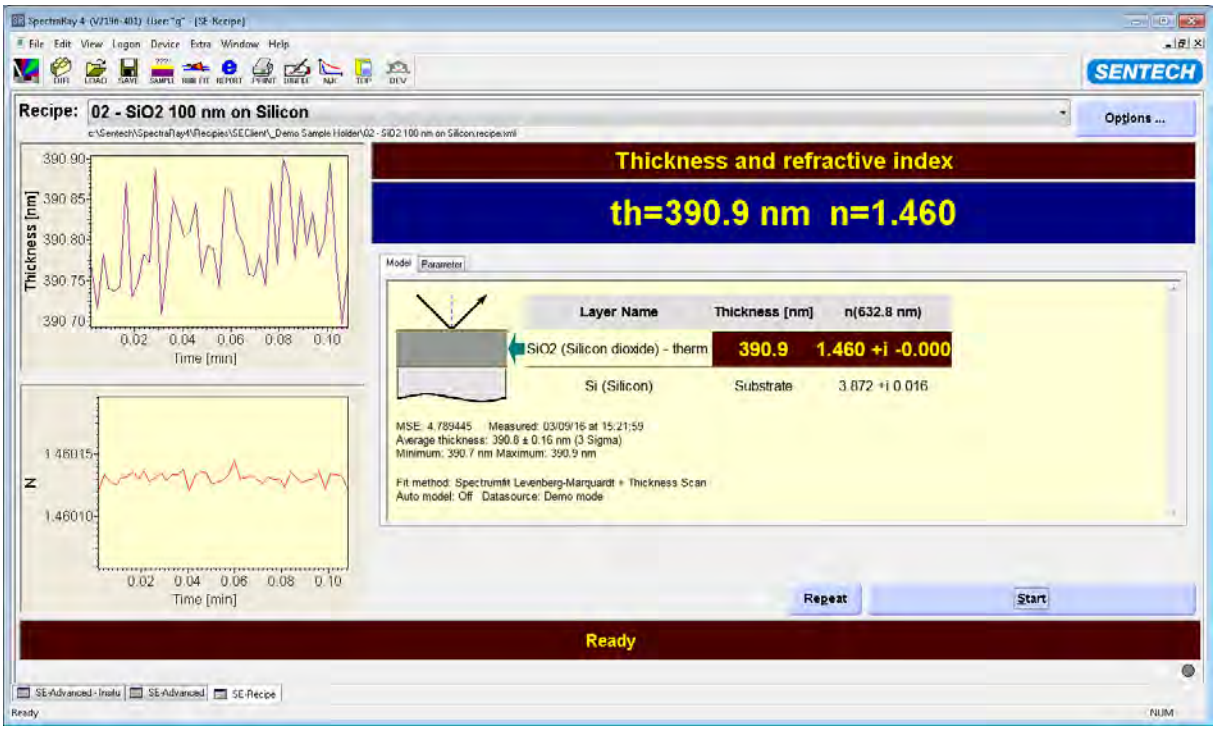


Fig. 4-20 Example for a continuous measurement with thickness result versus time and statistical values.

Depending on the settings for logging in the “Continuous Measurement Options” (see sec. 4.5.5.) different messages will appear at the end of a continuous measurement:

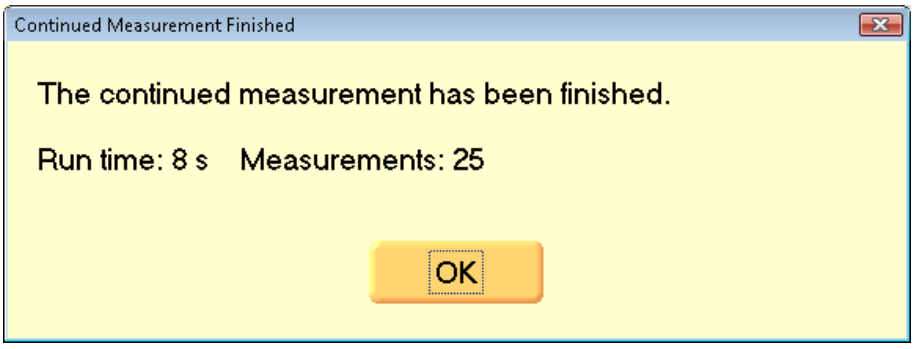


Fig. 4-21-4-22: Message if logging is disabled

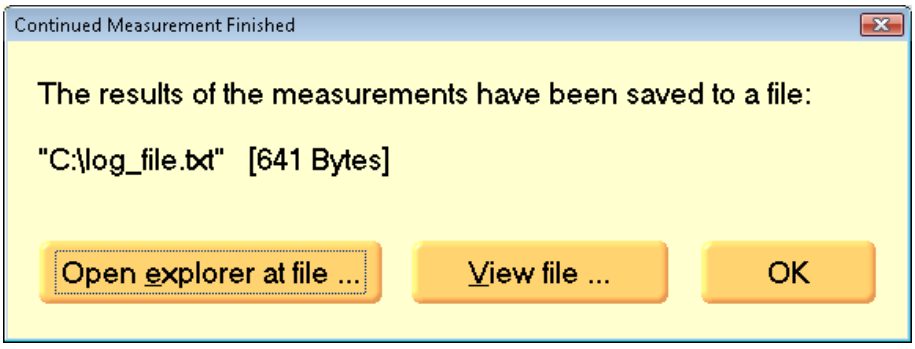


Fig. 4-23: Message if logging is enabled

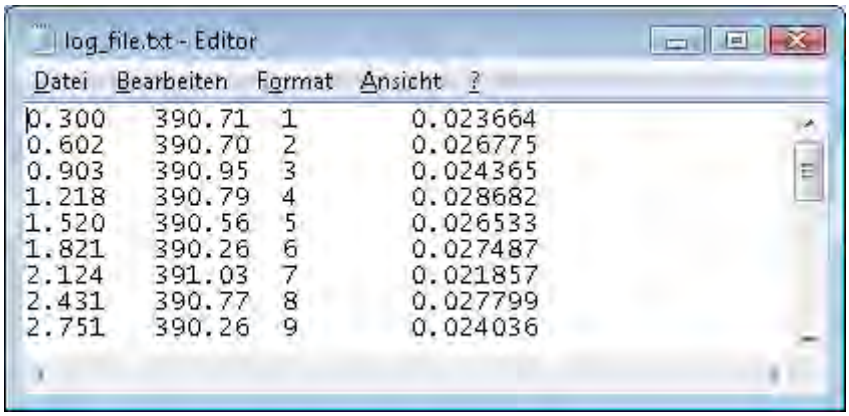


Fig. 4-24: Logging file of a continuous measurement.

4.5 Recipe Options

Clicking the blue button 

in the upper right corner of the Application Frame opens the last used register card in the “Recipe Options” window.

4.5.1 Model options

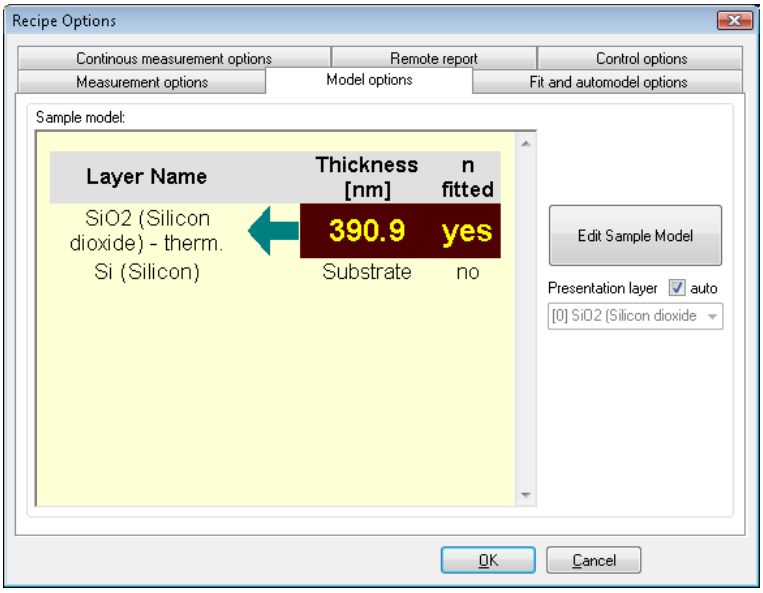
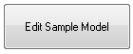


Fig. 4-25: The “Model options” tab in the recipe options

Clicking the button 

on the right side of the model options tab one may proceed to edit the sample model. The corresponding windows are described in section 4.5.8.1.
In this screen it is also possible to change the presentation layer for the main results. If “auto” is selected, the thickest fitted layer will be shown.

4.5.2 Sample measurement options

The “Measurements options” window can be accessed also by choosing “Edit” → “Measurement options …”.

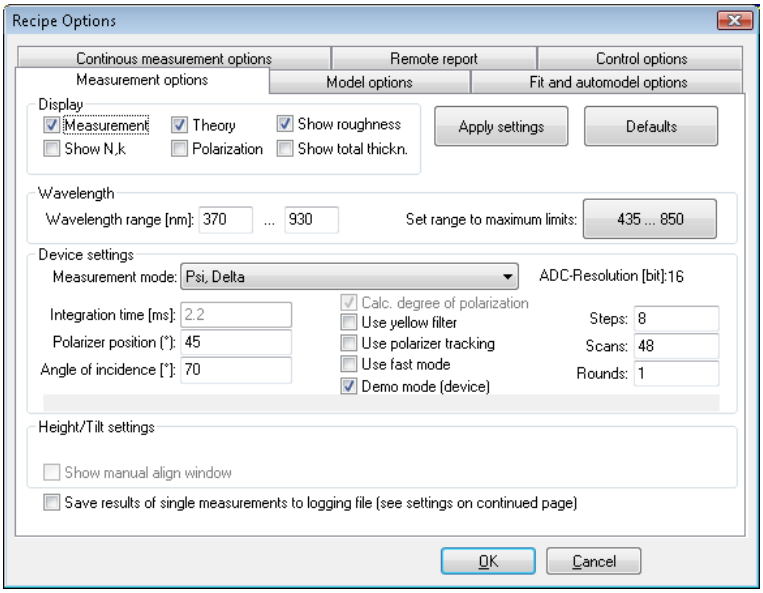


Fig. 4-26: Sample measurement options

4.5.2.1 Frame “Display”

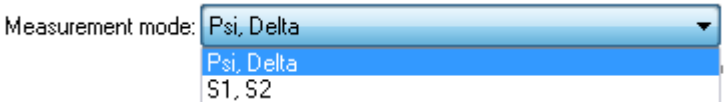
The frame “Display” allows checking the options “Measurement”, “Theory”, “Show roughness”, “Polarization” and “Show total thickn.” separately. If all are unchecked, no curve will be displayed.
It is also possible to select n, k. In this case values of n and k will be displayed. It is necessary to select “Report dispersions” in the “Fit and automodel options”-tab, because otherwise the values of n, k will not be transferred to the GUI.
“Default” inserts the default values, and “Apply settings” sends them to the measurement device. The same does “Ok”.

4.5.2.2 Frame “Wavelength”

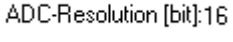
The Frame “Wavelength” allows to set a narrower wavelength range in the two text boxes or to reset it to the device limits with the right button.

4.5.2.3 Frame “Device settings”

The frame “Device settings” allows setting most important of the device driver settings.
Select one of two measurement modes:

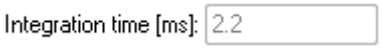


Each mode is another way to calculate the results from the measured spectra data.

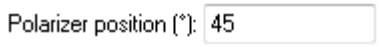


In this field the resolution of the Analog/digital converter of the spectrometer is shown (normally 16 bit).

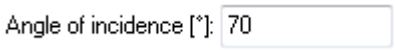
If this parameter is checked the degree of polarization is calculated. This parameter is checked by default.



In this field the last integration time of the last measurement is shown. It is not possible to set this value, because the device driver controls this value automatically. If this value is large (>=500 ms), it is possible that there is no sample on stage.

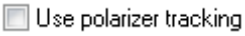


Here it is possible to set a fixed polarizer position for the measurement.

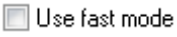


In this field the angle of incidence of this device is shown. It is a device specific value and will be set during calibration of the device. It is not possible to set this value here manually.

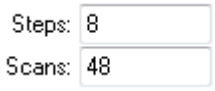
If this parameter is checked a yellow filter will be used during measurement. This is useful especially for measuring resists.



If this parameter is checked the system will try to find an optimal position for the polarizer during measurement. This is useful especially during creation of new recipes.



If this parameter is checked the device works in the so called “fast mode”. In this mode the device measures on the fly without stopping the analyzer. This results in a faster measurement, but accuracy will be a little bit lower than in step/scan mode (default mode).



Here the values for steps and scans for a step/scan mode measurement can be set. These values are not used during a fast mode measurement.

In this field it is possible to set used rounds for one measurement cycle.

With this parameter is checked it is possible to “simulate” a measurement without any hardware. This is sometimes useful for presentations.

4.5.2.4 Frame “Height/tilt settings”

With these settings you can modify the normal behavior of height/tilt control.

If not checked, no manual align window will be shown after a failed automatic height/tilt control action. It is useful to uncheck this option during long automatic tests.

4.5.3 Fit options

The “Fit and automodel options” window can be accessed also by choosing “Edit” → “Fit options …”.

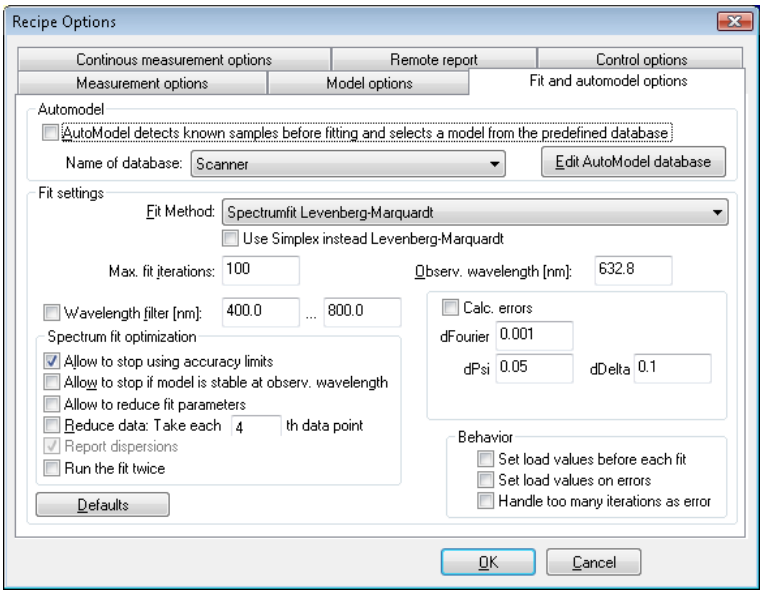
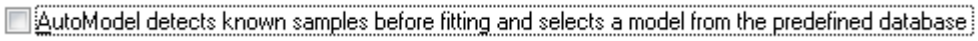


Fig. 4-27 The “Fit and automodel options” tab

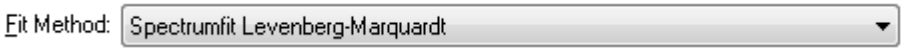
4.5.3.1 Frame “Automodel”



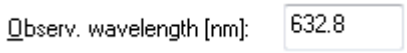
Checking this box enables the AutoModel feature during the fit process.

The box below allows selecting the database for the AutoModel feature. Click the button “Edit AutoModel database” to create, change or delete such a database (See Section 4.5.9 for explanations).

4.5.3.2 Frame “Fit settings”



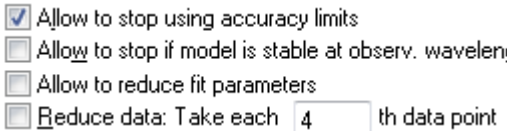
The “Fit Method” (Spectrum fit, Fourier transform, or combination of both) should be chosen according to the expected thickness. Use “Spectrum fit…” for thin and medium samples. “Fourier transform” may be chosen for medium and thick samples. The combination can be used to increase the quality of results for thick films.



The “Observation wavelength” is the wavelength for which the refractive index is displayed in the result screen, the edit layer screen, and in the print report.

Here the maximal count of iterations for the model fit can be set. If the error “Too many iterations” is displayed too often, you should increase this value.

The wavelength filter allows selecting the range used for fitting.

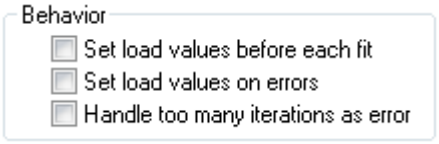


With these four check boxes one can customize the stop criteria for the fit process. “Reduce data” may be useful if there are no interferences in the spectrum.

If this parameter is checked the values of the dispersion (n, k) will be transferred from the analysis tool to the GUI. This is necessary to display these values in the GUI and to report the (n, k)-values. Normally this setting should be set.

If this parameter is checked, the analysis tool will start the fit twice to improve the success rate of the fit. Use this option, if the fit algorithm succeeded often in second step.

If this parameter is checked the fit component will calculate deviations of fitted values. The fields below this option show used (fixed) precisions for these values.



With these settings the behavior of the fit start settings can be modified. Normally the last values are used, because in most cases the same material will be measured again. Sometimes it is useful to change this behavior.

4.5.4 Display measured values only

To display the measured values without fitting choose the fit method “no Fit” in the “Fit and automodel options” tab. In this case, the selected measurement values (e.g. (Ψ, Δ) or (S1, S2)) at the observation wavelength will be displayed after the measurement as a numerical result instead of the thickness value.

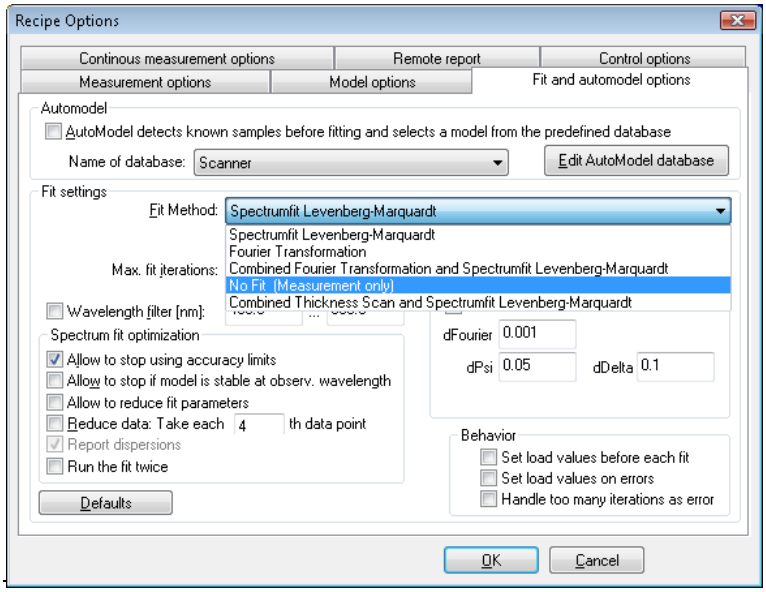


Fig. 4-28 The fit method “no Fit” in the “Fit and automodel options” tab

4.5.5 Continuous measurement options

The “Continuous measurement options” window can be accessed also by choosing “Edit” → “Continuous measurement options”.

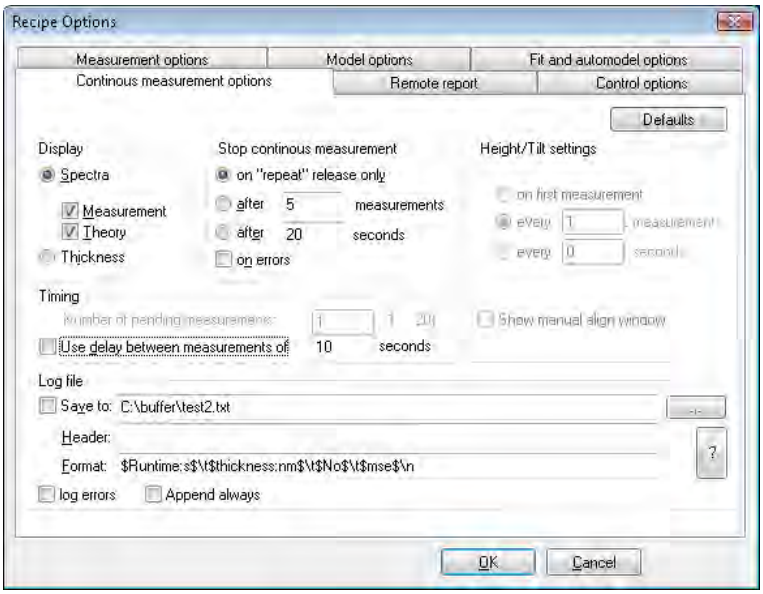
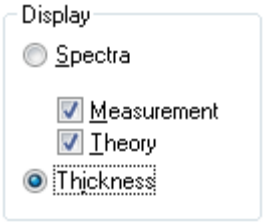


Fig. 4-29 The continued measurement options tab.

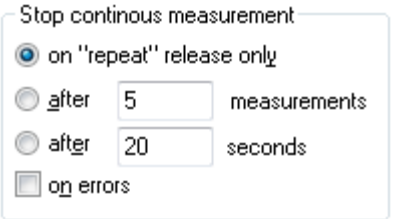
In this tab you can set measurement settings for a continuous measurement (after clicking “Repeat” and “Start” in main view).
Clicking the “Defaults” button sets the default settings.

Frame “Display”



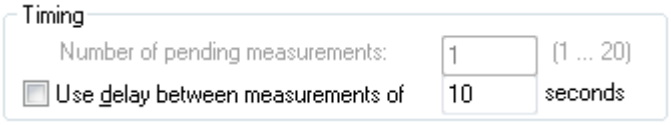
In the example, the continuous measurement options are set in the frame “Display” to display the thickness as a function of measurement time. If you select “Spectra”, every single measurement will displayed as described for single measurement steps.

4.5.5.1 Frame “Stop continuous measurement”



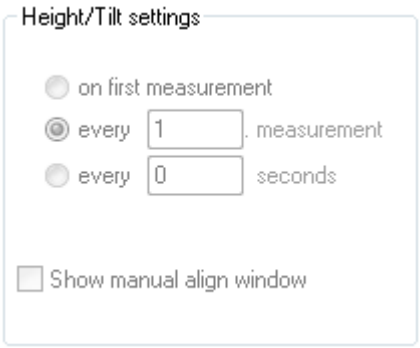
There are different possibilities to stop a continuous measurement: Clicking a button, after a predefined time or a count of measurements.
You can select in all modes to stop measurement after an error.

4.5.5.2 Frame “Timing”



The frame “Timing” allows the user software sending measurement requests for a “Number of … measurements” to the controller while the current measurement (including fitting) is not finished to obtain faster operation. “Use delay…”, on the other hand, allows selecting a certain time interval between the measurement, e.g. for stability measurements. The maximum allowed value is 3600 s.

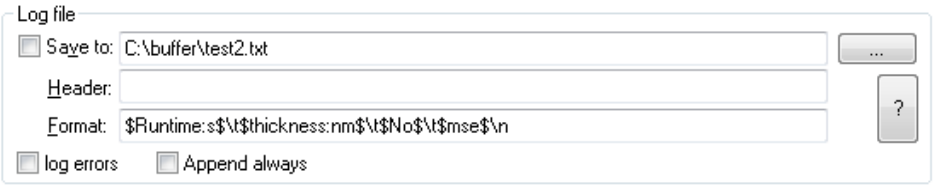
4.5.5.3 Frame “Height/tilt settings”



These settings are similar to the settings of a single measurement. Additional it is possible to specify, when height/tilt alignment should be repeated.

4.5.5.4 Frame “Log file”

The results are saved to the log file (see frame “Log file”). Clicking “…” allows changing name or path of the log file. For the format of the output file see below. Clicking “?” shows the text below in the result window.



4.5.5.4.1 Format of the log file

You can use variables to make a custom output. There is the following set of variable names and replaced content available. All these variables can be used within the normal output text when given within dollar signs. See the following example for logging file header lines:

```
; Date:\t$Date$ ($day$)\n; Time:\t$Time$\n; User:\t$user$\n\;Time [s],
Thickness [nm], No of Measurement, Mean Square Error (MSE)\n\n
```

Another example for line output during continued measurements:

```
$Runtime:s$\t$thickness:nm$\t$No$\t$mse$\t$th3sigma$\tEC:$code$\t$errmsg$\n
```

Some additional replacements are as follows: **\n** (carriage return + line feed), **\r** (carriage return), **\a** (line feed), \t (tab character), \\ (the backslash).
Alignment: Since a variable replacement has normally variable text length, there is a need to setup a minimum width and left or right alignment. For setting a minimum text length for a variable replacement, append a “&”

with the given minimum text length (filled with space characters). An additional "-" indicates right alignment instead of left alignment (default). Examples:

```
$No&6$    Number left aligned, at least 6 characters long
$No&-6$   Number right aligned, at least 6 characters long
```

Variable name	Replaced with content
code	Error code of measurement (0 is Ok, others are errors)
date	current data given as 11/02/01 (month, day, year with two digits)
day	name of weekday (like "Friday", depending on the locale settings)
ermsg	Error message text (empty if last error code was 0)
mse	Mean square error of last fitting result
no	Number of current measurement
runtime	runtime since start of continued measurement in display units
runtime:h	runtime since start of continued measurement in hours
runtime:min	runtime since start of continued measurement in minutes
runtime:s	runtime since start of continued measurement in seconds
subcode	detail code for errors (only applies if error code is not zero)
suberrmsg	detail text for errors (only applies if error code is not zero)
th1sigma	standard deviation of all measured thickness (1 sigma, display units)
th1sigma:a	standard deviation of all measured thickness (1 sigma, in A)
th1sigma:nm	standard deviation of all measured thickness (1 sigma, in nm)
th1sigma:um	standard deviation of all measured thickness (1 sigma, in µm)
thav	thickness average in display units
thav:a	thickness average in A
thav:nm	thickness average in nm
thav:um	thickness average in µm
thickness	thickness in display units
thickness:a	thickness in A
thickness:nm	thickness in nm
thickness:um	thickness in µm
thmax	largest thickness value in display units
thmax:a	largest thickness value in A
thmax:nm	largest thickness value in nm
thmax:um	largest thickness value in µm
thmin	smallest thickness value in display units
thmin:a	smallest thickness value in A
thmin:nm	smallest thickness value in nm
thmin:um	smallest thickness value in µm
time	current time given as 12:07:10 (hours, minutes, seconds)
user	current user (name given during login)
psi	psi value in display units
psi:deg	psi value in grade units
psi:rad	psi value in radian unit

psi:grade	psi value in new grade units (centesimal degree)
psi:500	psi value at wavelength 500 nm in display units
psi:500deg	psi value at wavelength 500 nm in grade
delta	delta value in display units
delta:deg	delta value in grade units
delta:rad	delta value in radian unit
delta:grade	delta value in new grade units (centesimal degree
delta:500	delta value at wavelength 500 nm in display units
delta:500deg	delta value at wavelength 500 nm in grade
s1	s1 value in display units
s1:500	s1 value in display units at wavelength 500 nm
s1c	s1c value in display units
s1c:500	s1c value in display units at wavelength 500 nm
s2	s2 value in display units
s2:500	s2 value in display units at wavelength 500 nm
s2c	s2c value in display units
s2c:500	s2c value in display units at wavelength 500 nm
refr	refraction index value (n) in display units
refr:500	refraction index value (n) in display units at wavelength 500 nm
absk	absorption coefficient value (k) in display units
absk:500	absorption coefficient value (k) in display units at wavelength 500 nm

Tab. 4-2: Format of the log file

4.5.6 Remote report

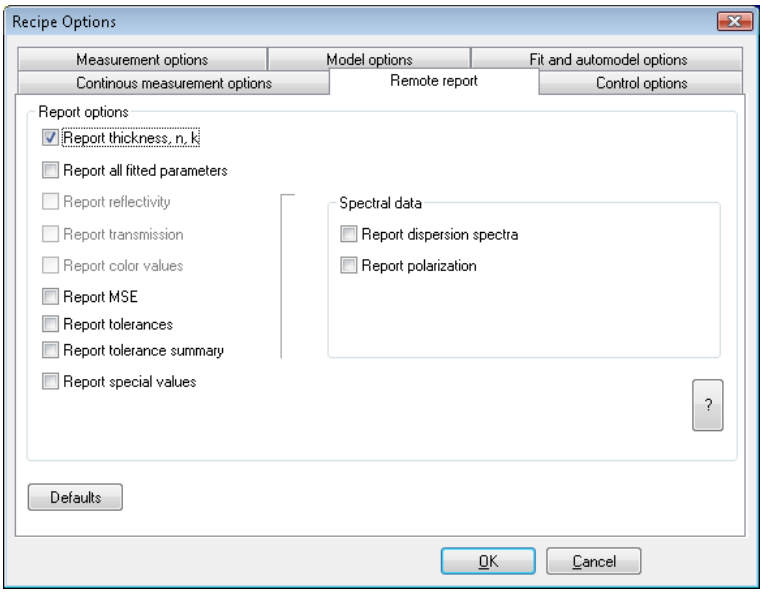


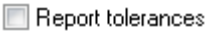
Fig. 4-30 The “Remote report” tab

Settings in this tab affect the format of results in the remote control of the measurement device. Grayed settings are not supported until now.

Fitted values of thickness, n and k are reported.

All fitted parameters are reported.

If checked, the value of MSE (mean square error) will be reported.



If checked, the values of tolerances will be reported.

If checked, a summary of tolerances will be reported.

If checked, special values will be reported.

4.5.7 Control options

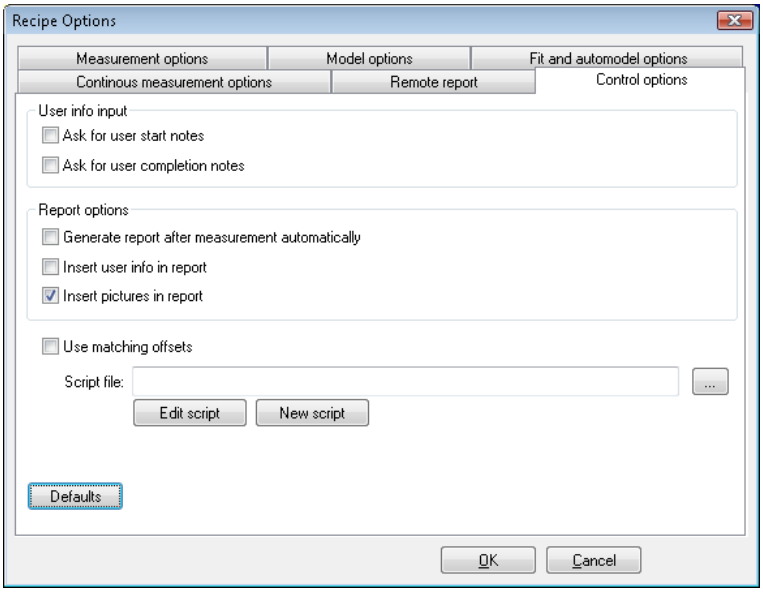


Fig. 4-31 The “Control options” tab

Settings in this tab affect the flow control of a measurement and report generation.

4.5.7.1 Frame “User info input”

Ask for user start notes

If this parameter is checked, a dialog will be displayed at the beginning of a measurement.

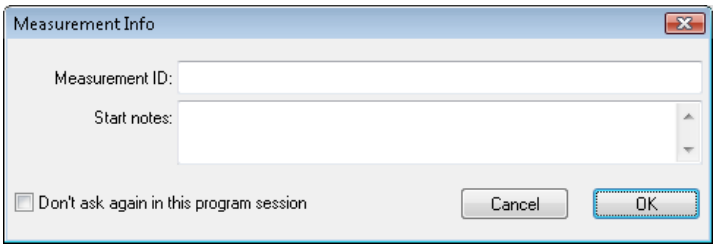


Fig. 4-32: Measurement start notes

The user can input some information about the measurement in the fields of this dialog.

Ask for user completion notes

If this parameter is checked, a dialog will be displayed at end of a measurement.

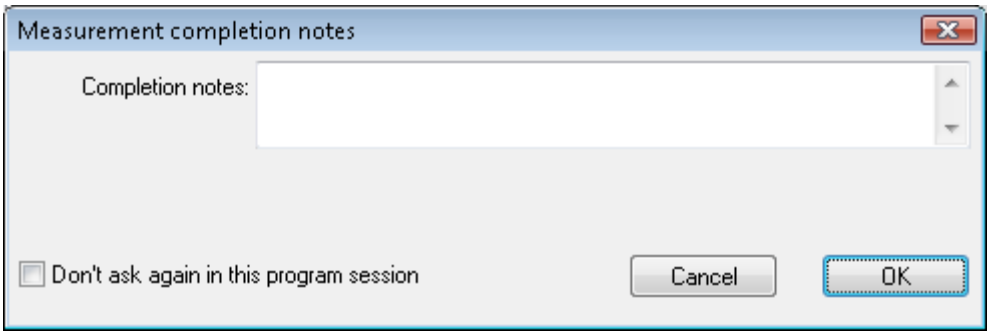


Fig. 4-33: Measurement completion notes

The user can input some information about the measurement in this dialog.

4.5.7.2 Frame “Report options”

Generate report after measurement automatically

If this option is checked, a report will automatically be generated after completing a measurement.

Insert user info in report

If this option is checked, the user info (start/completion notes, current login) will be inserted into the reports.

Insert pictures in report

If this option is checked, graphics of the measurement (as shown in left part of the main view) will be inserted into the reports.

4.5.7.3 Other control options

Selection of this option enables the software to use parameter based matching offsets in the presentation of results. This is useful to eliminate minor hardware dependent result differences between different measurement devices.

With this setting it is possible to realize some additionally functionality in the measurement sequence. It is useful for customizing and related things.

4.5.8 Edit model

If one wishes to measure layer stacks or materials not covered by the predefined recipes one may edit the sample model.

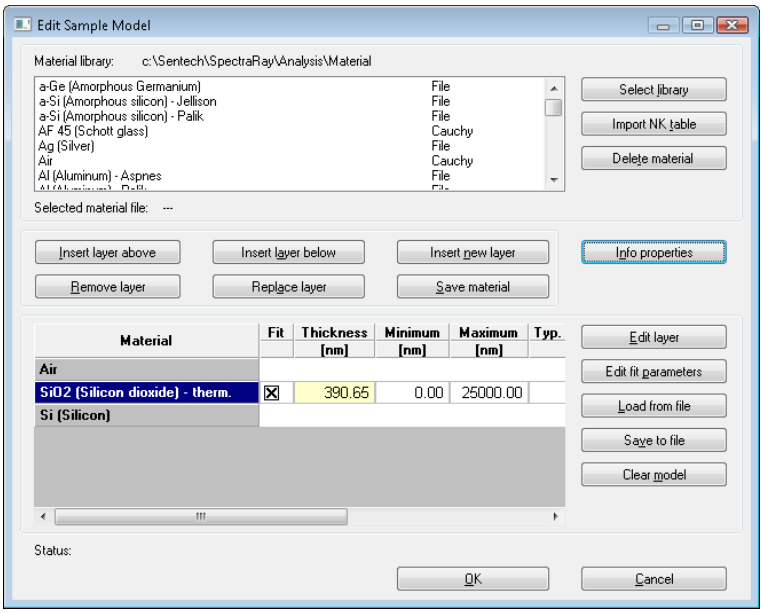


Fig. 4-34 The “Edit sample model” window

4.5.8.1 Edit Sample model

The “Model options” window can be accessed also by choosing  from the icon bar. To edit a sample model, three groups of functions are available (see Fig. 4-34): Choosing a type of a model (called material), adding, removing or replacing layers in the layer stack, and setting the properties and fit options of each layer.
Some examples will be given which would work in the current software version and use functions of the three groups.
We wish to choose a model type. After clicking the button “Select library” on the “Edit sample model” screen the following window appears:

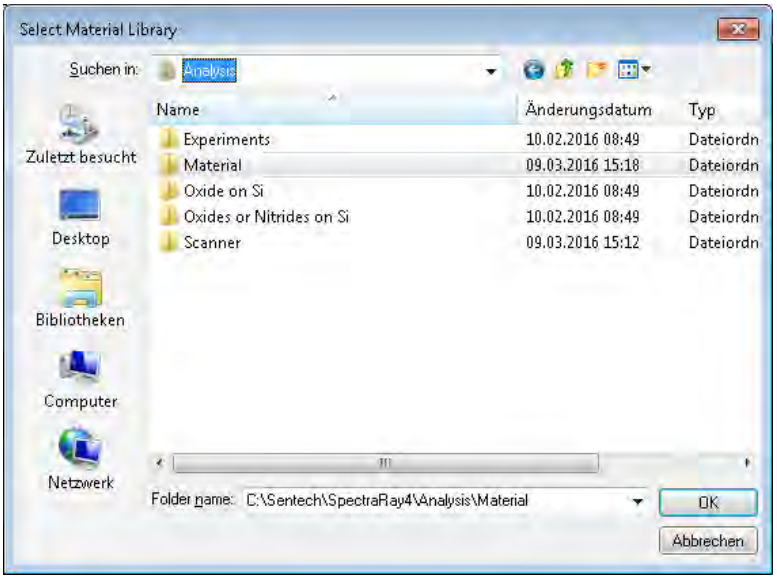
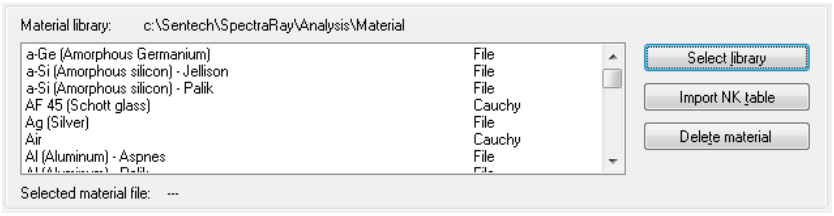


Fig. 4-35: Select a Folder with a material library

After selecting the folder “Material”, the files in this folder will be displayed in the scrollable text window of the edit sample screen (Fig. 4-34). In this window the most important information about the sample model is shown. It is updated when a recipe is selected from the list. In the example in Fig. 4-5 a silicon dioxide film of about 22 nm thickness on a silicon substrate is selected.



The top frame of the “Edit sample model” window contains the scrollable text window displaying the files in the selected folder, the already mentioned “Select library” button, the button “Import NK table”, which will be explained later, and the button “Delete material” which allows to delete a selected file.

The next frame contains the buttons “Insert new layer” which inserts a new layer in an empty layer stack, the buttons which “Remove…” and “Replace…” a selected layer, the buttons “Insert layer above” and “…below” which insert another layer above or below the selected layer. “Save material” saves the parameters characterizing the material model to a file.

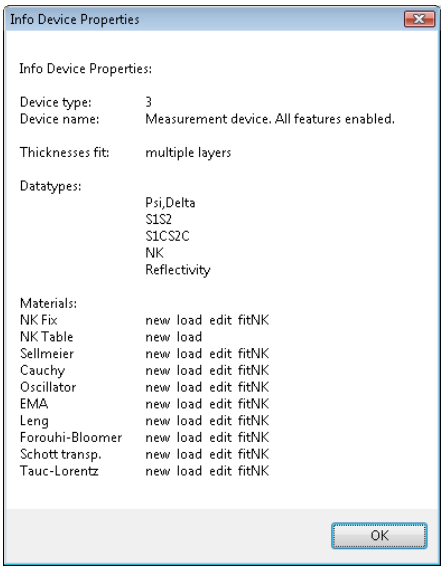


Fig. 4-36: Supported device options

Pressing the “Info Properties” button on the right side shows the small window containing the software version type together with the edit options available (see Fig. 4-36).

4.5.8.2 Edit layer

Clicking the Edit layer button in the "Edit sample model" window opens the following window:

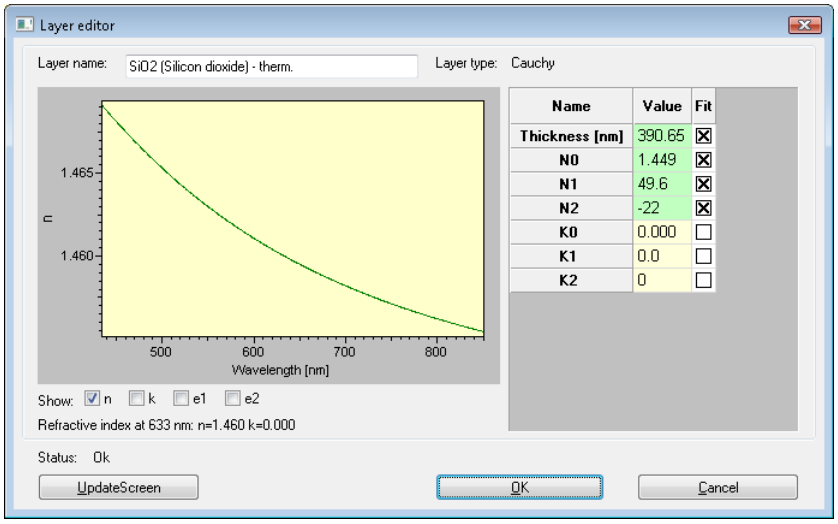


Fig. 4-37: The layer editor window

The file name in the text box can be changed by typing a different name. The diagram shows the spectral values of n, k, epsilon 1 or epsilon 2, if selected in the according check box. If no box is checked, nothing will be displayed in this area. The table on the right side shows the model parameters. If they are gray, they cannot be edited. If a box in the "Fit" column is checked, the parameter will be fitted.

4.5.8.3 Edit fit parameter list

Clicking Edit fit parameters button in the Edit sample model window leads to the following window:

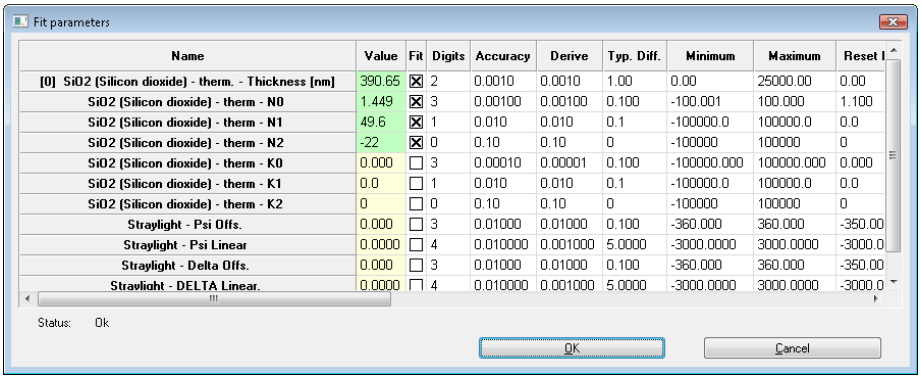


Fig. 4-38: The editable list of fit parameters.

The fit parameters list gives an overview over the values used in the edit layer window. The fit parameters list of a multilayer stack would show the set of parameters for all layers, beginning from the air side. Moreover, it shows auxiliary parameters for fit control like "accuracy".
The fit parameters list is an adjustable table, i.e. one may shift the columns to get a clear view on the values. Loading it again shows a table with default column widths. "Digits" gives the number of digits displayed in the "Value" column, "Accuracy" sets the limits when the fit can stop, "Derive" sets values for the fit optimization using the gradients. For the Fourier transform procedure, "Typ. Diff." sets the difference between data points; during the spectrum fit procedure it sets the beginning step width. "Minimum" and "Maximum" gives the expected range of the value. The starting value should lie in within this range. "Reset Min." or "Reset Max." are reset start values during a fit procedure if the value tends to leave the lower or upper limits (Min. < Res. Min ≤

Value ≤ Res. Max. < Max.). If some values are gray, e.g. in the basic version, they cannot be changed. Click "OK" to apply these values.

4.5.8.4 Save model or experiment

To save the model file, click 

button in the "Edit sample model" window, and type in a name (Fig. 4-39). A model characterizes a layer stack. An experiment contains the model, measurement data and additionally information like the measurement time. A recipe contains an experiment, the reference model, and all needed device settings like integration times.

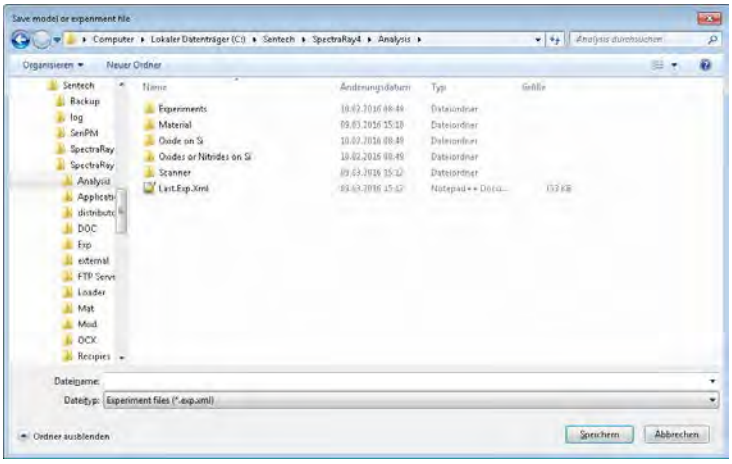


Fig. 4-39 Saving an experiment file in the Save model or experiment file window

4.5.8.5 Load model or experiment

To load a model or experiment, click 

button in the "Edit sample model" and choose a file (see Fig. 4-40).

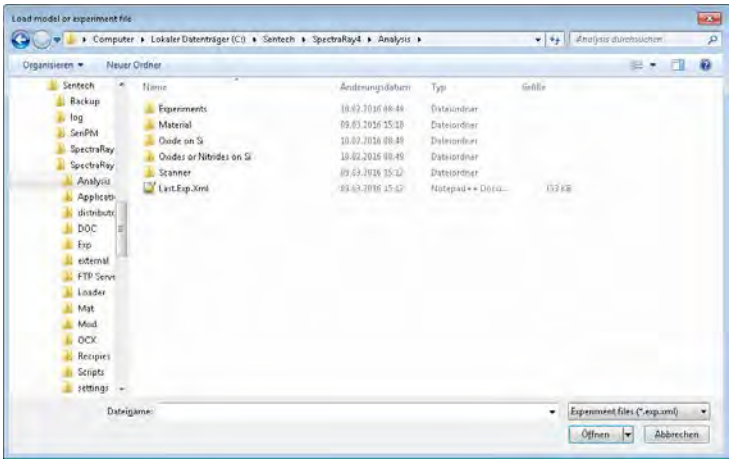


Fig. 4-40: Loading an experiment in the Load model or experiment window

4.5.8.6 Create a new Cauchy material

To model a new layer, a model type has to be selected. Clicking the Insert new layer button in the "Edit sample model" window brings the following window (Fig. 4-41):

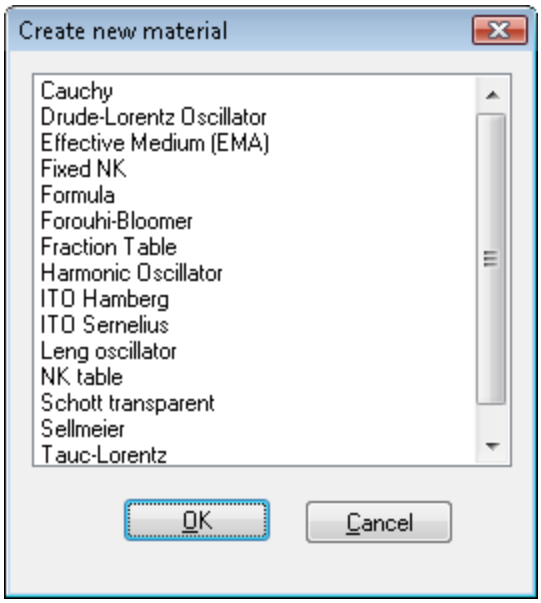


Fig. 4-41 Choose model type for the material

Now the new layer is shown in the "Edit Sample Model" window. Double clicking the new layer opens the "Layer editor" window (Fig. 4-42). In the example the name "NewCauchyMat" has been typed in. Additionally, in the table, values for thickness, n_o, n_1, and n_2 have been typed in.

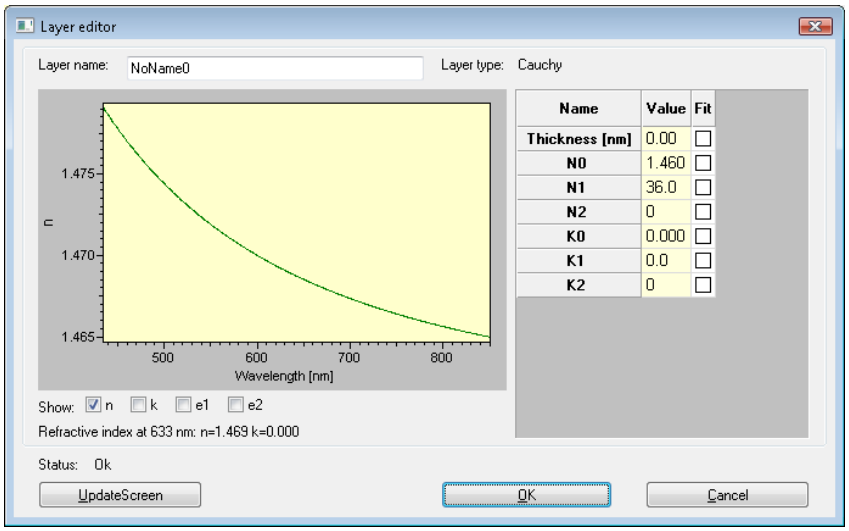


Fig. 4-42: Example for parameters of a new Cauchy layer with arbitrarily set values.

To save the material, click "save material" in the "Edit sample model" window and type in a name. Under this name the file is saved on the hard disk (NoName0 in the example).

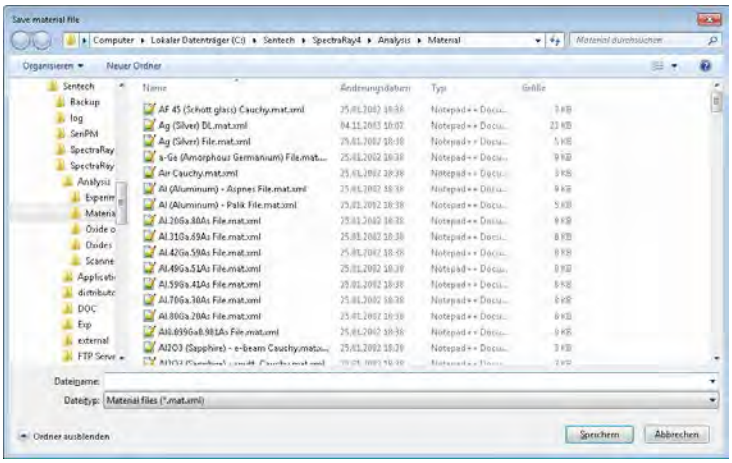


Fig. 4-43: Saving the material in a file

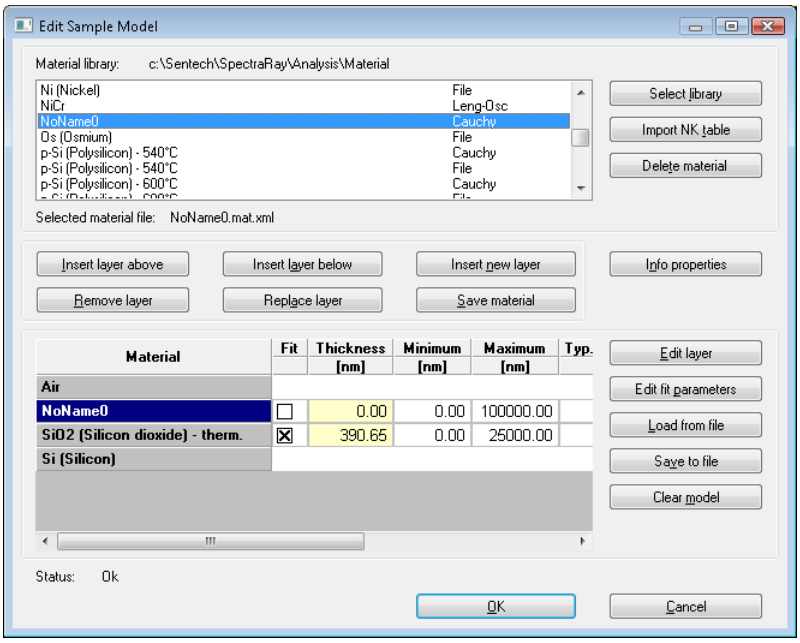


Fig. 4-44: The new material appears in the “Edit sample model” window

4.5.8.7 Create new NK table material

It is assumed that data from external sources (like books) have to be converted into a model. An ASCII table is needed as source with three columns: wavelength in nm, in ascending order, n and k (k<0). Fig. 4-45 shows an example of such a table. If one types the table manually, one should save it as ASCII or ANSI file (*.txt). If there are only zeros after the decimal point, they are not needed.

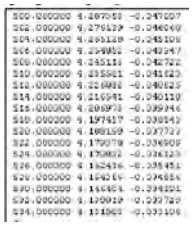


Fig. 4-45 Example for an (λ, n, k)-table

Clicking the Import NK table button in the top frame of the “Edit Sample Model” window brings the following window:

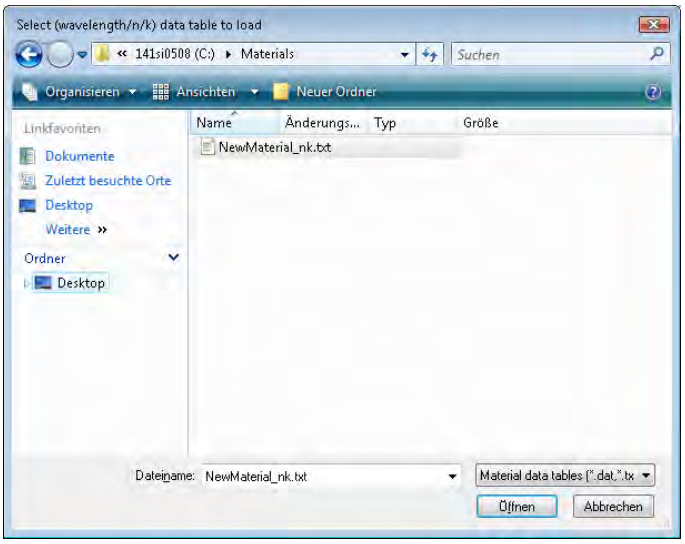


Fig. 4-46 Select a file containing an (λ, n, k) table

After selecting the file with the (λ, n, k) table, the following window appears:

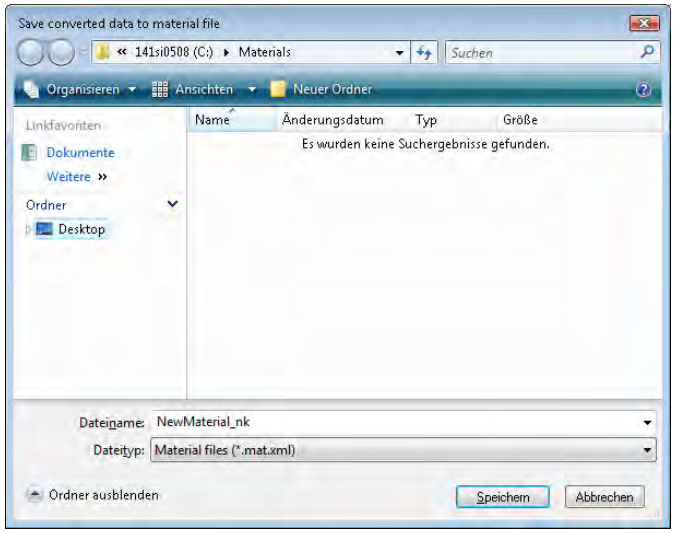


Fig. 4-47 Save the converted data table to a material file

After typing in a name (“NewMaterial_nk” in the example) the new material model can be found in the directory area of the Edit sample model window.

4.5.8.8 Theory on layer model types

4.5.8.8.1 Theoretical assumptions for a Cauchy-Layer

Most dielectric layers have a dielectric function ε(λ) near to a polynomial for a certain spectral range, but depends on the material. There are several polynomials suitable, but the Cauchy type is widely used for transparent and weakly absorbing films like photo resists, oxides or nitrides.

The Cauchy relation uses the first two even orders to approximate ε(λ) using coefficients for n and k (the wavelength λ given in nm):

$$n(\lambda) = n_0 + C_0 \frac{n_1}{\lambda^2} + C_1 \frac{n_2}{\lambda^4},$$

$$k(\lambda) = k_0 + C_0 \frac{k_1}{\lambda^2} + C_1 \frac{k_2}{\lambda^4},$$

$$C_0 = 10^2, \qquad C_1 = 10^7.$$

The coefficients C_0 and C_1 are used to avoid large numbers for n_1, k_1, n_2 and k_2 and their value agrees with most publications on Cauchy layers.

4.5.8.8.2 Theoretical assumptions for a NK-Layer with fixed refractive index and absorption

The simplest form of a dielectric function is a constant independent from any other parameter. This model is suitable for air (no high or low pressures), vacuum or for any measurement with single wavelength devices. Since at a fixed wavelength the dielectric function degrades to a dielectric constant

$$\tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2 \qquad \tilde{n} = n + ik \qquad \tilde{\varepsilon} = \tilde{n}^2$$

this layer type has only 2 constants: refractive index and extinction.

4.5.8.8.3 Theoretical assumptions for a Sellmeier layer

The Sellmeier relation works for transparent layers using the following formula:

$$n = \sqrt{1 + \sum_{i=1}^{3} \frac{A_i m}{m - B_i}}, \qquad k = 0, \qquad m = \left(\frac{\lambda}{1000}\right)^2, \qquad [\lambda] = \text{nm}.$$

4.5.8.8.4 Theoretical assumptions for a Drude-Lorentz oscillator layer

The dielectric properties of many materials in the far infrared and mid infrared spectral range can be described fairly well by the classical oscillator model. Mainly three contributions to the complex dielectric function $\tilde{\varepsilon} = 1 + \tilde{\chi}_{ve} + \tilde{\chi}_{ph} + \tilde{\chi}_{fc}$ are important:

1) The susceptibility of the valence electrons χ_{ve} which is a real constant in the IR range because the excitations of the valence electrons have much higher frequencies. As in general $\tilde{\varepsilon} = 1 + \tilde{\chi}$ a high frequency dielectric constant $\varepsilon_\infty = 1 + \chi_{ve}$ can be defined.

2) The excitation of a collective vibration of the atoms (which is called phonon) within a crystal by the incident light can be compared to an oscillator with center frequency Ω_0, strength Ω_p and damping Ω_τ, which is externally driven by the alternating electrical field of the light. The connection is given by a classical equation of motion. Often many vibrations (1...n) may be present. This leads to a frequency dependent susceptibility of the phonons $\tilde{\chi}_{ph}(\nu) = \sum_{k=1}^{k=n} \frac{\Omega_{pk}^2}{\Omega_{ok}^2 - \nu^2 - i\Omega_{\tau k}\nu}$.

Please note that we use capital letters $\Omega_{0,p,\tau}$ for the oscillator parameters in this case.

3) The presence of free charged carriers in a material, e.g. electrons in a metal or in a doped semiconductor, leads to a contribution $\chi_{fc} = \frac{\omega_p^2}{-\nu^2 - i\omega_\tau \nu}$, which looks like an oscillator with center frequency $\omega_0 = 0$.

Please note that we use small letters $\omega_{p,\tau}$ for the fit parameters in this case.
These spectroscopic values are connected with the values of the free charged carriers by the relations

$\omega_p = \sqrt{\frac{ne^2}{\varepsilon_0 m^*}}$ and $\omega_\tau = \frac{e}{m^* \mu}$, where n is the concentration, μ the mobility and m^* the effective mass of the carriers and ε_0 the permittivity of free space.

4.5.8.8.5 Theoretical assumptions for a Leng-Lorentz oscillator layer

The formula published by Leng [J. Leng, J. Opsal, H. Chu, M. Senko, D.E. Aspnes, "Analytic representations of the dielectric functions of materials for device and structural modeling", Thin Solid Films 313-314 (1998) 132-136] uses a damped oscillator model. SENTECH has expanded this formula by a non-constant offset in the real part and a constant offset in the imaginary part. The complete formula is shown below.

$$\epsilon(E) = \epsilon_\infty + \sum_{i=1}^{N} \left(\frac{C_{0_i}}{E^2} \left[e^{\imath\beta_i} (E_{g_i} - E - \imath\Gamma_i)^{\mu_i} + e^{-\imath\beta_i} (E_{g_i} + E + \imath\Gamma_i)^{\mu_i} \right.\right.$$
$$\left.\left. - 2\,\mathrm{Re}\left[e^{-\imath\beta_i} (E_{g_i} + \imath\Gamma_i)^{\mu_i} \right] - 2\imath\mu_i E\,\mathrm{Im}\left[e^{-\imath\beta_i} (E_{g_i} + \imath{\Gamma_i}^{\mu_i - 1} \right] \right] \right)$$
$$+ m_0 E^{x_0} + \imath k_0$$

It is recommended to use this formula for crystalline semiconductors or alloys.

4.5.8.8.6 Theoretical assumptions for a Forouhi Bloomer layer

The Forouhi Bloomer relation was developed to model the dielectric function of amorphous semiconductors [Reitano et al. "Spectroscopic ellipsometry of a-Si" Thin solid films, 233 (1993) 203-206]. A typical example of this material is a-Si which is difficult to model by means of other common dispersion relations. The dispersion uses five parameters for n and k in the following formulae:

$$n(E) = n(\infty) + \frac{B_0 E + C_0}{E^2 - BE + C},\quad k(E) = \frac{A(E - E_g)^2}{E^2 - BE + C},$$

$$Q = \frac{1}{2}\sqrt{4C - B^2},\qquad B_0 = \frac{-AB^2}{Q(2 + E_g B - E_g^2 + C)},\quad C_0 = \frac{AB(E_g^2 + C)}{Q(2 - 2E_g C)}.$$

4.5.8.8.7 Theoretical assumptions for a Schott transparent layer

This expression was developed for modeling Schott glass materials by means of six parameters

$$n = A_0 + A_1 m + \frac{A_2}{m} + \frac{A_3}{m^2} + \frac{A_4}{m^3} + \frac{A_5}{m^4},\qquad k = 0,$$
$$m = \left(\frac{\lambda}{1000}\right)^2,\ [\lambda] = \mathrm{nm}.$$

As it is clear the relation works for transparent materials.

4.5.8.8.8 Theoretical assumptions for a Tauc-Lorentz layer

The Jellison-Modine model [G.E.Jellison Jr., F.A.Modine, P. Doshi, A.Rohatgi" Spectroscopic ellipsometry characterization of thin-film silicon nitride", Thin Solid Films 313-314 (1998) 193-197] uses the Tauc-Lorentz formula. It has been developed for Silicon nitride and amorphous semiconductors. It is based on an oscillator expression for ε_2 and the Kramers-Kronig integral is used to obtain ε_1 (the software uses multiple oscillators, but here is the presentation for a single oscillator only):

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0C(E-E_g)^2}{(E^2-E_0^2)^2+C^2E^2}\frac{1}{E} & E > E_g \\ 0 & E \le E_g \end{cases}$$

$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{x\varepsilon_2(x)}{x^2 - E^2} dx$$

This layer type has 4N+1 constants if N is the number of oscillators (infinity is typically fixed at near 1).

4.5.8.8.9 Theoretical assumptions for a Cody-Lorentz layer

Ferlauto et al. introduced the Cody_lorentz layer in combination with an Urbach absorption tail [A.S. Ferlauto, G.M. Ferreira, J.M. Pearce, C.R.Wronski, R.W.Collins, Journal of Applied Physics, Volume 92, No. 5 (2002), 2424", Thin Solid Films 313-314 (1998) 193-197] as a modification of the Tauc-Lorentz formula. It has been developed for amorphous materials. It is based on an oscillator expression for ε_2 and the Kramers-Kronig integral is used to obtain ε_1 (the software uses multiple oscillators, but here is the presentation for a single oscillator only):

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0CE(E-E_g)^2}{\left(\left(E^2-E_0^2\right)^2+C^2E^2\right)\left((E-E_g)^2+E_P^2\right)} & E > E_t \\ \frac{E_1}{E}\exp\left(\frac{(E-E_t)}{E_u}\right) & E \le E_t \end{cases}$$

$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{x\varepsilon_2(x)}{x^2 - E^2} dx$$

This layer type has 7N+1constants if N is the number of oscillators (infinity is typically fixed at near 1).

4.5.9 AutoModel Database Editor

Under certain conditions it is possible to detect sample types by the AutoModel feature, a fast comparison with a spectrum library. One can use a measured spectrum (called experiment) to calculate sets of spectra of the same layer system, but with varying thicknesses. The AutoModel Database editor can be found in the main menu under Edit or in the Recipe options. It allows generating, modifying, or deleting the databases for the AutoModel feature.

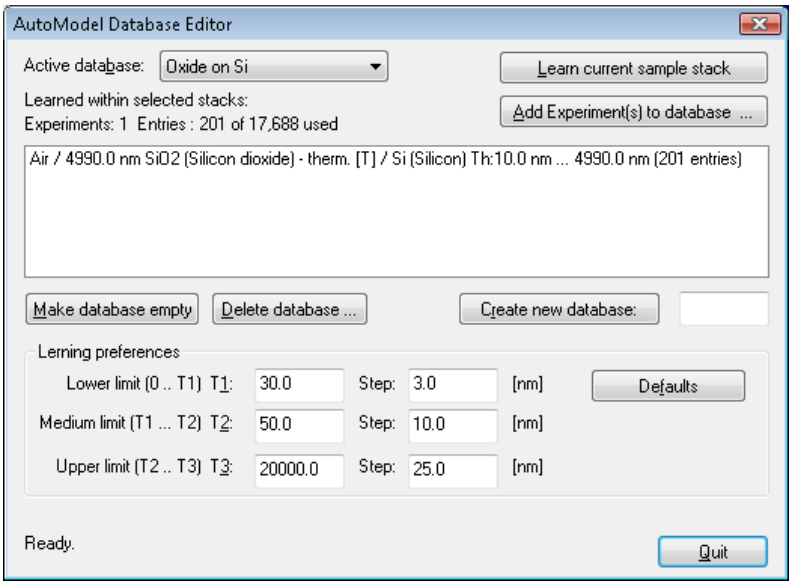


Fig. 4-48 The AutoModel Database editor.

To create a new database type a name right to the button "Create new database" and click the button. If you have just performed a measurement, you may click "Learn current sample stack" to let the software generate a set of curves with the current recipe. The frame "learning preferences" contains information on step width and range of the thicknesses for these calculations. Clicking "Defaults" sets the default values for the step widths and limits. With "Make database empty" you may delete the entries from the selected database. With "Delete database…" you may delete an active database, except the default database "scanner".
With "Add Experiment(s) to database" you may select a saved experiment and add it to the database (see chapter 4.5.9).

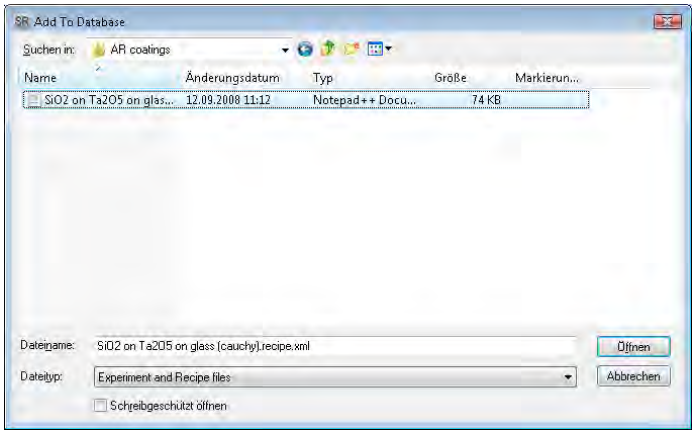


Fig. 4-49 Adding saved experiments to the AutoModel database.

4.6 Print reports

The report allows printing the curves of measurement and model together with a list of the fit parameters and fit options. This option is available from the menu "File\Print report" in the main menu or from the Print icon in the icon bar.
To print a report of the measurement on the windows default printer click:

If you want to print on a specific printer or if you would like to preview the report click:

Then the following preview window appears. You may also use menu “File\Show report” for a preview.

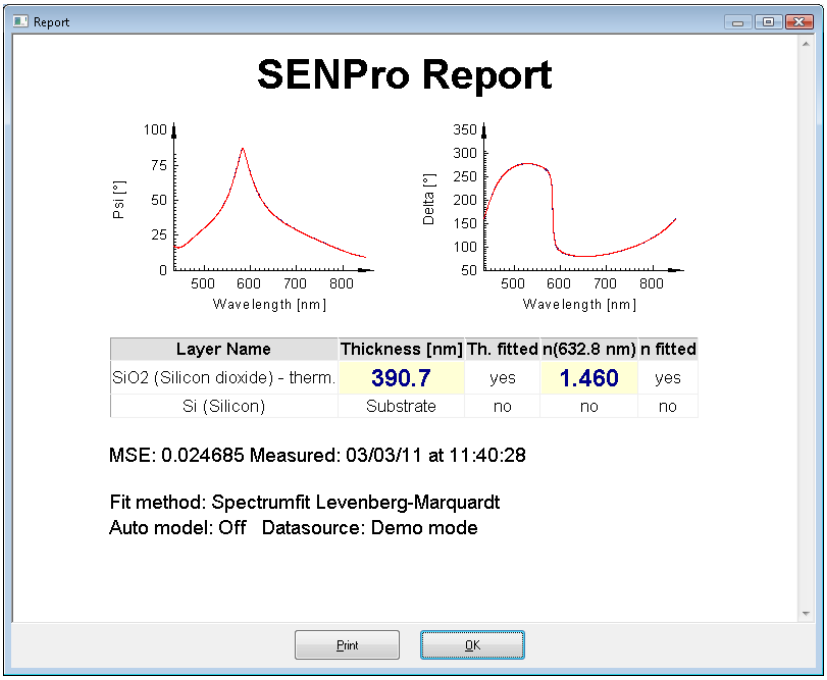


Fig. 4-50: Preview of a print report of a measurement showing the (Ψ, Δ) versus wavelength and the layer stacks with the used and fitted parameters. Click Print to select a printer, OK to leave without printing.

4.7 Print setup

The print setup window is available from “File\print setup” and allows selecting and changing the settings of the printer used for printing the reports.

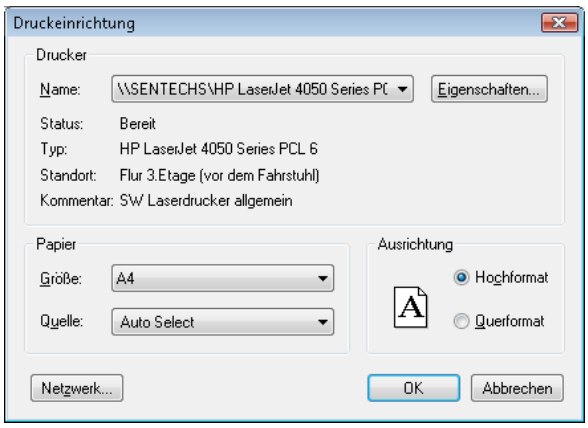


Fig. 4-51: The print setup window

5 SE-Advanced module

The SE-Advanced Module is a powerful software package designed for simulating, fitting and measuring data of spectroscopic ellipsometers (DUV, UV/VIS, NIR and MIR), single wavelength ellipsometers and for processing data of reflection and transmission measurements. The functionalities of this module are described in the following chapters.

5.1 Measurements

Clicking on  in the tool bar opens the measurement window shown below.

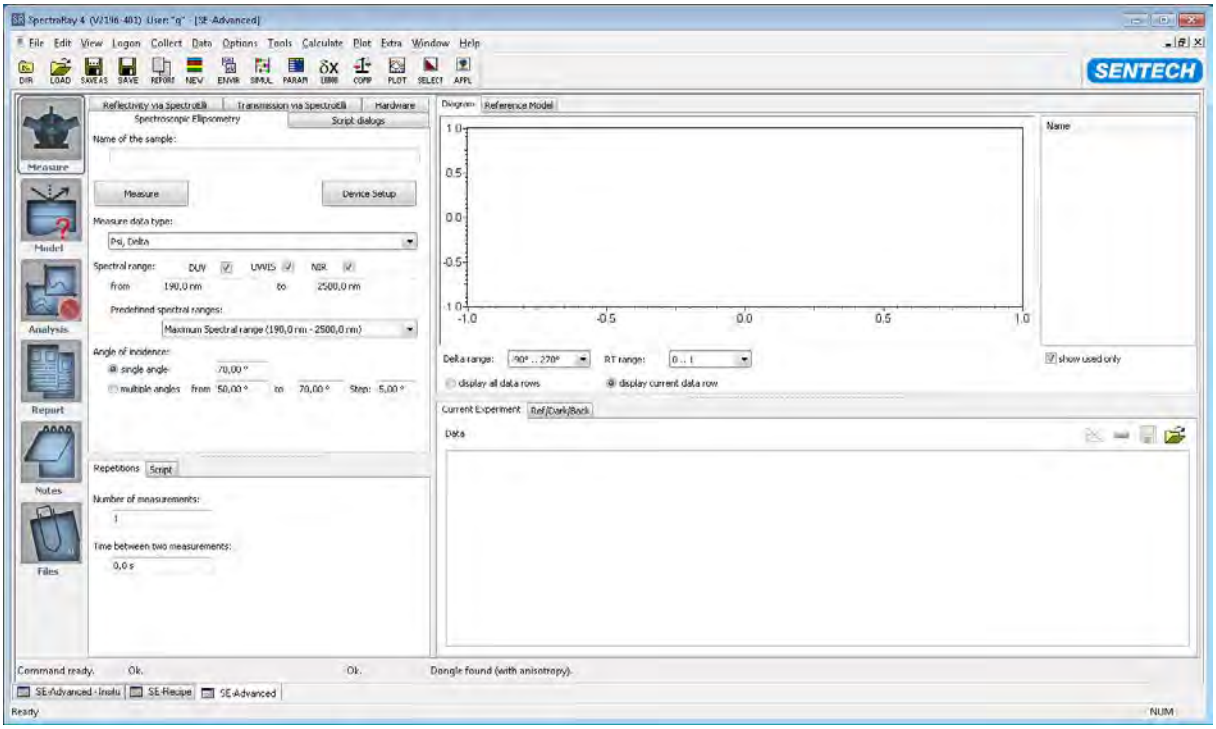


Fig. 5-1 Measurement settings

The measurement-window consists of 4 sub-windows for measurement settings, display of measured data and datasets. In the following sections the functions of these sub-windows will be described.

5.1.1 Measurement settings

The measurement settings tabs are located in the left part of the measurement window.

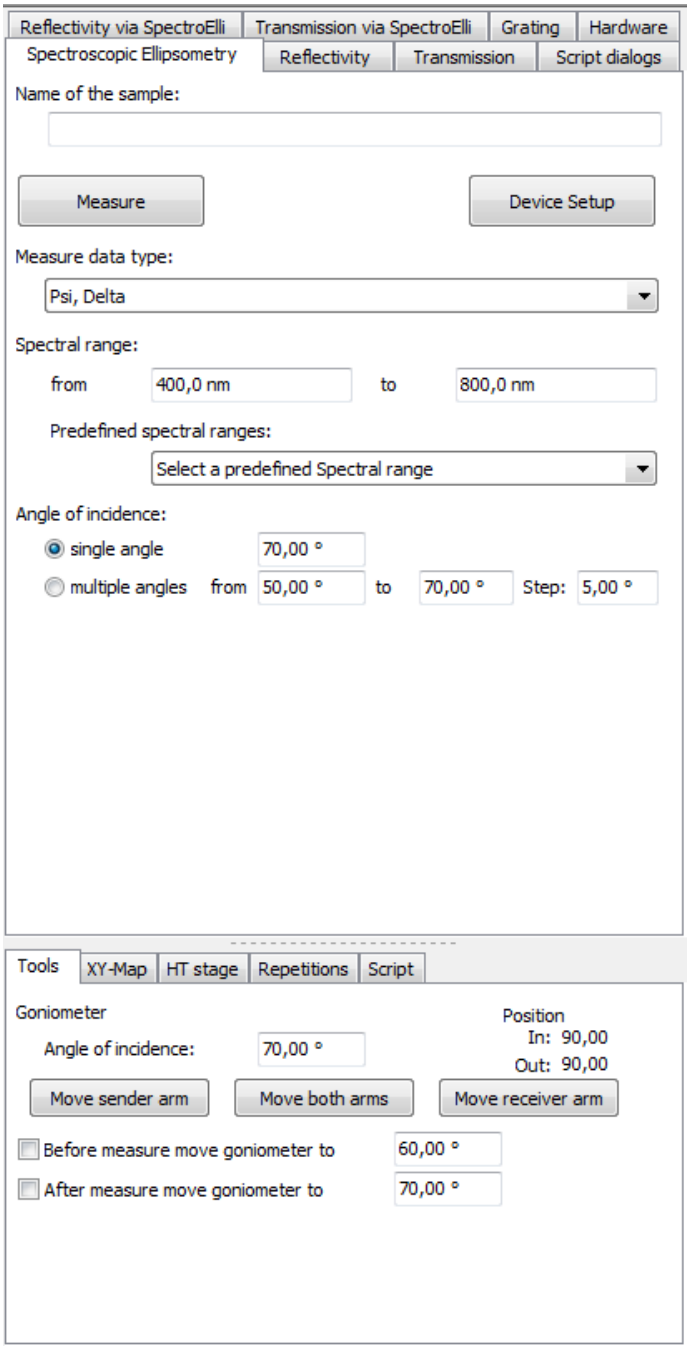


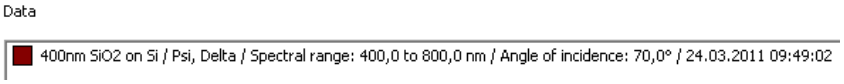
Fig. 5-2 Measurement settings in the measurement window

Here you have different tabs for all settings of the measurement devices. The number of tabs depends on the installed measurement devices and options.

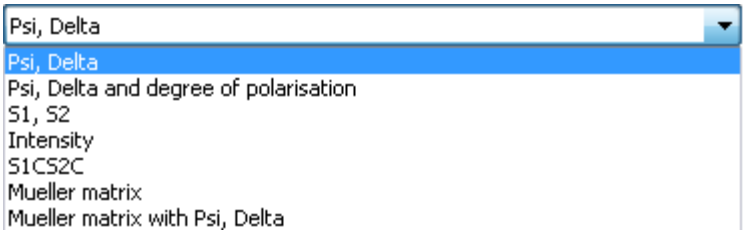
5.1.1.1 Spectroscopic ellipsometry

Fig. 5-2 shows in the upper part the measurement settings for ellipsometry measurements. You can choose a name for the sample you want to measure.

This name will be part of the title of the measured data set:



The title of the data set contains also the selected measurement mode,

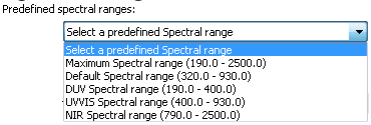


the selected spectral range,

the angle of incidence (or range of angles of incidence)

and date and time of the measurement.

It is also possible to select predefined spectral ranges.



Clicking on 

starts the measurement with the selected parameters. After the measurement is finished the resulting data set appears in the list in the lower right part of the measurement window and the curves are displayed in the upper right part of the measurement window (diagram).

Clicking on 

opens the device driver. Here you can set more specific parameters of the measurement (see chapter 1).

5.1.1.2 Spectroscopic Mueller matrix ellipsometry

Selecting the measurement mode “Mueller matrix” or “Mueller matrix with Psi, Delta” allows measuring the Mueller matrix of a sample. Depending on your ellipsometer setup you can measure all 16 elements of the Mueller matrix or only a subset (9 or 12 elements, see Fig. 5-3).

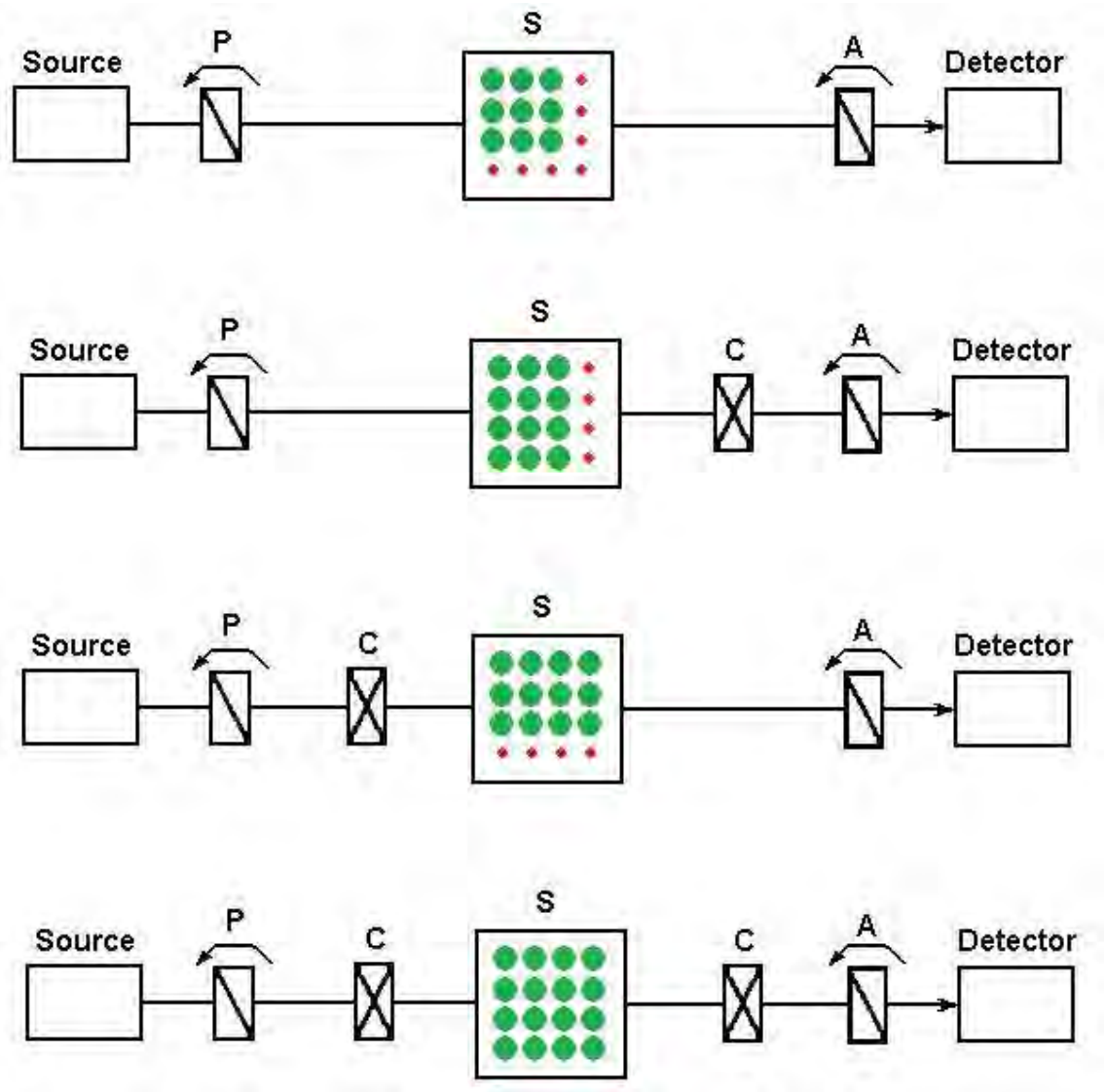


Fig. 5-3 Setups for Mueller matrix measurements

Fig. 5-4 shows the Mueller matrix measurement mode. For measuring the Mueller matrix the Fourier-coefficients s1/s2 without retarder and s1c/s2c with retarder at different polarizer positions have to be measured. “Pol. Steps” defines the polarizer step width for the Fourier-coefficient measurements. When 45 ° is selected only the minimal count of Fourier-coefficient measurements is made for calculating the Mueller matrix (PCSA: 6 measurements, PSCA: 7 measurements, PCSCA: 10 measurements). When 2° is selected additional measurements will be made with 2° step width between -90° and +90° of the polarizer. The additional measurements will be used for fitting the Mueller matrix elements to the measured curves so that you get elements with a higher accuracy.

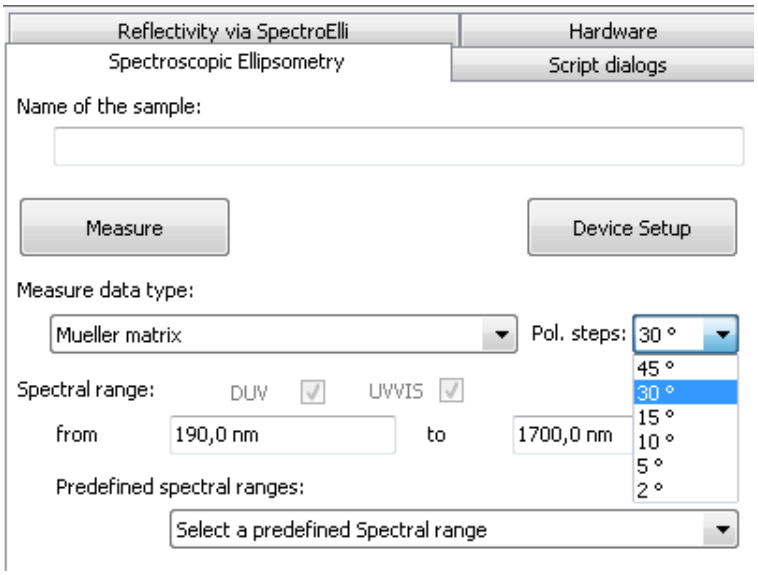


Fig. 5-4 Measurement mode Mueller matrix

After measuring the Mueller matrix a data set will be created containing the Mueller matrix elements, all the measured spectra of the Fourier-coefficients, maximum intensities and the properties of the retarders used for calculating the Mueller matrix elements (see Fig. 5-5-5-6).

Assuming an isotropic sample (Ψ,Δ)-spectra can be extracted from the Mueller matrix too (->measurement mode “Mueller matrix with Psi, Delta”).

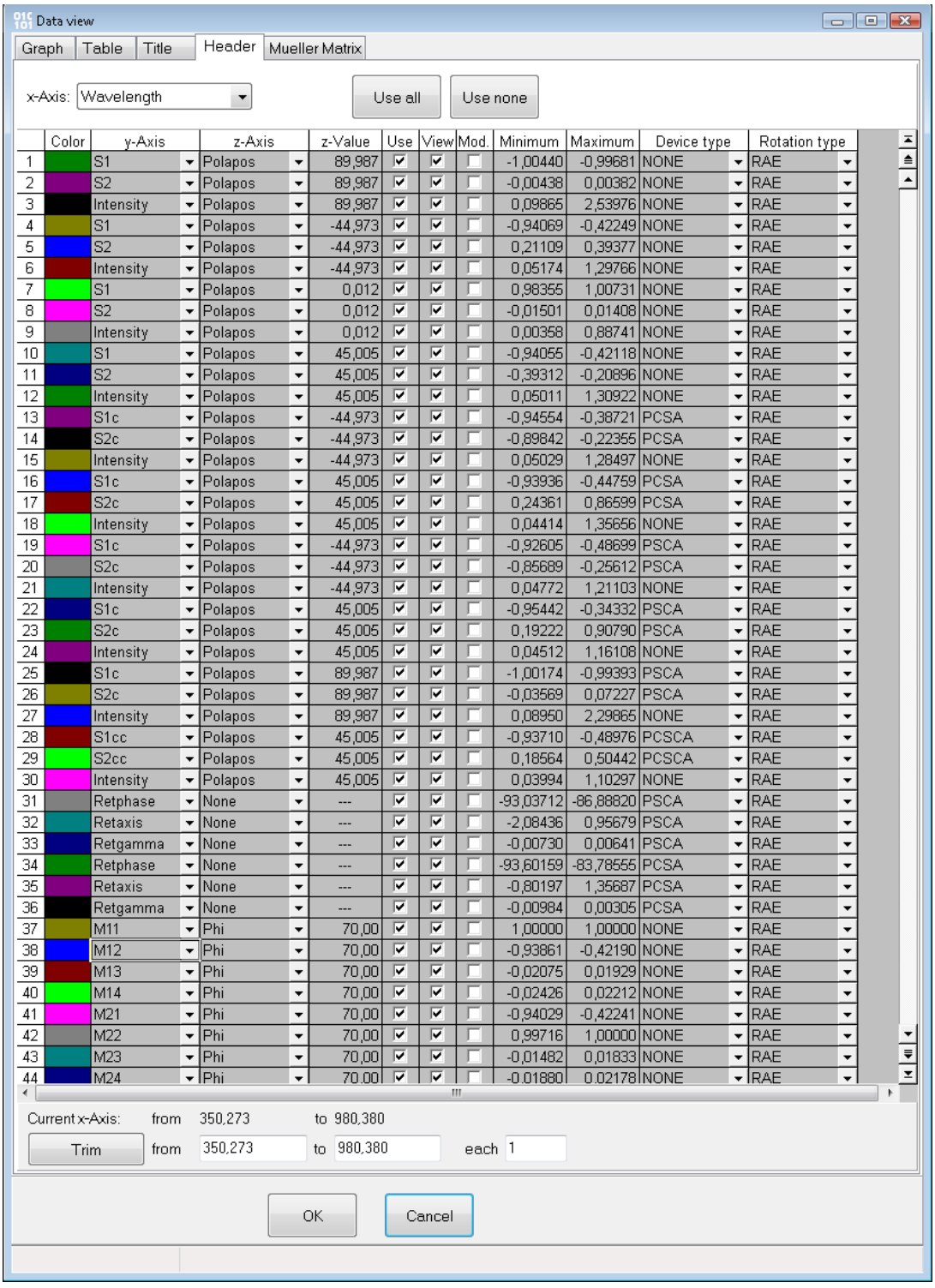


Fig. 5-5-5-6 Header-page of a Mueller matrix data set

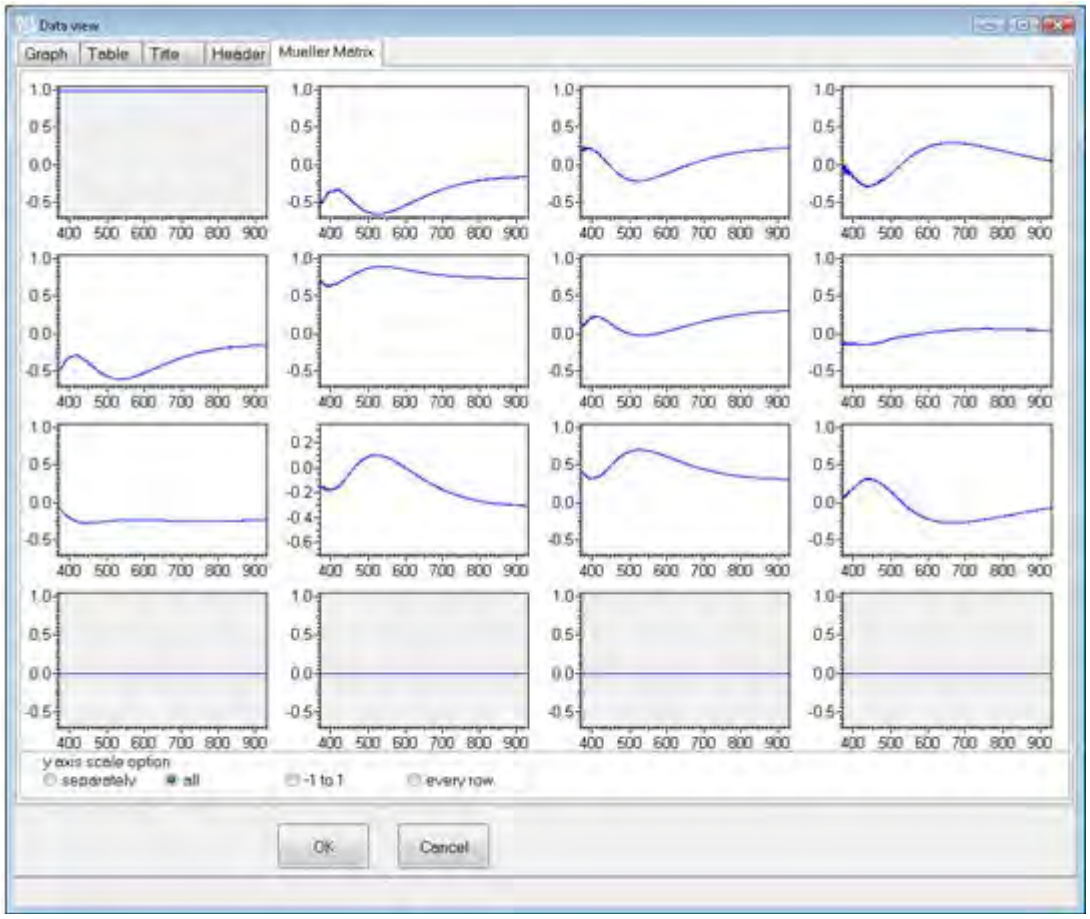


Fig. 5-7 Mueller matrix spectra

The 16 graphs in Fig. 5-7 show the 16 Mueller matrix elements in dependence of the wavelength. Depending on the measurement device 12 (PCSA[3] or PSCA) or 16 (PCSCA) elements can be measured. The first element M11 of the Mueller matrix is used for scaling and is fixed to 1 (-> grey background). The graphs in the 4th row also have a grey background and are set to zero because these elements were not measured (-> PCSA-device).

Fig. 5-8 shows a measurement of a complete Mueller matrix using a PCSCA device. This means that the ellipsometer has two retarders, one in the sender arm and one in the receiver arm. This is an extra option; the standard ellipsometers only have one retarder and only can measure 12 of the 16 elements.

[3] Setup principle of the ellipsometer with component list from source to detector (P-polarizer, C-retarder, S-sample, A-Analyzer).

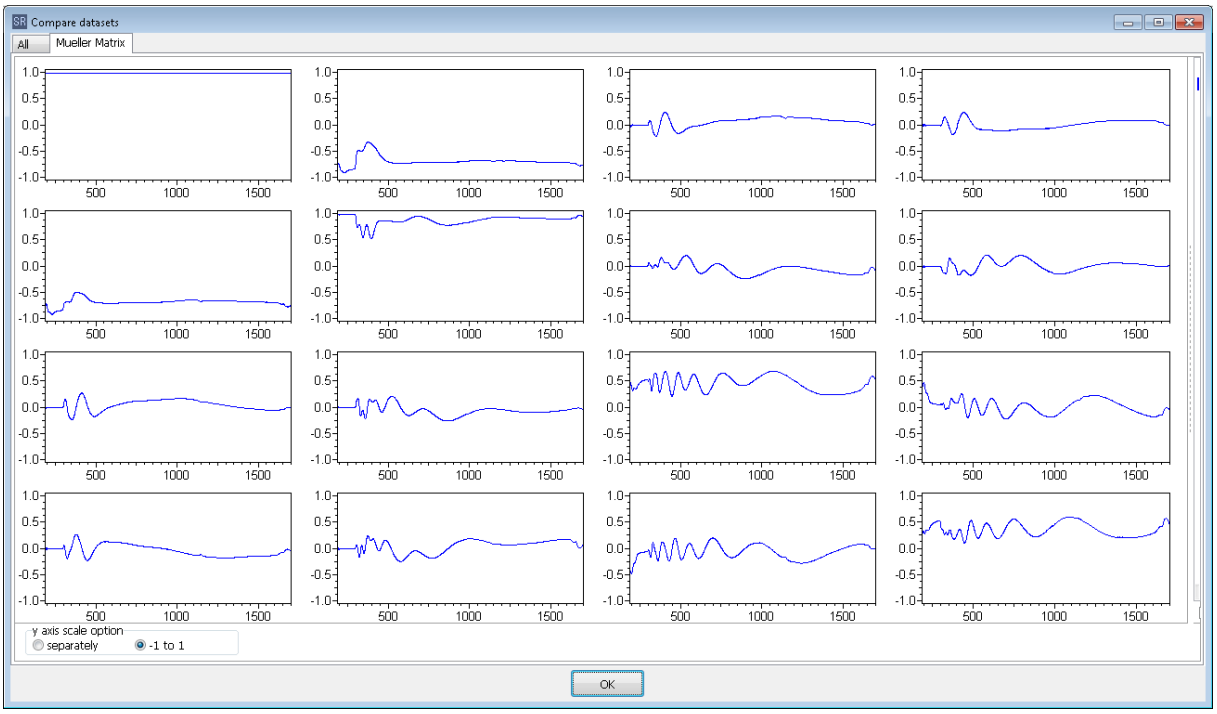


Fig. 5-8 Mueller matrix measurement with a PCSCA device

5.1.1.3 Reflectivity

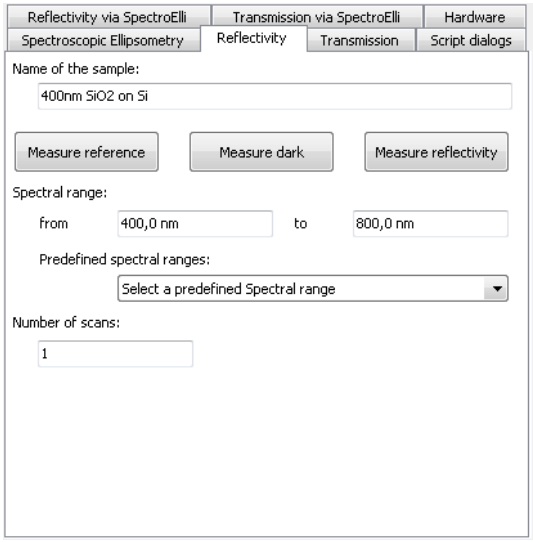
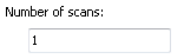


Fig. 5-9 Settings for reflectivity measurements

There are two possible configurations for measuring the reflectivity. It is possible to measure the reflectivity with the spectroscopic ellipsometer for s- or p-polarization and for different angles of incidence (see chapter 5.1.1.6). On the other hand you can measure the reflectivity with a special hardware configuration at an angle of incidence of 0° (additional (optional) hardware needed). Fig. 5-9 shows the tab for the settings of the reflectivity measurements with the special hardware configuration. Just like for spectroscopic ellipsometry you have the possibility to choose a name for the sample you want to measure and to select a specific or predefined spectral range. Additional you have to set the number of scans for averaging of the reflectivity measurement.



Before you can start your first measurement by clicking on 

you have to measure reference and dark spectra by clicking 

and 

. For the reference measurement you need a special reference sample (e.g. native oxide on Si) and a suitable reference model (“Refernce model”-tab in the upper right part). For the dark measurement you need a special tool which reflects all of the light out of the light path. Dark and reference measurements will also be stored in the list of the “Ref/Dark/Back” tab in the lower right part of the measurement window.
After the reflectivity measurement is finished the resulting data set appears in the list in the lower right part of the measurement window and the curve is displayed in the upper right part of the measurement window (diagram).

5.1.1.4 Transmission

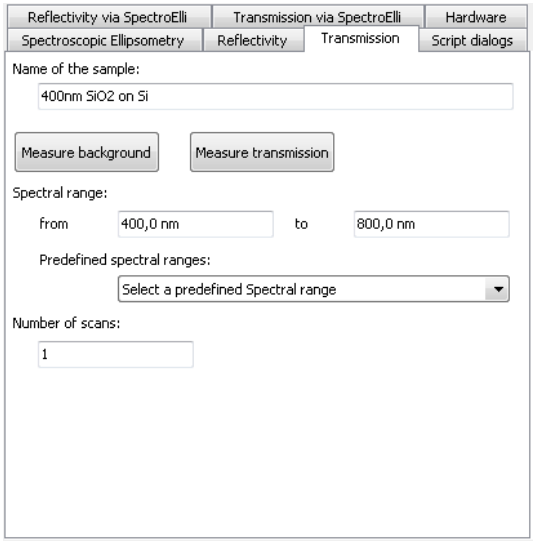
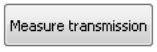


Fig. 5-10 Settings for transmission measurements

There are two possible configurations for measuring the transmission. It is possible to measure the transmission with the spectroscopic ellipsometer with a special transmission holder (see chapter 5.1.1.7). On the other hand you can measure the transmission with a special (optional) hardware configuration at an angle of incidence of 0°. Fig. 5-10 shows the tab for the settings of the transmission measurements with the special hardware configuration. This tab is mostly identical to the “Reflectivity”-tab.

Before you can start your first measurement by clicking on 

you have to measure a background spectrum without any sample in the light path by clicking 

. The background measurement will also be stored in the list of the “Ref/Dark/Back” tab in the lower right part of the measurement window.
After the transmission measurement is finished the resulting data set appears in the list in the lower right part of the measurement window and the curve is displayed in the upper right part of the measurement window (diagram).

5.1.1.5 Script dialogs

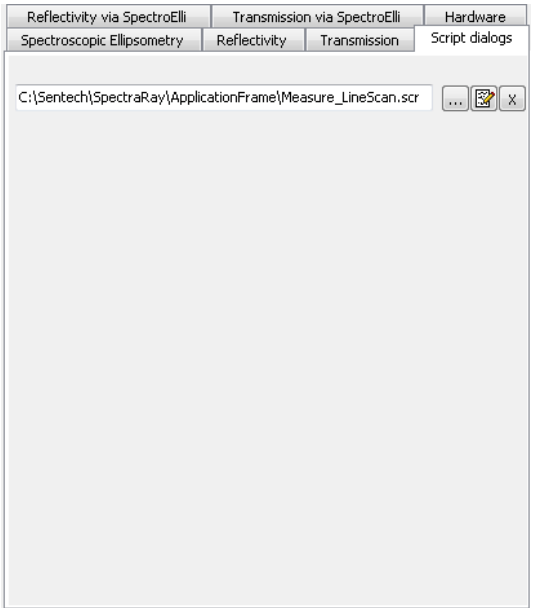


Fig. 5-11 Script dialogs tab

When you click on ... a file dialog will be opened and you can select and load a script file. The scripting allows creating an individual dialog for special measurement requirements as shown in Fig. 5-12.

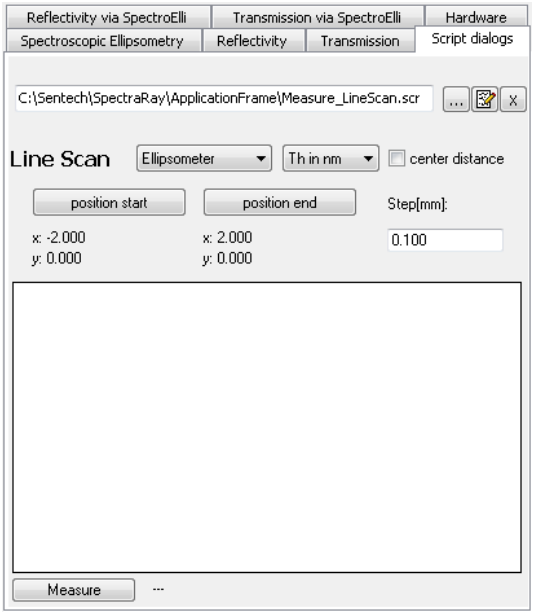


Fig. 5-12 Example for a script dialog

Clicking on opens the script editor for editing the selected script file.

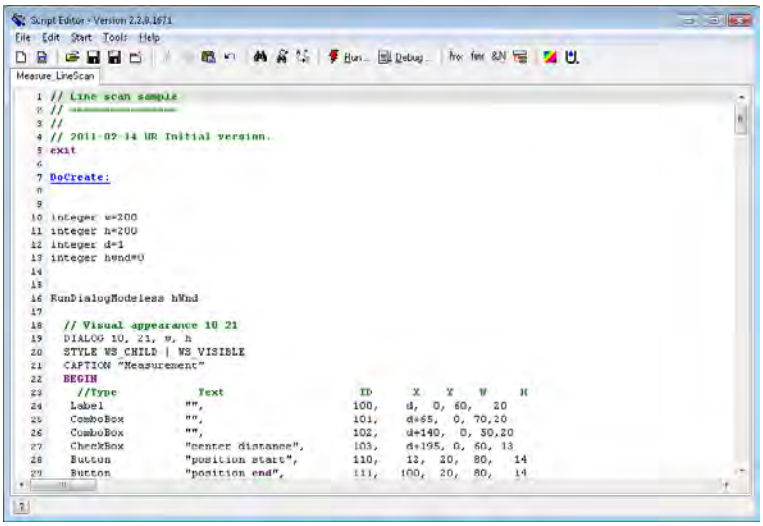


Fig. 5-13 Scripting example

Clicking on  unloads the selected script and the tab appears as shown in Fig. 5-11.

5.1.1.6 Reflectivity via SpectroElli

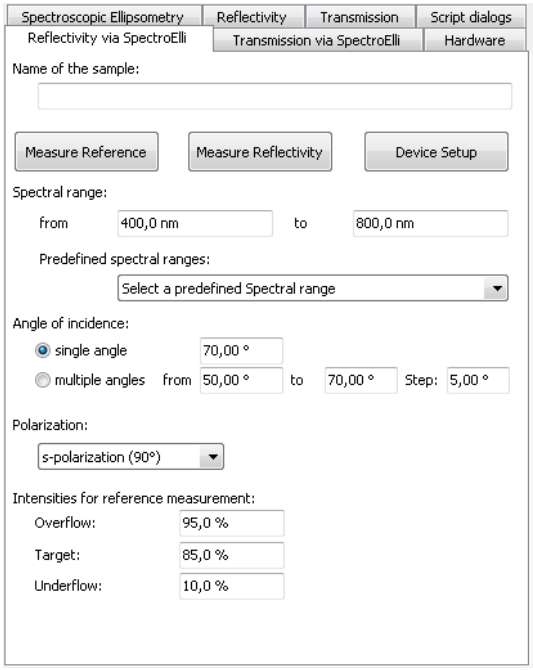
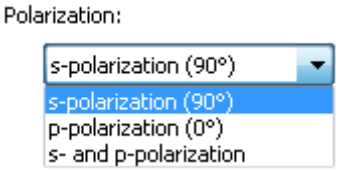


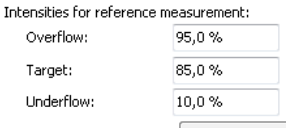
Fig. 5-14 Reflectivity via SpectroElli

There are two possible configurations for measuring the reflectivity. It is possible to measure the reflectivity with the spectroscopic ellipsometer for s- or p-polarization and for different angles of incidence. On the other hand you can measure the reflectivity with a special hardware configuration at an angle of incidence of 0° (see section 5.1.1.3). Fig. 5-14 shows the tab for the settings for reflectivity measurements with the spectroscopic ellipsometer.
Just like for spectroscopic ellipsometry you have the possibility to choose a name for the sample you want to measure and to select a specific or predefined spectral range.
You can measure the reflectivity at specific/multiple angles of incidence

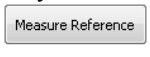
and for p- or s-polarization of the incident beam.



Finally you can set a maximum, minimum and target intensity for the automatic search of the integration time.



Before you can start your first measurement by clicking on 

you have to measure a reference spectrum by clicking 

. For the reference measurement you need a special reference sample (e.g. native oxide on Si) and a suitable reference model (“Refernce model”-tab in the upper right part).The reference measurements will also be stored in the list of the “Ref/Dark/Back” tab in the lower right part of the measurement window.

Clicking on 

opens the device driver. Here you can set more specific parameters of the measurement (see chapter 1).

5.1.1.7 Transmission via SpectroElli

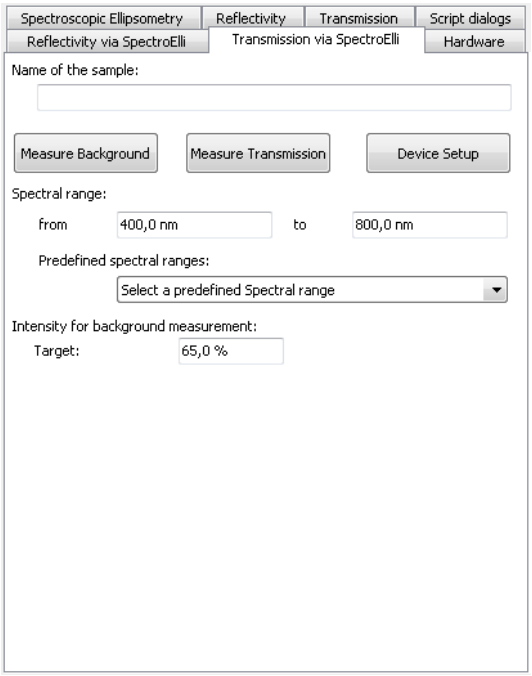
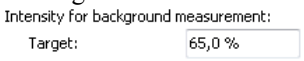


Fig. 5-15 Transmission via SpectroElli

There are two possible configurations for measuring the transmission. It is possible to measure the transmission with the spectroscopic ellipsometer with a special transmission holder. On the other hand you can measure the transmission with a special hardware configuration at an angle of incidence of 0° (see section 5.1.1.4). Fig. 5-15 shows the tab for the settings of the transmission measurements with the spectroscopic ellipsometer.
Just like for spectroscopic ellipsometry you have the possibility to choose a name for the sample you want to measure and to select a specific or predefined spectral range.
Finally you can set a target intensity for the background measurement.



Before you can start your first measurement by clicking on 

you have to measure a background spectrum without any sample in the light path by clicking 

. The background measurements will also be stored in the list of the “Ref/Dark/Back” tab in the lower right part of the measurement window. All the measurement will be made at 90° settings of the goniometer which means 0° angle of incidence on the sample which has to be mounted on a special transmission sample holder.

Clicking on 

opens the device driver. Here you can set more specific parameters of the measurement (see chapter 1).

5.1.1.8 Grating

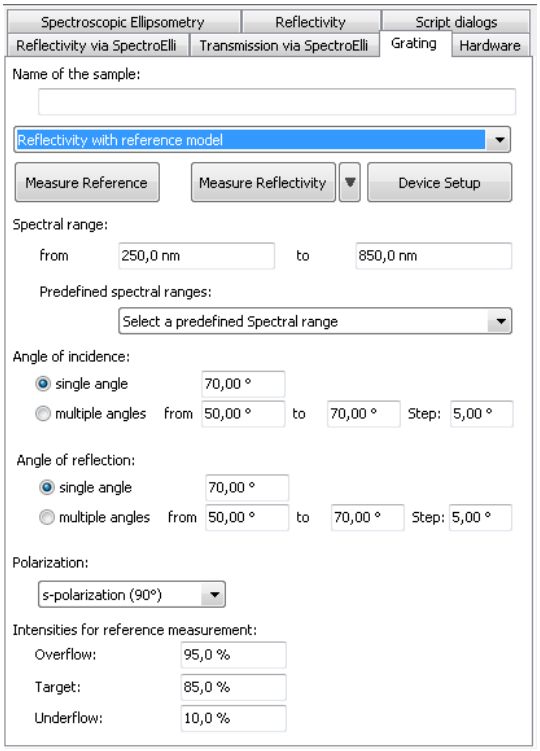
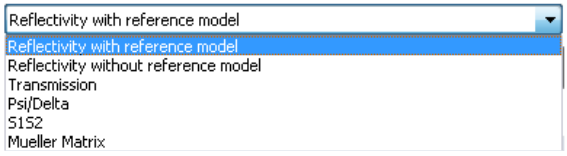


Fig. 5-16 Tab for measuring gratings

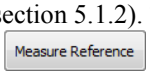
If this option is installed it allows measuring with different settings for sender and receiver arms. This may be interesting e.g. for measuring different diffraction orders of gratings. Just like for the other measurement options you have the possibility to choose a name for the sample you want to measure and to select a specific or predefined spectral range. There are several measurement modes like reflectivity, transmission, Psi/Delta, Fourier coefficients or Mueller matrix.



Usually the angles of the sender and receiver are identical. This measurement mode allows selecting different angles for the sender and for the receiver. For each mode you can select a single or multiple angles of incidence (angles of the sender arm) and a single or multiple angles of reflection (angles of the receiver arm).

This allows you to measure e.g. in reflection with an angle of incidence of 70° and different angles of reflection (e.g. on gratings) or in transmission with angle of incidence of 85° and an angle of reflection of 95° (special goniometer settings needed), which means an angle of incidence of 5° in the reference plane of the sample (e.g. on anisotropic transparent samples). In principle all combinations of incidence and reflection angles are possible.

5.1.1.8.1 Reflectivity with reference model

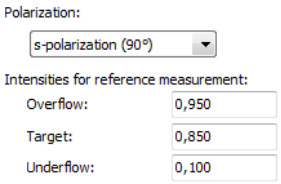
Fig. 5-16 shows the measurement settings for reflectivity measurements with a reference model. In this mode you have to create a reference model (see section 5.1.2). The reference measurement on a suitable reference sample (e.g. native oxide on Si) started by 

will be related to this reference model and the measured counts will be translated to a reflectivity (0…1). The reference measurement serves as a calibration of the measured intensity. This calibration allows evaluating the reflectivity for the following reflectivity measurements started by 

.

The button 

opens the device driver described in section 1. Similar to the reflectivity measurements via SpectroElli (see section 5.1.1.6) you can also set the polarization state of the incident beam and the intensities for the reference measurement.



5.1.1.8.2 Reflectivity without reference model

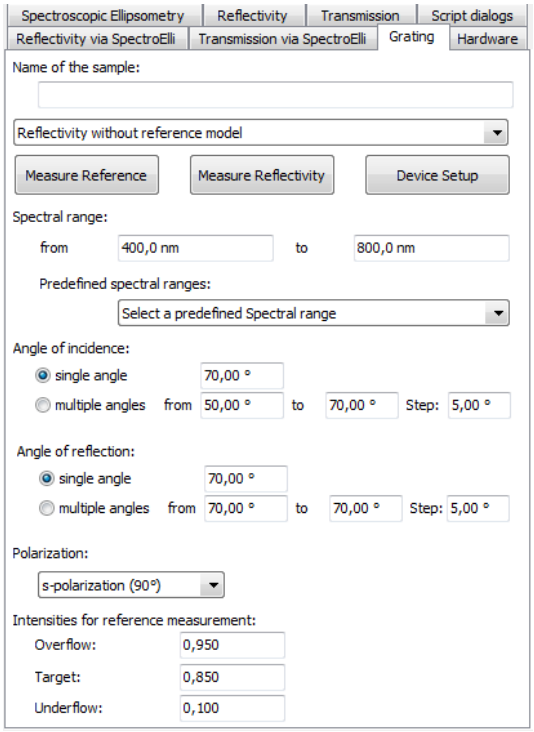
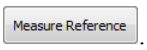


Fig. 5-17 Reflectivity without reference model

Fig. 5-17 shows the measurement settings for reflectivity measurements without reference model. You just have to make a reference measurement (for example the zero order of diffraction) by clicking 

. All other reflectivity measurements are related to this reference measurement only. So you just measure a relative reflectivity no absolute reflectivity. The measurement settings are identical to the “Reflectivity with reference model”-mode (see section 5.1.1.8.1).

5.1.1.8.3 Transmission

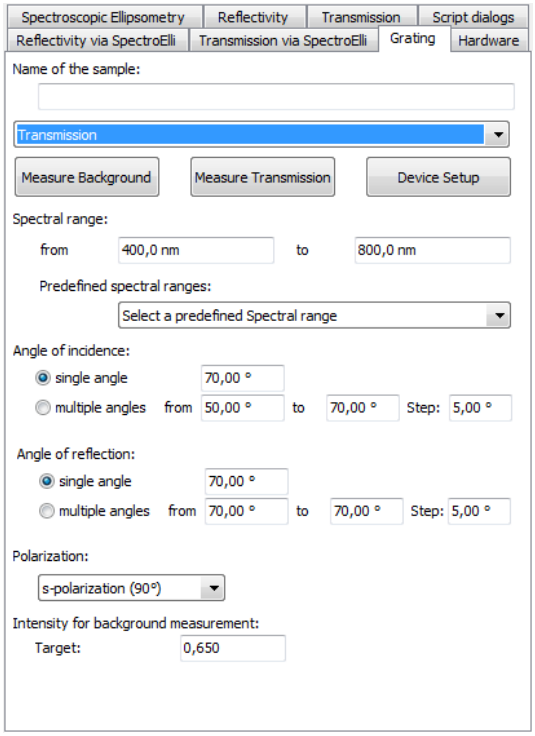


Fig. 5-18 Transmission of samples

Fig. 5-18 shows the measurement settings for transmission measurements of gratings. This tab allows measuring the transmission of samples for different angles. So you are able to measure the transmission for a fixed angle of incidence and fixed angle/multiple angles of the sender arm. The measurement settings shown in Fig. 5-18 are already described in the previous sections (see for example section 5.1.1.7).

5.1.1.8.4 Psi/Delta, S1S2 and Mueller Matrix

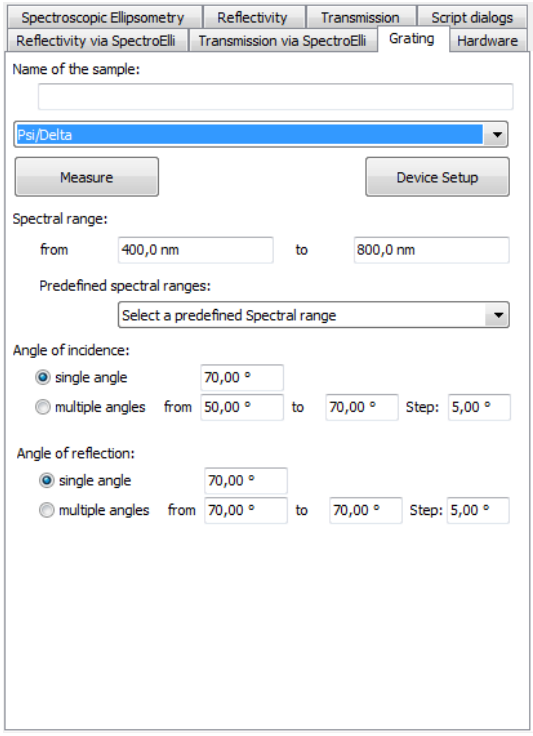


Fig. 5-19 Psi/Delta for the measurement of gratings

Fig. 5-19 shows the measurement settings for (Ψ, Δ) measurements of samples. This tab allows measuring the (Ψ, Δ)-spectra of samples for different angles of incidence and reflection. The measurement settings shown in Fig. 5-19 are already described in the previous sections (see section 5.1.1.1) with the only difference that different angles for sender and receiver can be set. It is also possible to measure S1/S2 and the Mueller matrix in the same way.

5.1.1.9 Hardware

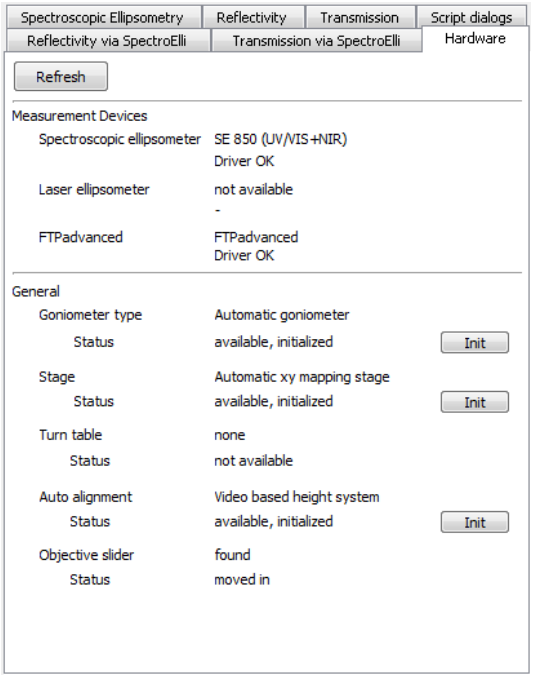


Fig. 5-20 Hardware tab

The hardware tab shows the installed hardware equipment and allows initializing the hardware like automatic goniometers or mapping stages by clicking on Init. Clicking on Refresh will search for connected hardware and update the hardware tab. In the upper part the installed measurement devices are listed. In the second part the installed options like automatic goniometer, mapping stage or turn table with their actual status are shown.

5.1.1.10 Tools

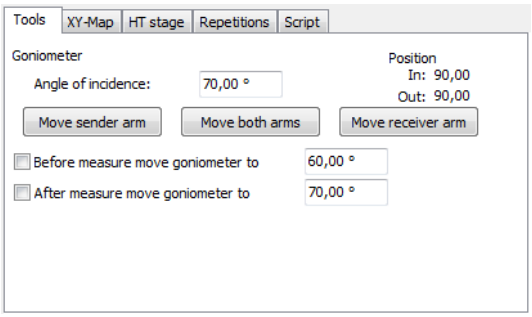


Fig. 5-21 Tools tab

The tools tab allows moving the goniometer arms to the desired position, if an automatic goniometer is installed. You just have to choose the desired angle of incidence Angle of incidence: 70,00 ° and click on Move sender arm, Move receiver arm or Move both arms to move the sender, receiver or both arms to this angle. The actual position is displayed in the upper right corner of this tab. “In” is the position the sender arm, “Out” the position of the receiver arm.

Position
In: 90,00
Out: 90,00

If Before measure move goniometer to 60,00 ° is checked, both arms are moved to the desired angle before each measurement.

If After measure move goniometer to 70,00 ° is checked, both arms are moved to the desired angle after each measurement.

5.1.1.11 XY-Map

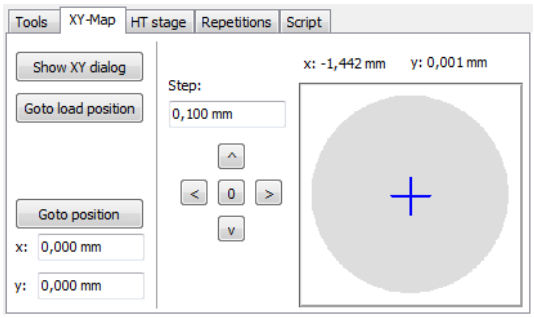
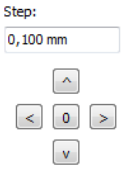
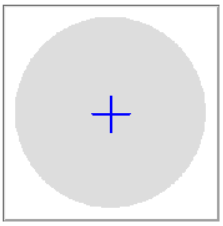


Fig. 5-22 XY-Map

If a mapping table is installed the XY-map tab allows moving the sample stage. By clicking on ^ the mapping table moves one step into the desired direction. The length of each step can also be set. Clicking on 0 moves the table to the center position.



You can also move the table just by clicking into

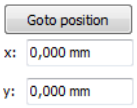


.

The table will move and the measurement spot on the sample will be located at the position you clicked before. The actual position of the stage is displayed too.

x: -1,442 mm y: 0,001 mm

By editing the desired x- and y-position and clicking on “Goto position” you can directly move the sample stage to a desired position.



Clicking on Show XY dialog opens another dialog for the advanced XY-mapping setup.

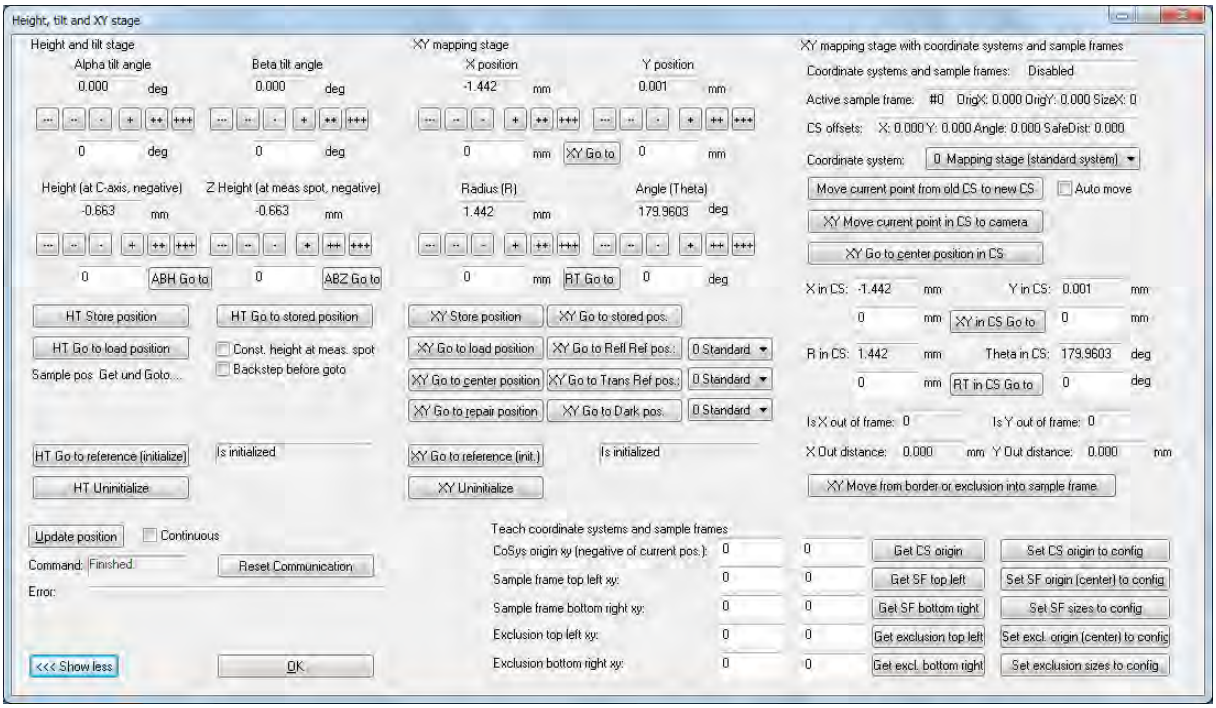


Fig. 5-23 Height, tilt and XY stage

Clicking on Goto load position moves the stage to the load position for easy sample loading.

5.1.1.12 HT stage

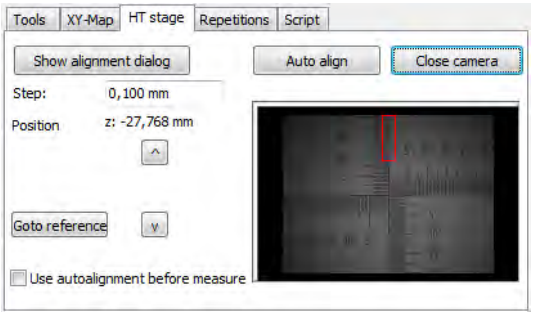


Fig. 5-24 HT stage

If a HT stage with a camera is installed the HT stage tab allows aligning the height and/or the tilt of the sample stage automatically or manually. Clicking on Auto align will start an auto alignment procedure. This procedure searches for the correct sample height by scanning the area in the red rectangle and finding the position with a maximum definition of the light cross. Close camera will close the camera, the video picture will disappear and the button will change to “Open camera”.

Show alignment dialog opens an advanced alignment dialog.

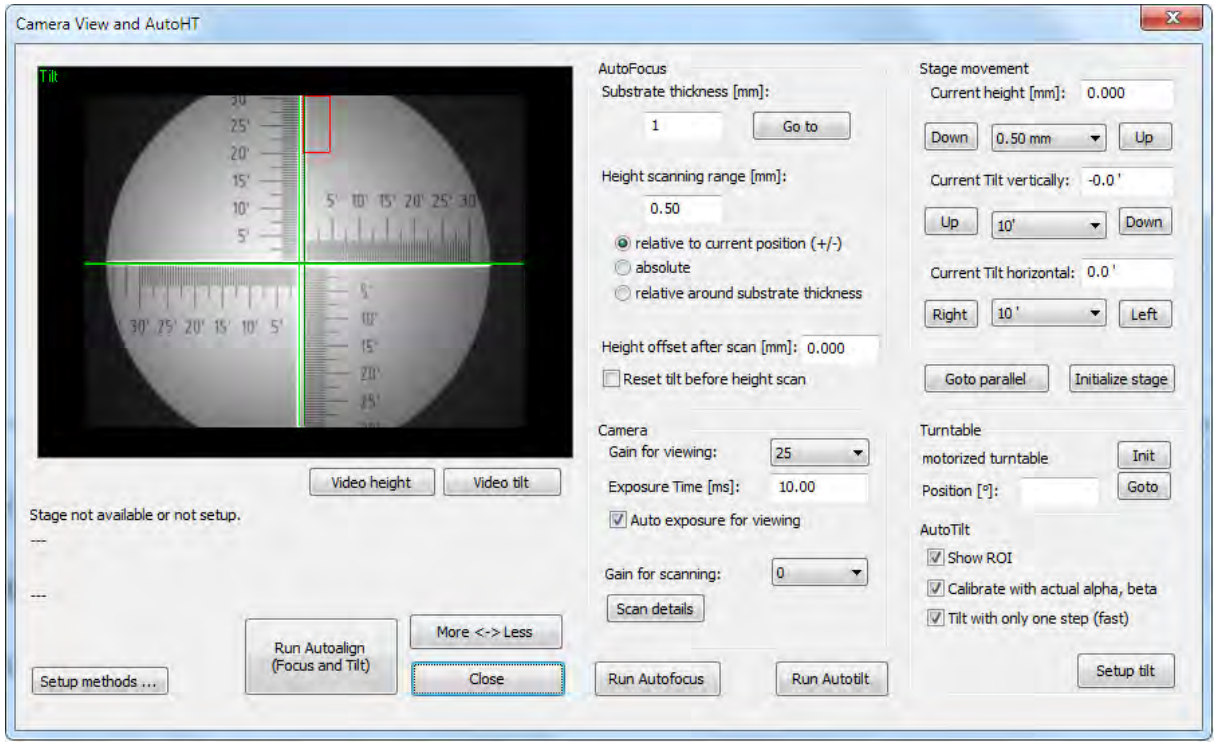
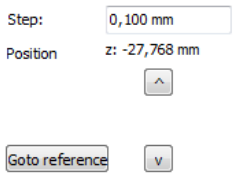


Fig. 5-25 Sample alignment

It is also possible to move the sample stage “manually” one step into the desired direction by clicking on . The length of each step can also be set. Clicking on “Goto reference” moves the table to the reference position. The actual height of the stage is also displayed.



If Use autoalignment before measure is checked an automatic height alignment of the sample is performed before each measurement.

5.1.1.13 Repetitions

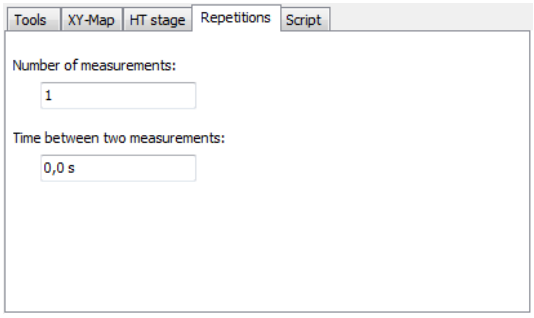


Fig. 5-26 Repetitions

The repetition tab allows setting repetitive measurements with a desired number of measurements (max. 100) and a desired time between two measurements.

5.1.1.14 Script

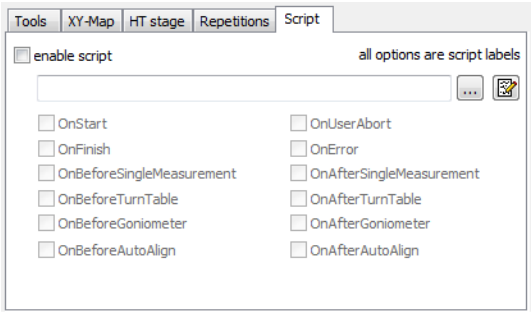
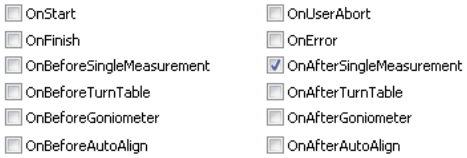


Fig. 5-27 Script

The script tab allows using additional scripts for your measurement. By checking enable script you can use a script which you have loaded by clicking on ... . allows editing the selected script by starting the script editor.
If you check one of the checkboxes the script will be executed at the selected position marked by the corresponding label in the script.



In this example the script is executed after each single measurement at the label “OnAfterSingleMeasurement:”.

5.1.2 Diagram/Reference model

Two tabs, the diagram and the reference model, are located in the upper right part of the measurement window.

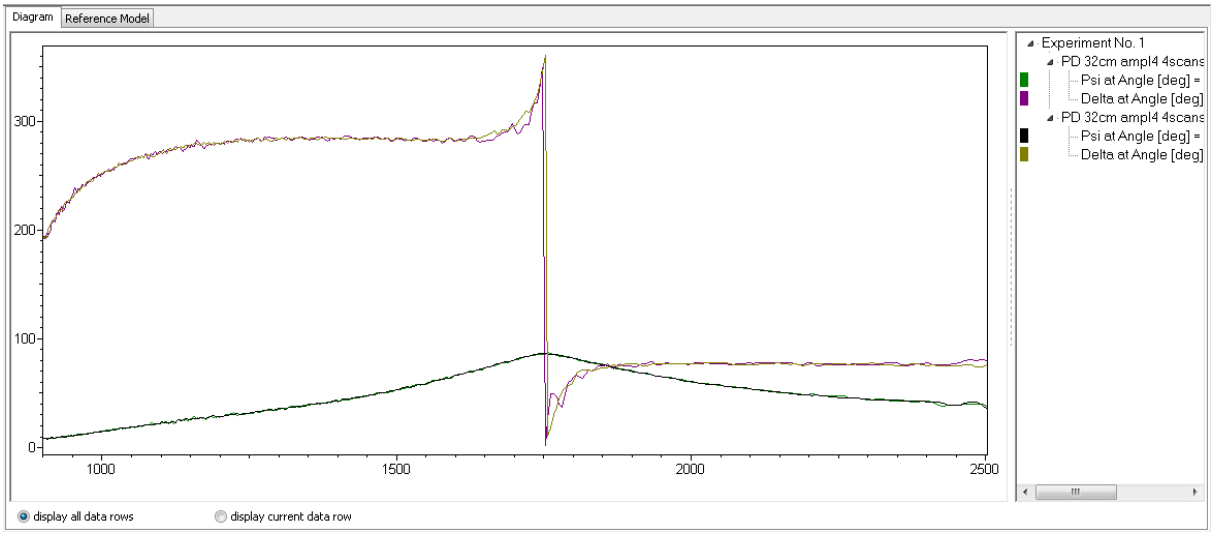
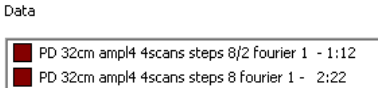


Fig. 5-28 Diagram – display all data rows

In the diagram tab the selected data sets are displayed as shown in Fig. 5-28. You can select two different display modes. If display all data rows is selected all selected rows of all listed data sets are displayed (see Fig. 5-28).



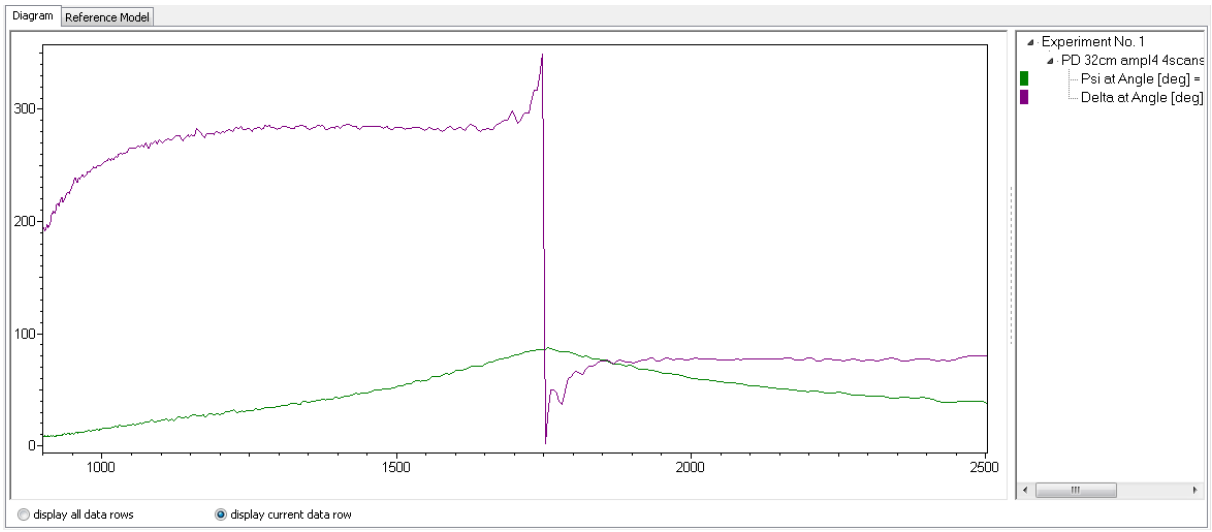
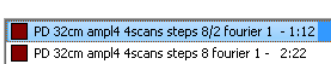


Fig. 5-29 Diagram – display current data row

If display current data row is selected all selected rows of the last marked data set are displayed (see Fig. 5-29).



The tab for the reference model contains the model for the reference measurements of the reflectivity measurements (see Fig. 5-30). Clicking on allows loading a model. Clicking on allows editing layers of a selected model.

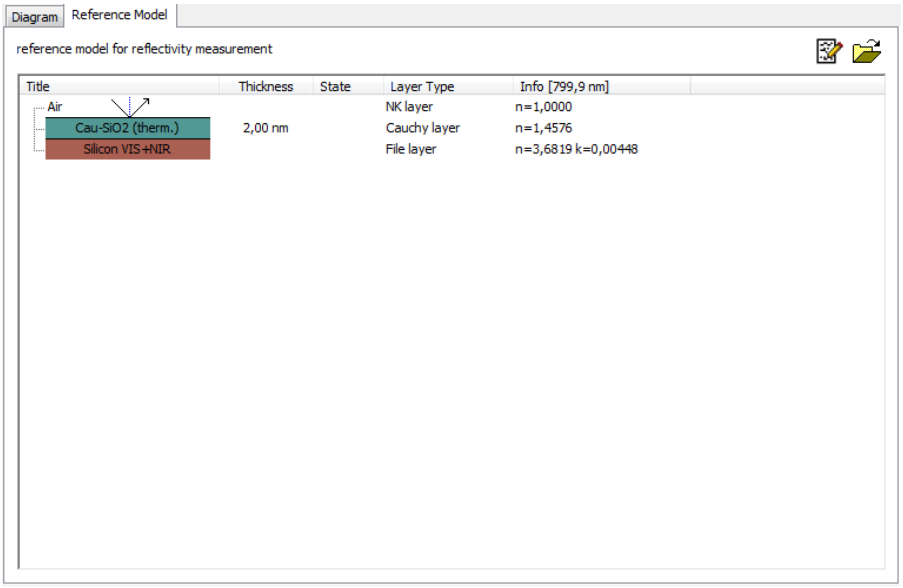


Fig. 5-30 Reference model

5.1.3 Listed data sets

Two tabs are located in the lower right part of the measurement window. The first tab is a list of all data sets of the current experiment.

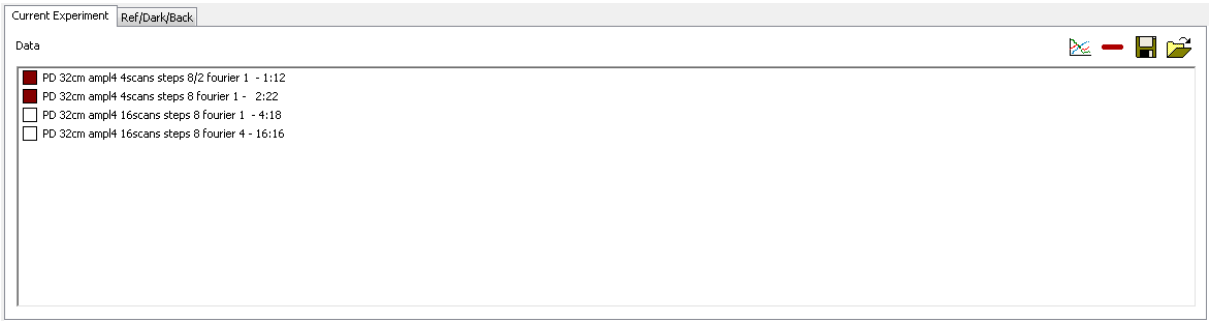
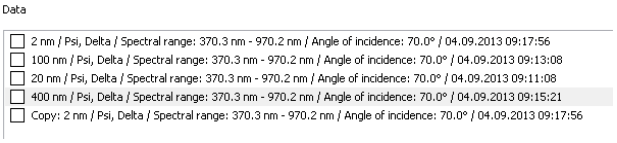


Fig. 5-31 Data sets of the current experiment

This list is identical to the data list in the model window (see section 5.2). Using Drag&Drop you can sort/move data sets or remove data sets from your list. Pressing the CTRL-key of your keyboard **after** dragging a data set will create a copy of the dragged data set after dropping it to the list at the end of the list.
Dropping a dataset to a folder inside the explorer on the left side will save the data set in the selected directory.



The second tab “Ref/Dark/Back” contains a list of the current reference, dark and background spectra used for transmission and reflectivity measurements.

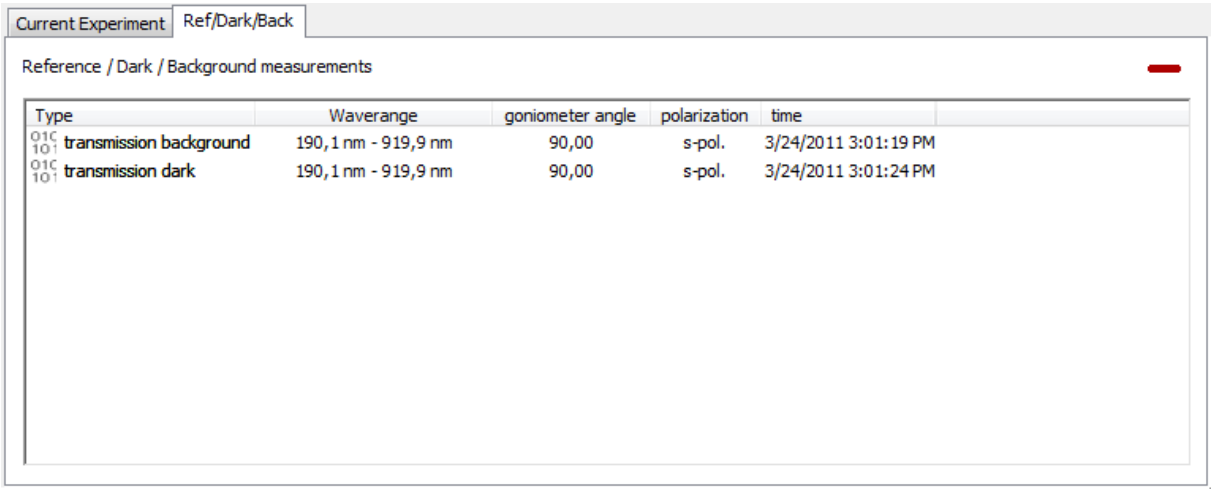


Fig. 5-32 Background and dark data for transmission measurements

5.2 Modeling a sample

5.2.1 Retrieving data of samples

When measuring samples with ellipsometry or reflectometry the interaction of light with your sample causes a change in intensities or polarization of the incident beam. This change is measured and contains the information on your sample. Any reflectance measurement does not measure sample parameters directly! In all cases the reflecting light is theoretically calculated using a theoretical description of the sample (i.e. the model) and compared with the measured behavior. If both are identical within error limits we assume the sample description to be correct and the parameters of the model to be equal to those of the real sample.

The first step to get a result of any measurement is to select or create the sample description, a theoretical counterpart to all sample properties. This description should be precise enough to cover all effects and properties of interest but easy enough to be handy.
After a model was created you may want to study the process of reflecting or transmitting light. This covers the calculation of R, T or ψ and Δ (the ellipsometric angles) for different wavelengths, angles or other parameters. This is called the simulation, the second important function of SpectraRay.
If you measured data you may want to compare and fit theoretical model and measurements. This is done by fitting the theoretical model by varying one or more parameters. This requires extensive handling of sample descriptions and data sets and creates the third task of SpectraRay.

The reason why you use this software is to measure thicknesses and dielectric constants of your samples. The following sections describe how you can get them:

- modeling your sample
- simulation of the measurement
- measuring, editing, importing and exporting the data
- fitting the data
- printing the results

5.2.2 General information and example

A sample consists of a stack of materials within an ambient medium. For absorbing substrates the bottom ambient can be neglected (this is the case for c-Si substrates in the UV and VIS). In case of layers on glass substrates the bottom medium must be used as well as backside reflections (from the glass).
So we have to define a stack of layers each with its own properties. Such properties are the dielectric function, the thickness and non-ideal behavior. An ideal layer is homogeneous, plane and creates no stray light. Non-ideal layers may have thickness variations within the measurement spot, may cause depolarization and may reflect incoherent (thick substrates). The instrument you measure with has some parameters as spectral or angular resolution (monochromator or focusing spot). All these parameters must be set up properly before fitting the data.
The modeling section of this software provides all tools necessary for understanding and fitting measured data. These tools consist of layer types and a set of other settings called the environment. All together is called a model which can be saved and loaded.
For pattern practicing we want to analyze an oxide on silicon which was measured by a SE400adv single wavelength ellipsometer (this is a typical application for the SIMULATION package) at a series of 100 angles locations. These data are stored in the “LaserelliAngle Dep.exp” in the \exp subdirectory. We open this experiment (an experiment is the combination of a model and relating data) by the “File/Load” menu item or simply by double clicking on the file in the explorer window. Since we want to create the model ourselves we delete the current model by “File/New/Model”. The screen should appear as follows.

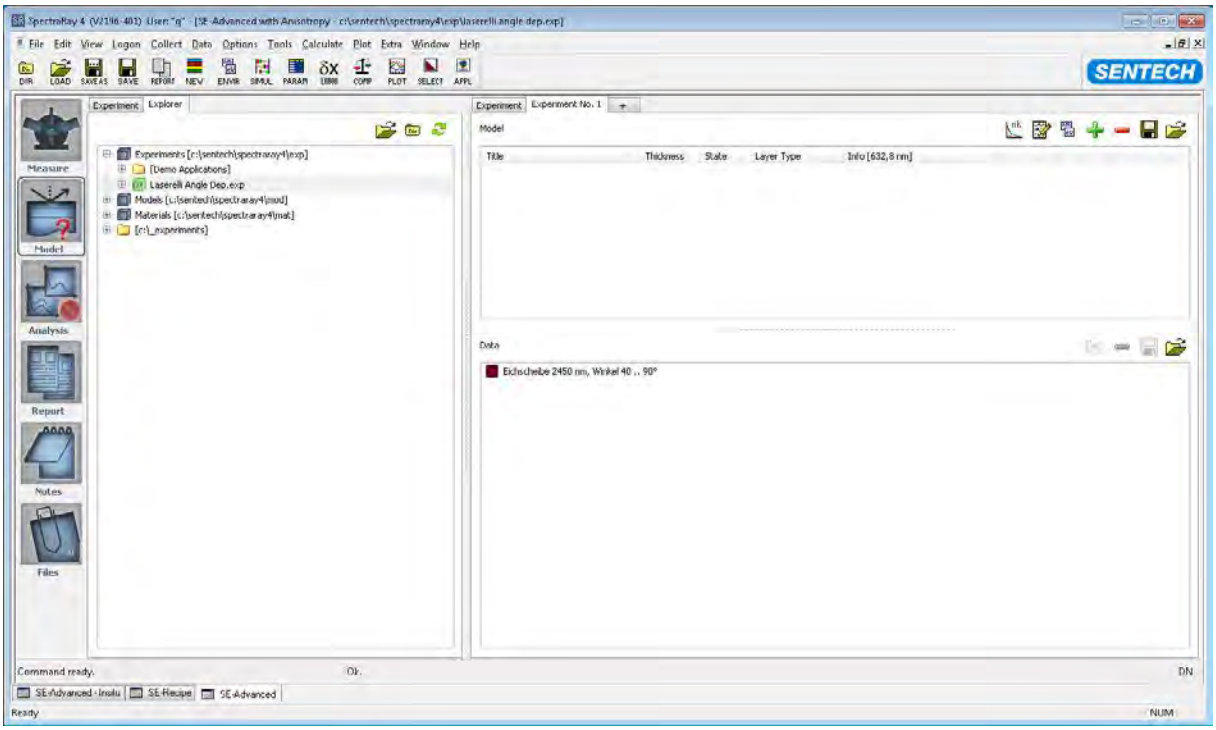


Fig. 5-33 Main screen with “Laserelli Angle Dep.exp” loaded and a new (empty) model created

The silicon oxide on silicon requires adding three materials: Air/oxide/c-Si. SpectraRay contains a large set of pre-manufactured layer descriptions which can be used for defining this sample. The ambient medium air is inserted first. After that we add “c-Si” and “therm. SiO_2”. This can be done by dragging the material name and dropping it onto the model box at the desired position[4]. It is also possible to resort the layer stack or to remove a layer on the same way. Using the menu “Edit\Materials\Insert file” is also possible.

Now the layers are stacked on each other, but have default values. For example we need to set the thickness of the oxide to the guess of 2400 nm. We can double-click a layer within the model listbox to open the layer specific editor.

5.2.3 Working with directories

SpectraRay uses experiments, models, materials and data. Though a file load/save function is included, file lists for drag&drop allow a much quicker and easier way to access data and materials than the file oriented way. Fig. 5-34 shows the locations of the directories which will be displayed in the explorer list for drag&drop. You can also select custom directories for your own files.

Material directory	this directory is used to search for material files *.mat which are displayed within the material list in the explorer on the main screen and for loading materials
Measurements directory	this directory is used to fill the listbox of data files in the main screen
Applications directory	this directory is used for script files
Models directory	this directory is used to search for model files *.mod which are displayed within the model list in the explorer on the main screen and for loading models

[4] see also Appendix A: Drag&Drop Overview

Experiments directory this directory is used to search for experiment files *.exp which are displayed within the experiment list in the explorer on the main screen and for loading experiments

Recipes directory this directory is used to search for recipe files *.rcp which are displayed within the recipe list in the explorer on the main screen and for loading recipes

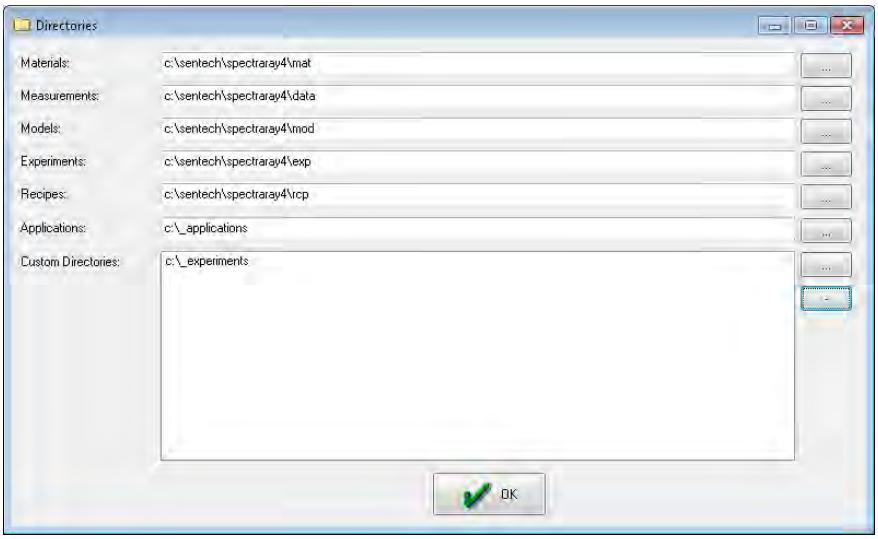


Fig. 5-34 Directories for materials and data

The load and save function of SpectraRay offers a series of file formats. Depending on the selection the saving/loading affects a whole experiment, a model or only the data.

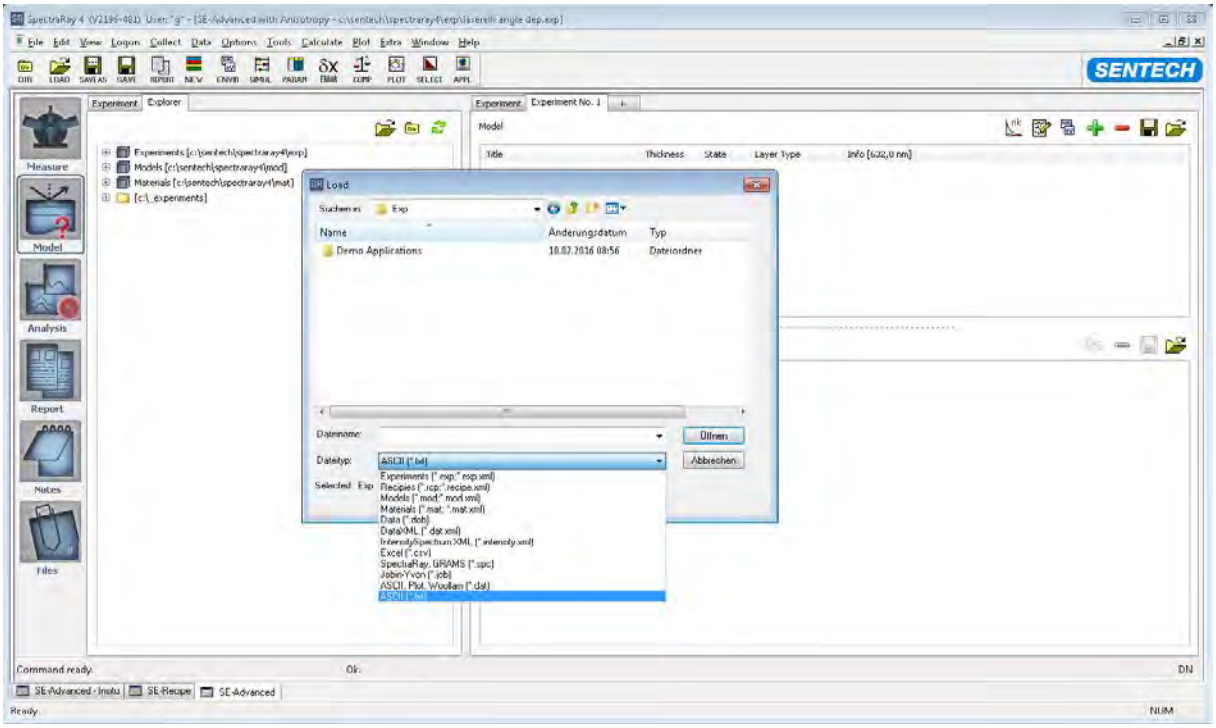


Fig. 5-35 Loading files of different types

5.2.4 Layer types

Stacking layers is a rather complicated process, since each layer has its own dielectric function and layers can be a combination of other layers (e.g. effective medium approximation).
A stack assumes the top and bottom layer to be semi-infinite, because ambient definitions are needed on the top and bottom of the sample. For this reasons the top and bottom layers do not have a thickness property. All other layers have a thickness property. This difference is the same between materials and layers (the latter always have a thickness). When a layer combines two materials (for example the effective medium approximation layer), the thickness property belongs to the combined layer only.
The behavior of the thickness property depends on the function a material is used for. The layer/material editor shows the thickness property only if it is used. The same applies to the model listbox where the top and bottom layer do not have the thickness property and act as ambient materials.
All other properties specifying the dielectric function and the so called transfer matrix are layer specific and they are displayed permanently. Since real materials have different dielectric functions we need a theoretical counterpart to meet or approximate the real function by appropriate theoretical functions. These theoretical functions could be for example a splined table or a polynomial.

5.2.4.1 Creation of new layers

The menu entry “File\New\Layer” opens a list of available layers types. The desired type can be selected from the list and a new layer will be created after clicking OK. The layer types are sorted according to their main functions in a number of groups. Not all layer types appear in these groups. The subgroup 'All layers' at the end of the list contains all available layer types including the seldom used special layers.

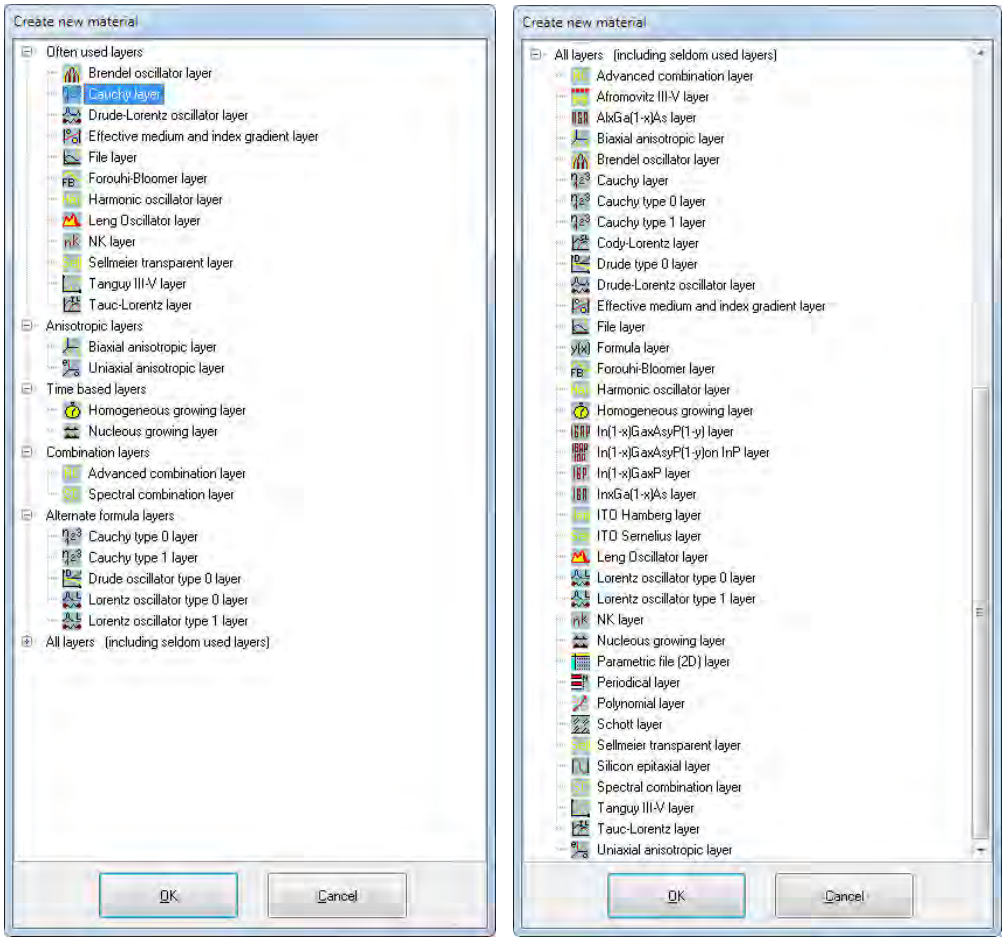


Fig. 5-36: Available layer types

5.2.4.2 Overview over layer types

A rough general overview over the available layer types and their main field of usage is given in Tab. 5-1.

L	Dispersion	Used for ...	Example
H	Fixed n and k	Constant dispersion	Only air
H	Cauchy	transparent dielectric materials Photoresist Glass	SiO_2, Al_2O_3, Si_3N_4, TiO_2 PMMA BK7, quartz
H	Tauc-Lorentz	Absorbing dielectric materials amorphous materials	Si_3N_4, TiO_2 a-Si, a-C
H	Drude-Lorentz	Metals TCO (transparent conductive oxide)	Au, Ag, Cu, Cr, Ni ITO, ZnO:Al
H	File-Layer	Table of wavelength, n, k, no fit parameters substrates	Good for all Si, Ge, GaAs, quartz
M	Leng-Lorentz	Crystalline indirect semiconductors polycrystalline indirect semiconduct. conjugated polymers (OLED, OFET)	c-Si, c-Ge, c-SiGe poly-Si MEH-PPV, P3HT
M	Brendel	Absorption (vibration) bands in the MIR	SiO2, SiN, CH-bonds
M	Sellmeier	Like Cauchy but for broader spectral range (VIS + NIR)	SiO_2
M	Tanguy III/V	Bandgap of direct semiconductors, also II/VI	GaAs, GaN, AlGaN ZnSe
L	Hamberg Sernelius	TCO (transparent conductive oxide)	ITO, ZnO:Al, SnO_2:F
L	Afromovitz	III/V semiconductors (specific)	GaAs, InP, InGaAsP
L	Formula	New non implemented dispersions	Good for all
L	Schott glass	Specific for glasses from Schott	AF45
H	EMA (effective medium approximation)	Mixture of two materials Roughness Interface Gradient	 mixture: Air / layer mixture: layer1 / layer2
M	Biaxial anisotropic	Direction dependent dispersion	Crystalline quartz
M	Periodical group	Bragg reflectors	20x (SiO_2 / TiO_2)
L	Table (2D)	Parameter dependent data of e.g. - Temperature - composition	 Si (0 deg C … 1000 deg) Si_xGe_{1-x}
L	Homogeneous growing layer	In-situ applications, thickness changes with time	Good for all
L	Nuclei growth	In-situ applications, island growth	Metallic film growth
L	Epitaxial Si profile	MIR, Si epitaxial layer growth	Si doping concentration and gradient

Tab. 5-1 The most important dispersions: Level of usage: High (used very often), Medium (sometimes) Low (seldom)

5.2.4.3 General remarks on layer editors

The dialogs used to define the various layers have a number of common components which are described here. In the following paragraphs only the special properties of the various layers are described.

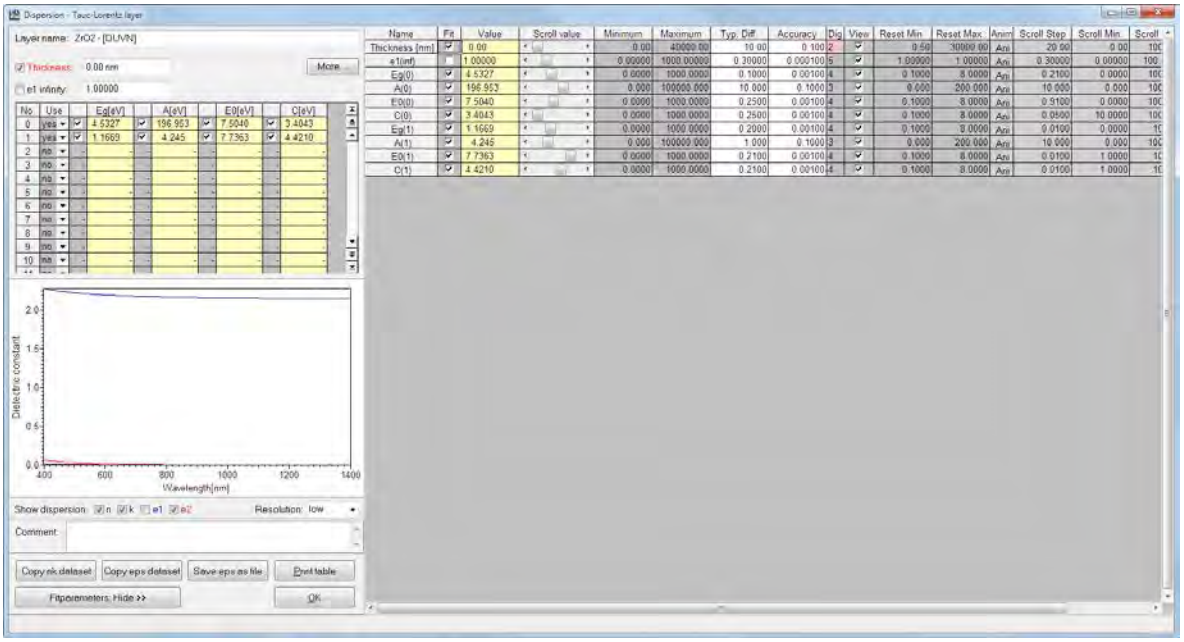


Fig. 5-37 General properties of layer editors

A typical editor a layer is shown in Fig. 5-37. Most of the items shown here are present in the special layers described in the following paragraphs.

The top left edit field contains the name of the material. The name can be edited. This is especially useful if the material data is changed due to the individual properties of the material in a certain sample.

The thickness of the layer is entered in the top left edit field. The thickness can be entered as a physical number. Expressions as “100 nm” or “1.35 mm” are accepted.
If the layer is used as top ambient or as lower substrate the thickness field is not shown as the top and bottom layer are supposed to be infinite 'half-spaces'.

In the example the thickness is selected as a fit parameter by the checkbox left to the edit field. The text appears in red color to indicate the selection.

The table on the left side allows to enter the parameters of a number of oscillators - one oscillator per line.
Each oscillator can be activated for calculation in the column 'Use'.
Each individual parameter can be activated for fit by the checkbox left to the value.

The button 'Fitparameters: show' or 'Fitparameters: hide' on the lower left side opens or closes the table on the right side. This table also holds the parameter values - one parameter per line.
For each parameter additional values can be entered to influence the behavior during the fit procedure. Most importantis the checkbox 'Fit' which activates the parameters for the fit procedure.
The minimum and maximum values define the allowed range for the parameter and the fit will not give values outside this range. This may help to stabilize the fit procedure and give reasonable results if the range is suitable. It may also lead to bad results if the real value is outside the allowed range.
Further explanations on the values in the table can be found in chapter 8.2.1.

The diagram on the left side shows the dispersion of the n, k, ε_1 and ε_2 values depending on the selection in the checkboxes below the diagram.

The spectral range for the diagram is defined by the environment settings, see chapter 5.2.6.

The 'Resolution' list box can be used to calculate a lower or higher number of points within the given spectral range.

The buttons 'Copy nk dataset' and 'Copy eps dataset' can be used to create a dataset in the databox of the main screen.

The button 'Save eps as file' can be used to save the current material dispersion as a table consisting of the wavelength and the selected entries n, k, e1 and e2 if they are selected.

The 'Comment' field allows to enter a comment, for example the source of dispersion data from literature or from certain samples etc.

5.2.4.4 Advanced combination layer

This layer type is an advanced version of the Spectral combination layer described in chapter 5.2.4.32.

Theoretical assumptions:

Dispersion relations of materials can in many cases be described by model functions. But these model functions usually give a good description in a certain spectral range only.

For example a transparent conducting material may be described by a Tauc-Lorentz model in the visible range where it is highly transparent and a Drude model for the infrared range where the conductivity leads to a 'partially metallic' behavior of the material.

The combination of these contributions allows to setup a combined model for the dispersion in the whole spectral range.
The combination has to be done in terms of the complex dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2$. The contributions to ε are added to give the resulting dielectric function.

$$\boldsymbol{\varepsilon = \varepsilon_1 + i\varepsilon_2 = \varepsilon_{1\infty} + \sum_{c=1}^{c\_max} (\varepsilon_{1,c} - \varepsilon_{1\infty,c}) + i \sum_{c=1}^{c\_max} \varepsilon_{2,c}}$$

The constant part $\varepsilon_{1\infty}$ has to be treated in a special way. If the individual contributions have their own $\varepsilon_{1\infty,c}$ this value has to be subtracted. In addition one common final $\varepsilon_{1\infty}$ for the resulting dispersion is added. This procedure avoids multiple ambiguous fit parameters.

This procedure works for all contributions that have their own $\varepsilon_{1\infty}$ in their formulas. This is the case example in Drude-, Lorentz-, Cody-Lorentz-, Harmonic-, Leng-, Tauc-Lorentz, Hamberg- and Sernelius-formulas.

In other contributions a separate $\varepsilon_{1\infty,c}$ is not available, for example in Cauchy-, Forouhi-Bloomer-, Schott-, Sellmeier-, Tanguy-formulas and in the File-layer. In these cases no subtraction of $\varepsilon_{1\infty,c}$ should take place and the resulting $\varepsilon_{1\infty}$ should be set to 0.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Advanced combination layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor is shown in Fig. 5-38 with a typical example for the dispersion of TCO. The individual contributions for this example are a Tauc-Lorentz and a Drude term. They are shown in Fig. 5-39. In the experiment view the combination layer appears together with the contributions as shown in Fig. 5-40.

The diagram of the spectral combination layers shows the combined dielectric function as continuous line and the individual contributions as broken or dotted line.

The contributions can be loaded from a new layer ( ), from a directory with material files ( ) or from the already existing layers in the layer stack ( ).
The entries in the list can be selected by a mouse click.
The selected contribution can be edited ( ) or deleted ( ).

The contributions are shown in the list. The usage can be selected for each contribution.
The $\varepsilon_{1\infty,c}$ value of each contribution is automatically subtracted in the case of all layer types that have their own $\varepsilon_{1\infty,c}$ values as discussed above.
For other layers nothing is substracted, but in this case the combined $\varepsilon_{1\infty}$ should be set to 0 as discussed above.

The combined dispersion and the dispersion of the contributions can be selected for display below the diagram.

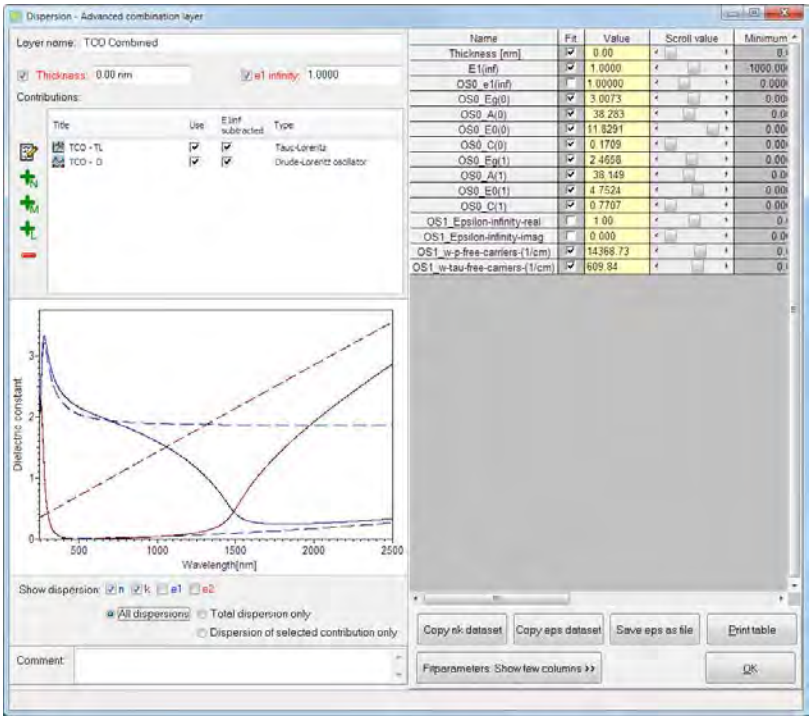


Fig. 5-38 Advanced combination layer editor

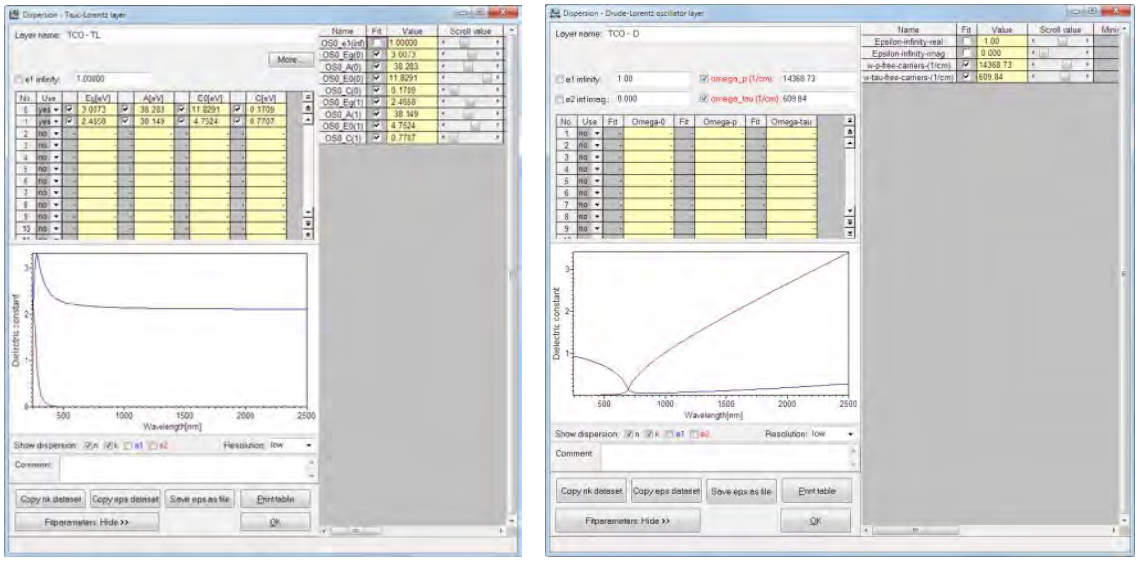


Fig. 5-39 Contributions of advanced combination layer

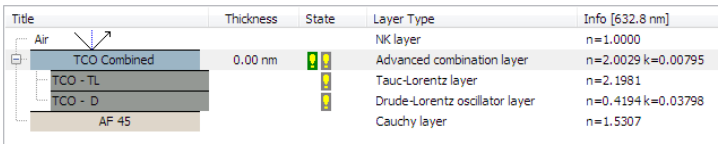


Fig. 5-40 Advanced combination layer in the experiment view

5.2.4.5 Afromovitz layer

Theoretical assumptions:

A description of the dielectric function of the system $In_{1-x}Ga_xAs_yP_{1-y}$ has been developed by Afromovitz [Solid State Communications, Vol. 15, pp. 59-63, 1974].
The condition for the lattice mismatch in the system gives a relation between the compositions x and y:

$$y = \frac{2.202 \cdot x}{1 + 0.0695 \cdot y}$$

The model was proposed by Wemple and DiDomenico [Phys. Rev. B 3, 1338 (1971)] and uses energies E_g, E_0 and a strength E_d all related to the composition:

$$E_g(y) = 1.35 - 0.75 \cdot y + 0.12 \cdot y^2$$
$$E_0(y) = 3.391 - 1.652 \cdot y + 0.863 \cdot y^2 - 0.123 \cdot y^3 \qquad [E_i]=eV$$
$$E_d(y) = 28.91 - 9.278 \cdot y + 5.626 \cdot y^2$$

The model introduced by Afromovitz calculates the dielectric function as follows:

$$\varepsilon(E, y, \Gamma) = 1 + \frac{E_d(y)}{E_0(y)} + \frac{E_d(y)}{E_0(y)^3}(E + i \cdot \Gamma)^2 + \frac{E_d(y)}{2E_0(y)^3\left[E_0(y)^2 - E_g(y)^2\right]}(E + i \cdot \Gamma)^4 \cdot Ln\left[\frac{2E_0(y)^2 - E_g(y)^2 - (E + i \cdot \Gamma)^2}{E_g(y)^2 - (E + i \cdot \Gamma)^2}\right]$$

The refractive index is calculated using the simple formula n=Re(ε) but the absorption is expanded by a second order polynomial above the band gap:

$$k = \mathrm{Im}[\varepsilon] \qquad if\ E < E_g$$
$$k = \mathrm{Im}[\varepsilon] + c(E - E_g) + d(E - E_g)^2 \qquad if\ E \geq E_g$$

Standard values for the parameters and their meaning are:

Parameter	Default value	Description
Gamma	0.001	Damping at E_g [eV]
x	0.0	Composition x [1]
C1	2.202	Coefficient in composition formula [1]
C2	0.0695	Coefficient in composition formula [1]
Eg-0	1.35	Polynomial for E_g coefficient 0 (constant) [1]
Eg-1	-0.72	Polynomial for E_g coefficient 1 (linear) [1]
Eg-2	0.12	Polynomial for E_g coefficient 2 (second order) [1]
E0-0	3.391	Polynomial for E_0 coefficient 0 (constant) [1]
E0-1	-1.652	Polynomial for E_0 coefficient 1 (linear) [1]
E0-2	0.863	Polynomial for E_0 coefficient 2 (second order) [1]
E0-3	-0.123	Polynomial for E_0 coefficient 3 (third order) [1]
Ed-0	28.91	Polynomial for E_d coefficient 0 (constant) [1]
Ed-1	-9.278	Polynomial for E_d coefficient 1 (linear) [1]
Ed-2	5.626	Polynomial for E_d coefficient 2 (second order) [1]
c	0.0	Linear factor for k [1]
d	0.0	Second order factor for k [1]

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Afromovitz layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

An example is given in Fig. 5-41 and Fig. 5-42 showing n and k respectively.

Note: The dispersion relation is defined near the band gap only. The energy range should be limited to approx. 0.5...2 eV.

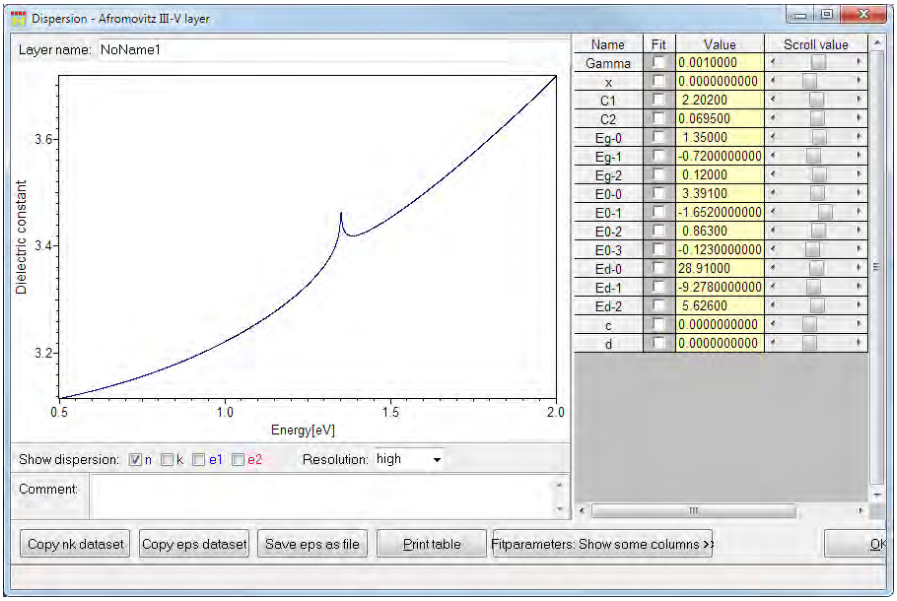


Fig. 5-41 Example for an Afromovitz layer (n)

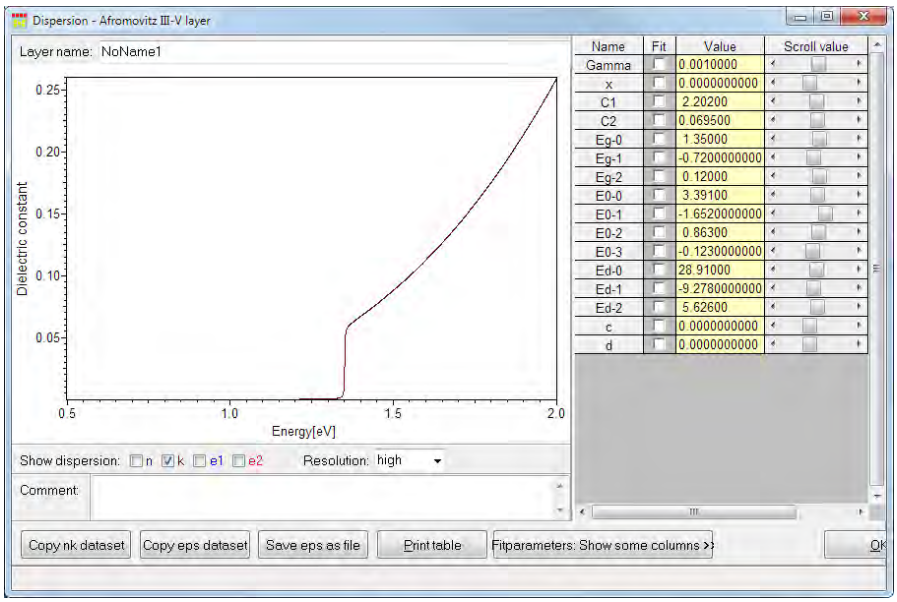


Fig. 5-42 Example for an Afromovitz layer (k)

A comparsion for GaAs between the Tanguy layer (see chapter 5.2.4.33) and the Afromovitz layer shows that the Tanguy layer can describe the material more precise.

5.2.4.6 Al(x)Ga(1-x)As, In(1-x)Ga(x)As(y)P(1-y), In(1-x)Ga(x)P, In(x)Ga(1-x)As layers

Theoretical assumptions:

Special dispersion relations have been set up for the different ternary and quaternary III-V semiconductor systems similar to the Afromovitz layer described in chapter 5.2.4.5.

Creating a new layer

A growing layer is created by “File\New\Layer” and selecting the layer type as for example “In(1-x)Ga(x)P layer ”. This creates the new layer and opens the editor. The values can be edited, especially the composition - in this example Ga-x.

Editing the layer

An example for the editors of these layers is given in Fig. 5-43 and Fig. 5-44.

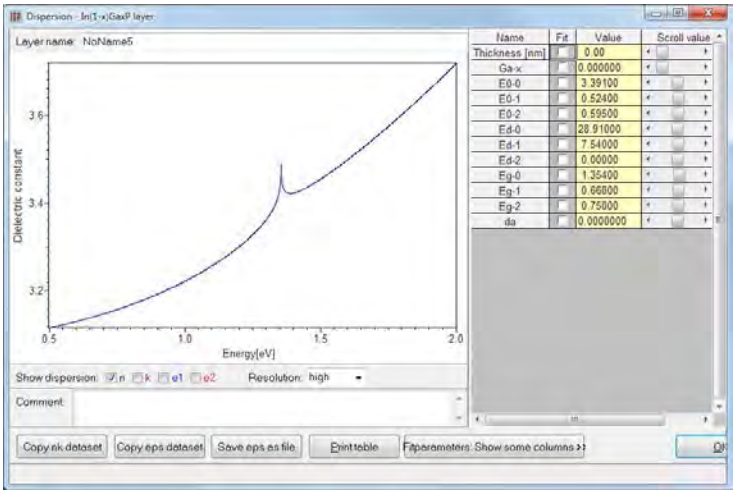


Fig. 5-43 Example for In(1-x)Ga(x)P editor (n)

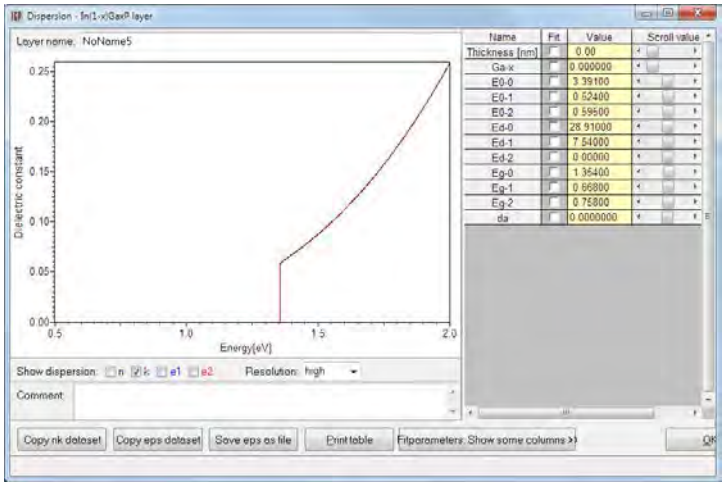


Fig. 5-44 Example for In(1-x)Ga(x)P editor (k)

5.2.4.7 Biaxial anisotropic layer

Theoretical assumptions:

In general the dielectric function of a material can be different in all three dimensions - mainly due to the crystalline order which leads to the anisotropy. This effect can be expressed by the dielectric tensor which is given here in the normalized form in the main axis coordinate system:

$$\underline{\underline{\tilde{\varepsilon}}}_{Ci} = \begin{pmatrix} \tilde{\varepsilon}_{xi} & 0 & 0 \\ 0 & \tilde{\varepsilon}_{yi} & 0 \\ 0 & 0 & \tilde{\varepsilon}_{zi} \end{pmatrix}$$

The orientation of the sample coordinate system relative to the measurement system is described by three Euler angles α, β and γ.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Biaxial anisotropic layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor is shown in Fig. 5-45Fig. 5-103 with a simple example for $CaCO_3$ which is a typical material that shows a strong anisotropy.

The different dispersions along the axis X, Y and Z have to be defined as 'submaterials'. After creation of a new layer all sublayers are simple NK-layers. It is possible to load other material definitions from the material library ('From materials...') or from the already existing layers in the layer stack ('From layers...').
The editors for the sublayers can be opened in order to setup all parameters ('Edit...').

The diagram shows the n, k, e1 and e2 values of the different dispersions versus the spectral scale which is defined by the environment.
Above the diagram the refractive index is shown at the wavelength and the sample rotation defined by the environment as shown in Fig. 5-46.

The biaxial anisotropic layer appears in the main layer stack together with its 'submaterials' as shown in Fig. 5-47.

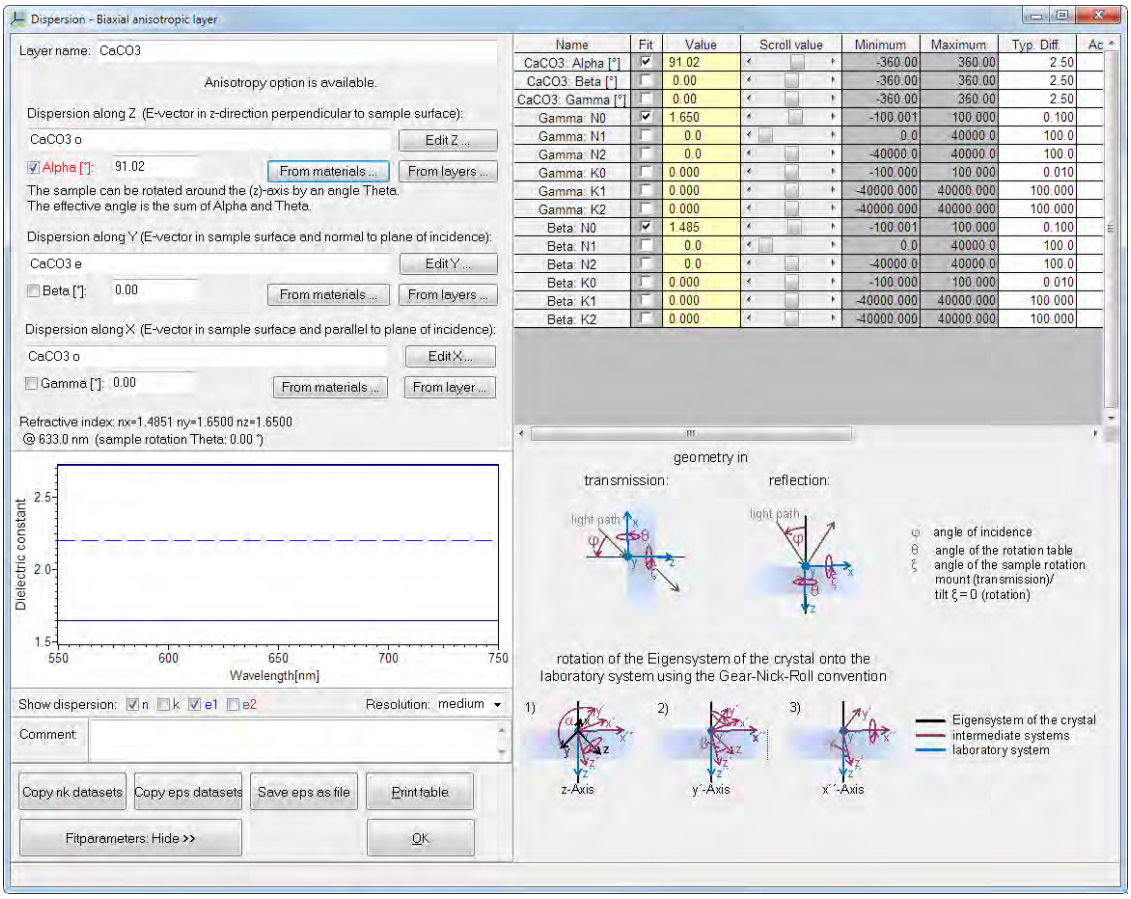


Fig. 5-45 Example for biaxial layer

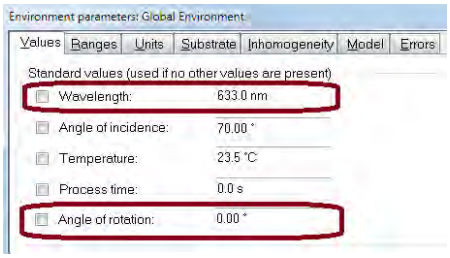


Fig. 5-46 Definition of observation values for display

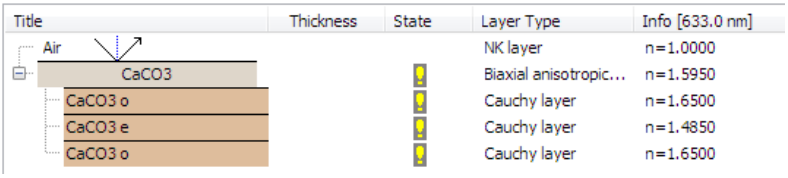


Fig. 5-47 Appearance of biaxial anisotropic layer in the main layer stack

The rotatable sample stage is used to acquire different ellipsometric spectra for different sample rotation angles θ (Theta). Fig. 5-48 shows the direction of the rotation of the sample on the sample stage.

The rotation angle is given in the measurement dataset either as z-axis type or as x-axis type as shown in Fig. 5-49

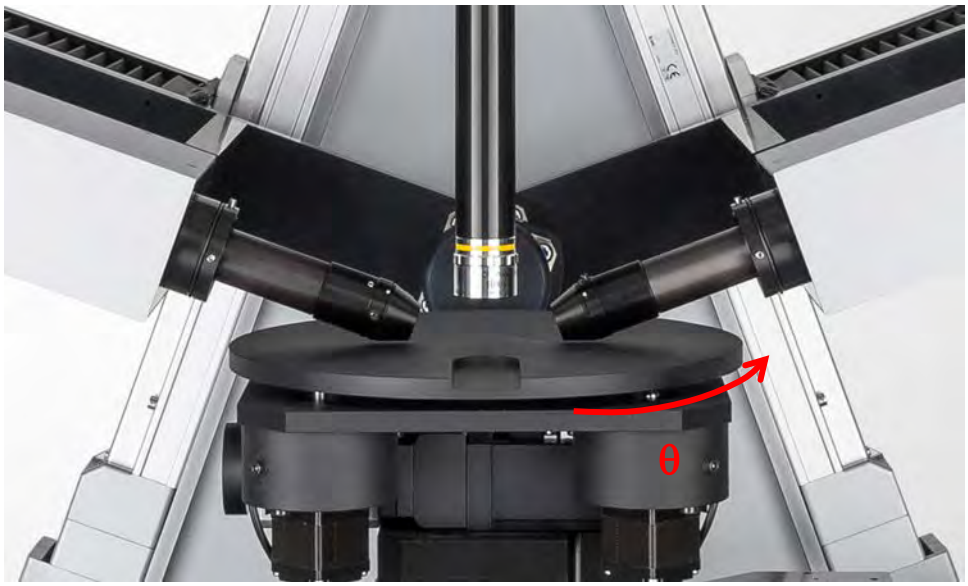


Fig. 5-48 Sample on rotatable sample stage and angle θ

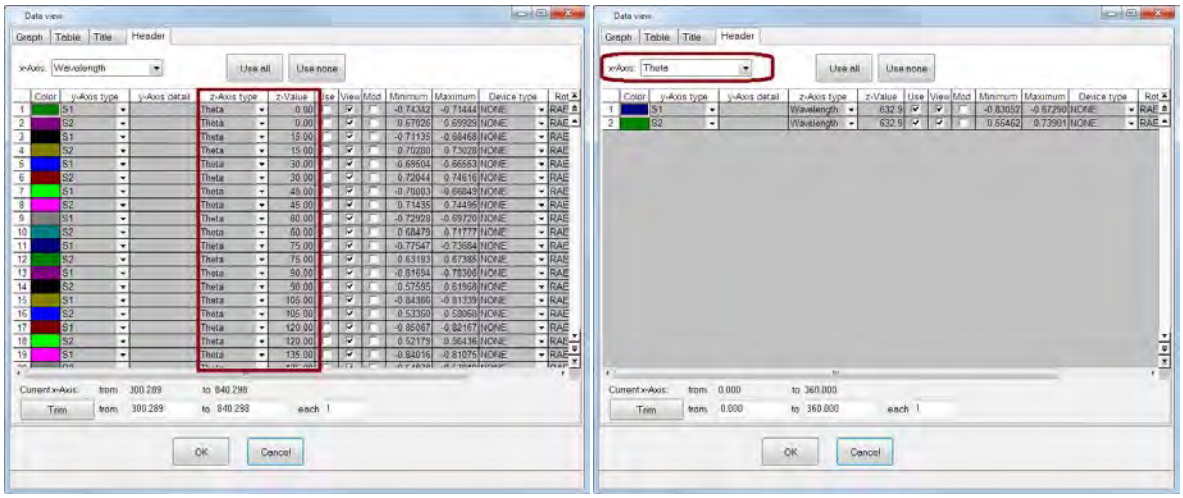
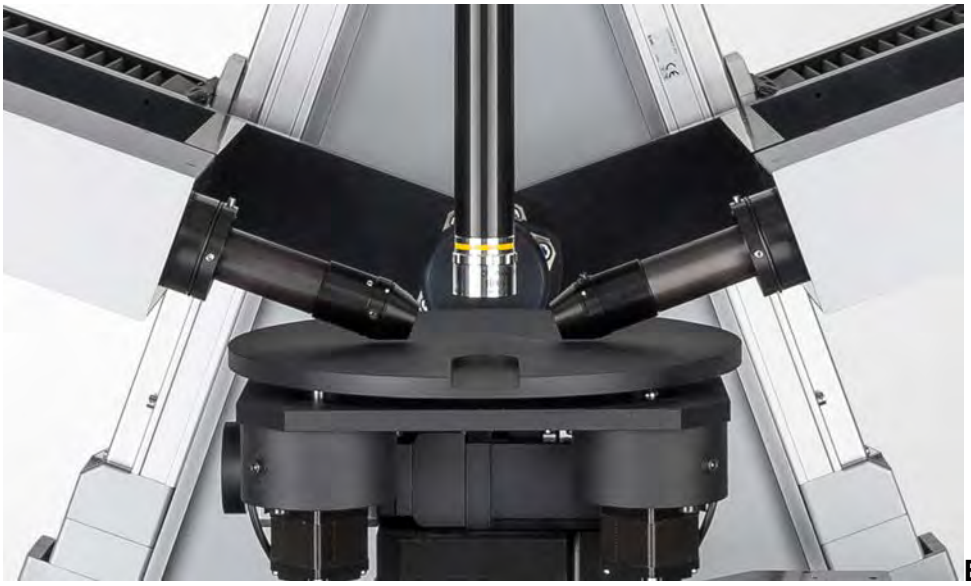


Fig. 5-49 Sample rotation angle in data sets

For more detailed discussions of anisotropic samples see chapter 8.7.4.



5.2.4.8 Brendel oscillator layer

Theoretical assumptions:

The Brendel oscillator model is designed to describe vibration absorption bands of molecules in the MIR spectral range. It is based on an oscillator model. Due to an inhomogeneous environment in amorphous materials the centre frequency of each individual oscillator is influenced. The Brendel oscillator describes the standard deviation of the Gaussian distribution of the centre frequency of the oscillator. Beyond that it is very useful to describe also metallic films. Especially metals like gold are showing strong benefits when described using the Brendel oscillator model.

$$\varepsilon(\nu) = \varepsilon_\infty + \sum_{k=1}^{m} \chi_k(\nu)$$

Gaussian distribution — Oscillator

$$\chi_k(\nu) = \frac{1}{\sigma_k\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left\{-\frac{(x-\nu_{0k})^2}{2\sigma_k^2}\right\} * \frac{\nu_{Pk}^2}{x^2 - \nu^2 + i\nu_{Tk}\nu}\, dx$$

χ_k	Susceptibility of the Brendel oscillator k
ν_{0k}	Resonance frequency / cm^{-1}
ν_{Tk}	Damping of the oscillator / cm^{-1}
ν_{Pk}	Oscillator strength / cm^{-1}
σ_k	Standard deviation of the centre frequency / cm^{-1}
k	Oscillator index

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Brendel oscillator layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

An example for the Brendel oscillator with damping of the oscillator term $\nu_{Tk} > 0$ and standard variation of the center frequency $\sigma_k > 0$ is given in Fig. 5-50.

Looking at the formula two special cases can be discussed:

If the standard deviation σ_k becomes 0 the Brendel oscillator becomes a standard Lorentz-oscillator. An example is shown in Fig. 5-51 with the relevant values indicated at the peak in ε_2.

If the damping of the oscillator ν_{Tk} becomes zero and the standard deviation σ_k is not zero the Brendel oscillator takes the shape of a Gaussian oscillator. An example is shown in Fig. 5-52 with the relevant values indicated at the peak in ε_2.

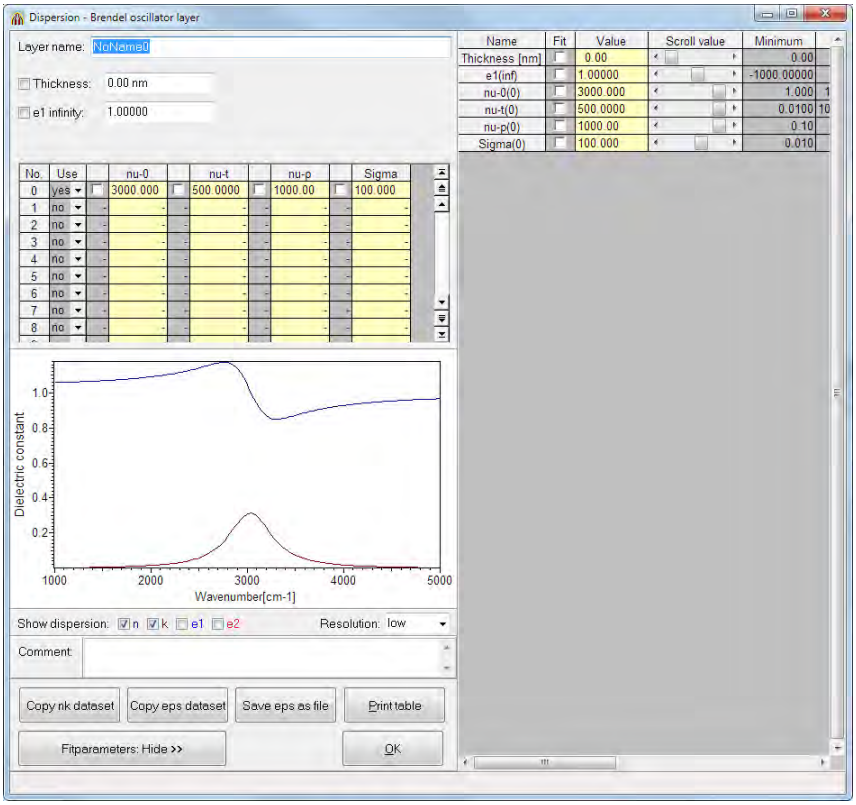


Fig. 5-50 Brendel oscillator with damping and standard variation

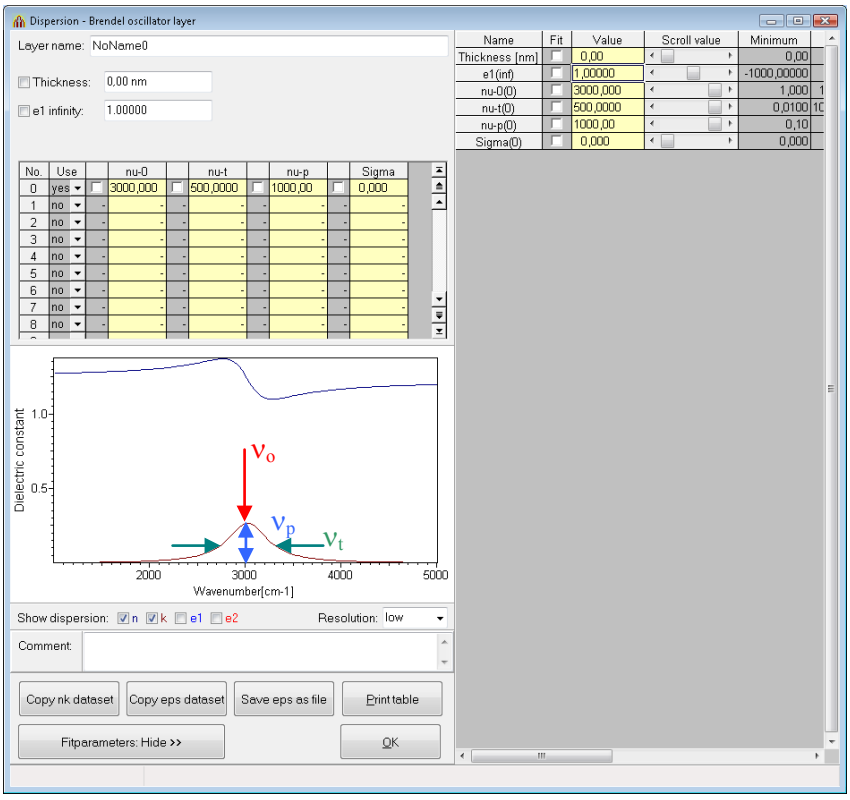


Fig. 5-51 Brendel oscillator with standard deviation equal to 0 (like Lorentz-oscillator)

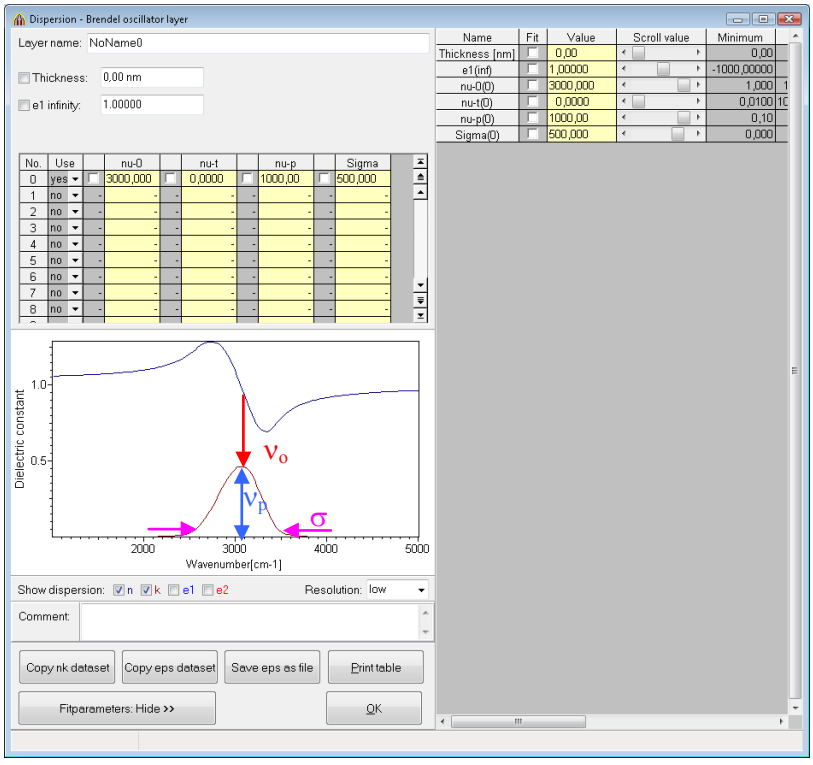


Fig. 5-52 Brendel oscillator with damping equal to 0 (like Gaussian-oscillator)

5.2.4.9 Cauchy-Layer

Theoretical assumptions:

Most dielectric materials have a dielectric function which is very similar to a polynomial for a certain spectral range. This is in many cases true for the visible spectral range from approximately 400 nm to approximately 900 nm wavelength, but depends on the material. For example the Cauchy formula works well for SiO_2, Al_2O_3, Si_3N_4 and TiO_2. There are several polynomials suitable, but the Cauchy type is widely used (if special formulas are preferred use the formula layer type).

The Cauchy relation uses the first two even orders to approximate the refractive index using coefficients for n and k:

$$n(\lambda) = n_0 + C_0 \frac{n_1}{\lambda^2} + C_1 \frac{n_2}{\lambda^4} \qquad [\lambda] \text{ - nm} \qquad C_0 = 10^2 \qquad C_1 = 10^7$$

$$k(\lambda) = k_0 + C_0 \frac{k_1}{\lambda^2} + C_1 \frac{k_2}{\lambda^4} \qquad [\lambda] \text{ - nm} \qquad C_0 = 10^2 \qquad C_1 = 10^7$$

$[n_i]$, $[k_i]$: dimensionless

The coefficients C_0 and C_1 are used to avoid large numbers for the dimensionless parameters n_1, k_1, n_2 and k_2 and their values agree with most publications on Cauchy layers.

Creating a new layer

A new Cauchy layer is created by “File\New\Layer” and selecting the layer type “Cauchy layer”. This creates the new layer and opens the editor. The name of the new layer and its properties n_0, n_1, n_2, k_0, k_1, k_2 can be entered.

Editing the layer

The editor for Cauchy layers is shown in Fig. 5-53. The settings can be made as explained in chapter 5.2.4.3.

Typical values after creation of a new Cauchy layer are shown in Tab. 5-2.

Typical values for commonly used materials are given in Tab. 5-3.

In the case of transparent materials it is advisable not to select the K0, K1 and K2 values for fit in order to stabilize the results.

Note: The parameter n_0 is frequently confused with the refractive index at 632.8 nm. But the value for n at any wavelength has to calculated according to the formula.

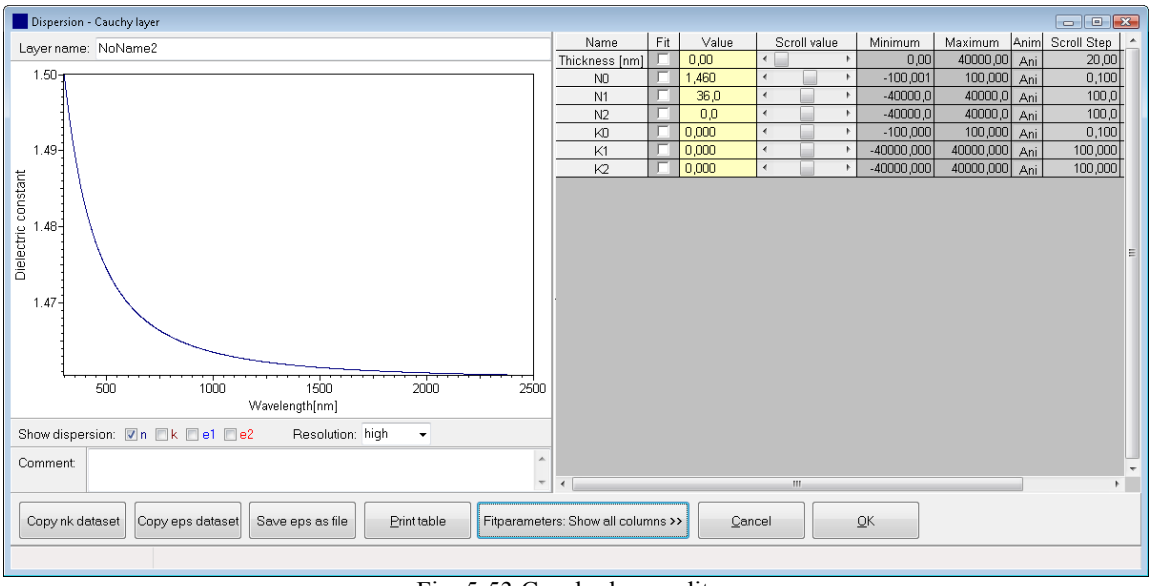


Fig. 5-53 Cauchy layer editor

Name	Fit	Value	Typ. Diff.	Minimum	Maximum	Reset Min.	Reset Max.	Accuracy
Thickness [nm]	0	0.0	20	0.0	40000	0.5	30000	0.1
N0	0	1.460	0.100	-100.001	100	1.100	2	0.001
N1	0	0.000	100	-40000	40000	0.000	20	0.010
N2	0	0.000	100	-40000	40000	0.000	20	0.010
K0	0	0.000	0.1	-100	100	0.000	1	0.001
K1	0	0.000	100	-40000	40000	0.000	20	0.010
K2	0	0.000	100	-40000	40000	0.000	20	0.010

Tab. 5-2 Default setup of fit parameters after a new Cauchy layer was created

Name	N0*1000	N1	N2	K0*1000	K1	K2
Air	1000	0	0	0	0	0
Al	6736	-32439	44009	10136	-9078	-2847
Al2O3 (sputt.)	1586	72	0	0	0	0
Al2O3 (e-beam)	1637	45	26	0	0	0
Al.099Ga.901As	3411	1002	2205	0	0	0
Al.804Ga.196As	3053	35	3169	0	0	0
Au (substrate)	1220536	-6870669	9839144	0	0	0
BK7	1501	73	-57	0	0	0
c-GaAs (substrate)	3559	157	4326	0	0	0
c-GaP (substrate)	3058	596	1781	0	0	0
c-Ge (substrate)	1825	22037	-27027	0	0	0
c-InP (substrate)	3501	-872	4499	0	0	0
c-Si	3445	1320	1693	46	-530	1700
Ceramic N58 (substrate)	2100	0	0	0	0	0
Compact Disc (substrate)	12970	-20910	20608	0	0	0
Cr (substrate)	8198	-9433	15902	0	0	0
GeO2	1571	136	-14	0	0	0
H2O	1325	29	-11	0	0	0
In.53Ga.47As (substrate)	3715	-1117	9696	0	0	0
InSbO	1888	324	142	0	0	0
ITO	1636	975	-337	129	-400	463
LiF	1385	24	-3	0	0	0
MgF2	1376	36	-33	0	0	0
MgO	1650	295	134	0	0	0
MgO (e-beam)	1590	295	134	0	0	0
PERMALLOY (Fe-Ni)(substrate)	12970	-20910	20608	0	0	0
Photoresist AZ1350H exp.	1602	92	80	0	0	0
Photoresist AZ1350J non exp.	1626	57	147	0	0	0
Photoresist AZ1350J exp.	1608	90	48	0	0	0
Photoresist AZ2400 non exp.	1608	61	98	0	0	0
Photoresist AZ2400 exp.	1603	71	66	0	0	0
Photoresist AZ111 non exp.	1580	46	91	0	0	0

Photoresist AZ111 exposed	1574	47	66	0	0	0
Photoresist HPR204 non exp.	1616	76	152	0	0	0
Photoresist HPR204 exposed	1608	97	52	0	0	0
Photoresist HPR206 non exp.	1615	48	193	0	0	0
Photoresist HPR206 exposed	1609	85	91	0	0	0
Photoresist KFTR non exp.	1535	18	78	0	0	0
Photoresist KFTR exposed	1523	55	18	0	0	0
Photoresist KODAK 809 n.e.	1593	25	18	0	0	0
Photoresist KODAK 809 exp.	1578	64	60	0	0	0
Photoresist PMMA	1474	47	0	0	0	0
Photoresist PMMA Copolymer	1481	46	0	0	0	0
Photoresist POLYGRAM	1560	0	0	0	0	0
Photoresist S1818-J2	1640	0	0	0	0	0
Photoresist SP-25	1680	0	0	0	0	0
Photoresist TERPOLYMER	1490	46	0	0	0	0
Photoresist 111S,111H	1650	0	0	0	0	0
Photoresist 1300,1400	1627	0	0	0	0	0
Polyimide Ciba-G P13N	1646	97	216	0	0	0
Polyimide du Pont RC5057	1675	111	229	0	0	0
Polyimide du Pont PI2550	1662	82	224	0	0	0
Polyimide du Pont PI2525	1663	52	266	0	0	0
Polyimide Gulf Therm. 600	1660	113	195	0	0	0
Polyimide Hitachi PIQ	1690	-17	451	0	0	0
Polyimide Monsanto 703	1657	-18	449	0	0	0
Polysilicon 900°C	3485	1792	1342	138	-530	1700
Polysilicon 650°C	3758	1792	1342	460	-530	1700
PSG (thermal)	1455	35	0	0	0	0
Sheet metal (substrate)	3300	4500	0	0	0	0
SiO2 (therm.)	1452	36	0	0	0	0
SiO2 (Pliskin)	1462	36	0	0	0	0
SiO2 (sputt.)	1456	43	-4	0	0	0
SiO2 (CVD)	1429	34	0	0	0	0
Si3N4	1985	123	29	0	0	0
SixNy (PECVD)	2068	152	241	0	0	0
SiOxNy	1765	103	0	0	0	0
Ti	4776	-15529	20161	4111	-5468	2977
TiO2	2368	-376	1800	0	0	0
ZnO	1924	163	387	0	0	0

Tab. 5-3 Cauchy coefficients for a series of materials valid in the wavelength range 500 nm … 900 nm (same as in the FTPadv software)

The refractive index is increasing towards shorter wavelengths. Fig. 5-54 shows the normal dispersion of SiO_2. The refractive index is increasing from n=1.46 at λ=850 nm to n=1.49 at λ=300 nm.

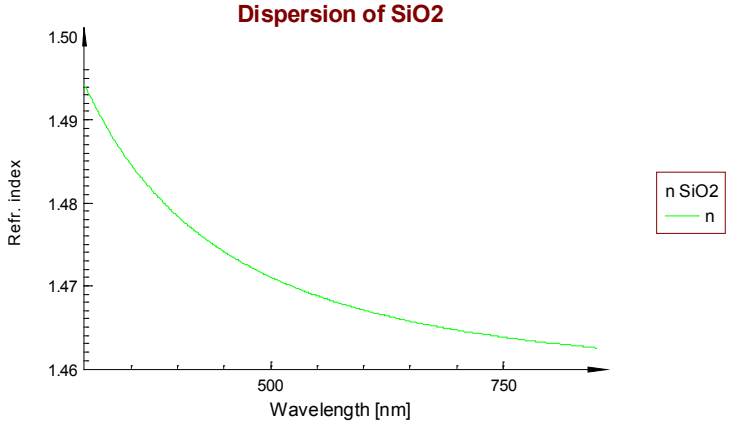


Fig. 5-54 Cauchy dispersion of SiO_2

In general the dispersion is getting stronger when the refractive index is increasing. This behavior can be seen in Fig. 5-55where the dispersion is shown for different dielectric materials.

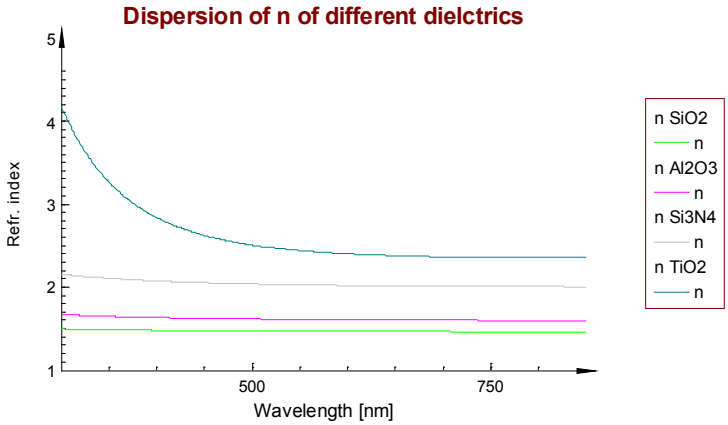


Fig. 5-55 Cauchy dispersion of different dielectrics

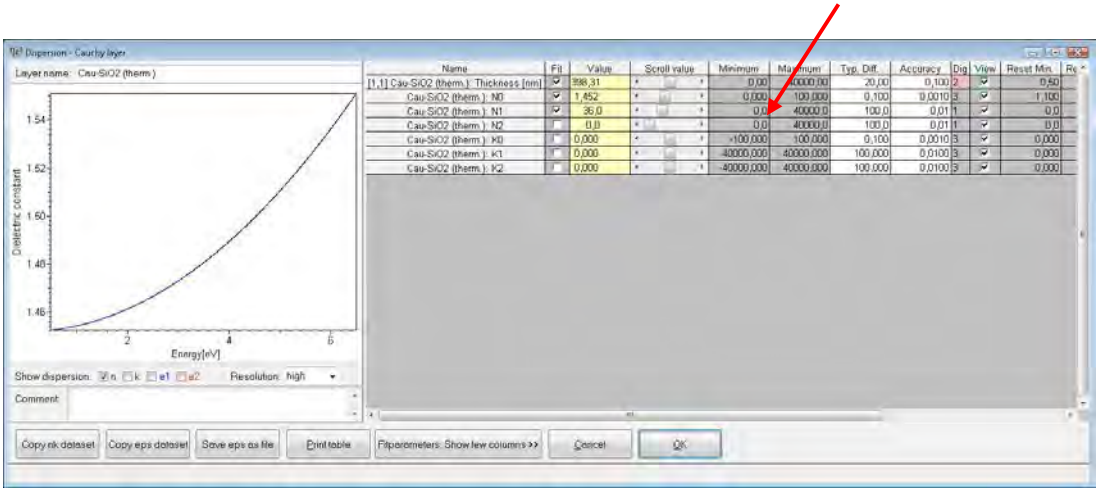


Fig. 5-56 Cauchy layer minimum values

In order to obtain a normal dispersion the values of n_1 and n_2 shouldn't become negative. The Minimum value in the parameter list can be set to zero to obtain positive values (indicated by the red arrow in Fig. 5-56).

Otherwise the following behavior might happen: the dispersion becomes negative as shown in Fig. 5-57. This is called abnormal dispersion. It is an allowed and physical correct solution only when an extinction k is present. It is an unphysical solution when k=0.

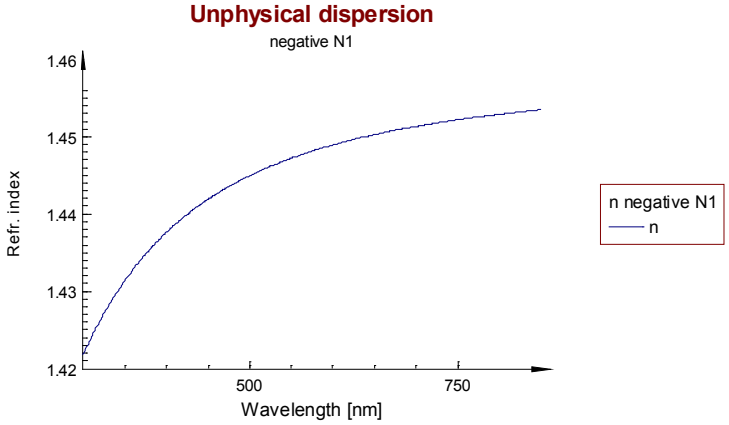


Fig. 5-57 Cauchy layer unphysical solution

Anormal dispersion:

In case the material is not completely transparent the dispersion is changing its behavior where the absorption starts.

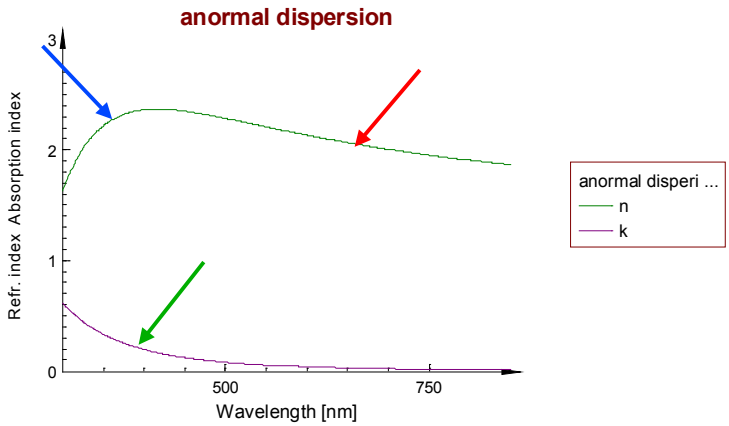


Fig. 5-58 Cauchy Anormal dispersion

The red arrow in Fig. 5-58 indicates the spectral range where the refractive index shows normal dispersion. The blue arrow indicates the spectral range where the refractive index shows abnormal dispersion. This behavior is allowed when the material shows an extinction k as indicated by the green arrow.

Usually different types of dispersion formulas (like Tauc-Lorentz) are used when this behavior should be described correctly. This is necessary because of the existing physical relation between n and k. This is called the Kramers-Kronig (KK) relation. It means: if the dispersion of k is known in the full spectral range (from zero to infinity) then the dispersion of n can be calculated using the Kramers-Kronig integral. The Cauchy dispersion doesn't obey this KK relation and should be replaced if necessary as mentioned above.

5.2.4.10 Cauchy type 0 and Cauchy type 1 layer

Theoretical assumptions:

In addition to the Cauchy formulas described in chapter 5.2.4.9 similar formulas are used alternatively. They do not use the scale factors C_0 and C_1 in the formula for n and they use different formulas for k.

Cauchy-type0 layer:

$$n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4} \qquad [\lambda] \text{ - µm, } [A_n]\text{: dimensionless, } [B_n] - \mu m^2,\ [C_n] - \mu m^4$$

$$k(\lambda) = A_k \cdot e^{B_k(E-C_k)} \qquad [\text{E}] \text{ - eV, } [A_k]\text{: dimensionless, } [B_k] - eV^{-1},\ [C_n] - eV$$

Cauchy-type1-layer:

$$n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4} \qquad [\lambda] \text{ - µm, } [A_n]\text{: dimensionless, } [B_n] - \mu m^2,\ [C_n] - \mu m^4$$

$$k(\lambda) = 10^{A_k} \cdot e^{B_k(E-C_k)} \qquad [\text{E}] \text{ - eV, } [A_k]\text{: dimensionless, } [B_k] - eV^{-1},\ [C_n] - eV$$

Important: As the parameters A_k and C_k are totally correlated in both types of layers the parameter C_k can be set manually but it should *not* be selected for fit, otherwise ambiguous results will occur.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Cauchy type 0 layer” or “Cauchy type 1 layer” depending on the desired type. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for Cauchy type 0 layer is shown in Fig. 5-59. The editor for Cauchy type 0 layer is shown in Fig. 5-60. The settings can be made as explained in chapter 5.2.4.3.

In the case of transparent materials it is advisable not to select the A_k, B_k and C_k values for fit in order to stabilize the results.

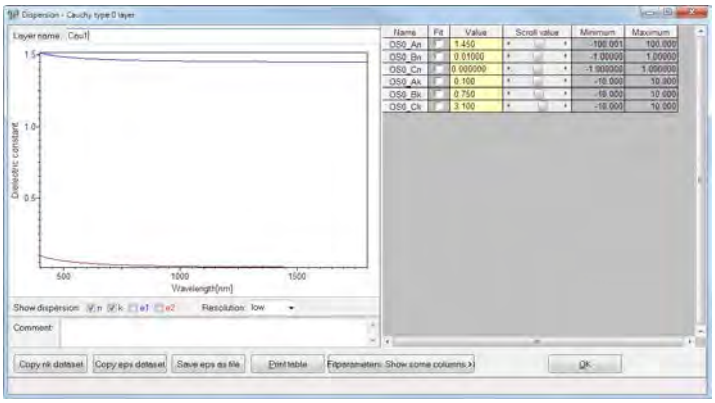


Fig. 5-59 Cauchy type 0 layer editor

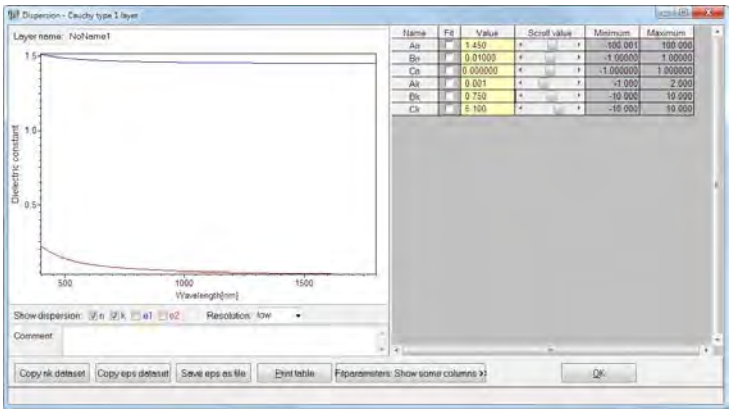


Fig. 5-60 Cauchy type 1 layer editor

5.2.4.11 Cody-Lorentz-Layer

Theoretical assumptions:

The Cody formula was derived on the assumptions of parabolic bands and a constant dipole matrix element (instead of parabolic bands with a constant momentum matrix element like in the Tauc-theory). The Cody-Lorentz-layer is a combination of the Cody formula and a Lorentz oscillator. Together with the Urbach absorption tail the layer gives us enhanced capabilities in the modeling of amorphous materials like a-Si:H[5].

The so called Urbach-Cody-Lorentz-layer is shown below.

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0CE(E-E_g)^2}{\left((E^2-E_0^2)^2+C^2E^2\right)\left((E-E_g)^2+E_P^2\right)} & E > E_t \\ \frac{E_1}{E}\exp\left(\frac{(E-E_t)}{E_u}\right) & E \le E_t \end{cases}$$

$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{x\varepsilon_2(x)}{x^2 - E^2} dx$$

A, E_0 and C are the parameters of the Lorentz-oscillator (A = amplitude, E_0 = resonance energy, C = oscillator width). E_g and E_p are the parameters of the Cody-formula (E_g = band gab energy, E_p = transition energy (E_g + E_p) that separates the absorption onset behaviour from the Lorentz-oscillator behavior). E_t and E_u are the parameters of the Urbach absorption tail which describes the weak exponentially increasing absorption with increasing E below the band gap (E_t = transition energy between Cody-Lorentz and Urbach tail, E_u = Urbach energy). All parameters are energies and therefore have the unit “eV”.

Creating a new layer

A new Cody-Lorentz layer is created by “File\New\Layer” and selecting the layer type “Cody-Lorentz layer”. This creates the new layer and opens the editor. The name of the new layer and its properties E_g, A, E_0, C, E_p, E_t, E_u can be entered. If you want to use a Cody-Lorentz layer without Urbach tail just set E_t and E_u to zero and deselect them for fitting. In this case the Urbach-part is deselected and the following formula is used:

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0CE(E-E_g)^2}{\left((E^2-E_0^2)^2+C^2E^2\right)\left((E-E_g)^2+E_P^2\right)} & E > E_g \\ 0 & E \le E_g \end{cases}$$

$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{x\varepsilon_2(x)}{x^2 - E^2} dx$$

[E_g], [A,], [E_0,], [C], [E_p], [E_t,], [E_u] : eV

Editing the layer

The editor for Cauchy layers is shown in Fig. 5-61. The settings can be made as explained in chapter 5.2.4.3.

Typical values after creation of a new Cauchy layer are shown in Tab. 5-4.

[5] A.S. Ferlauto, G.M. Ferreira, J.M. Pearce, C.R.Wronski, R.W.Collins, Journal of Applied Physics, Volume 92, No. 5 (2002), 2424

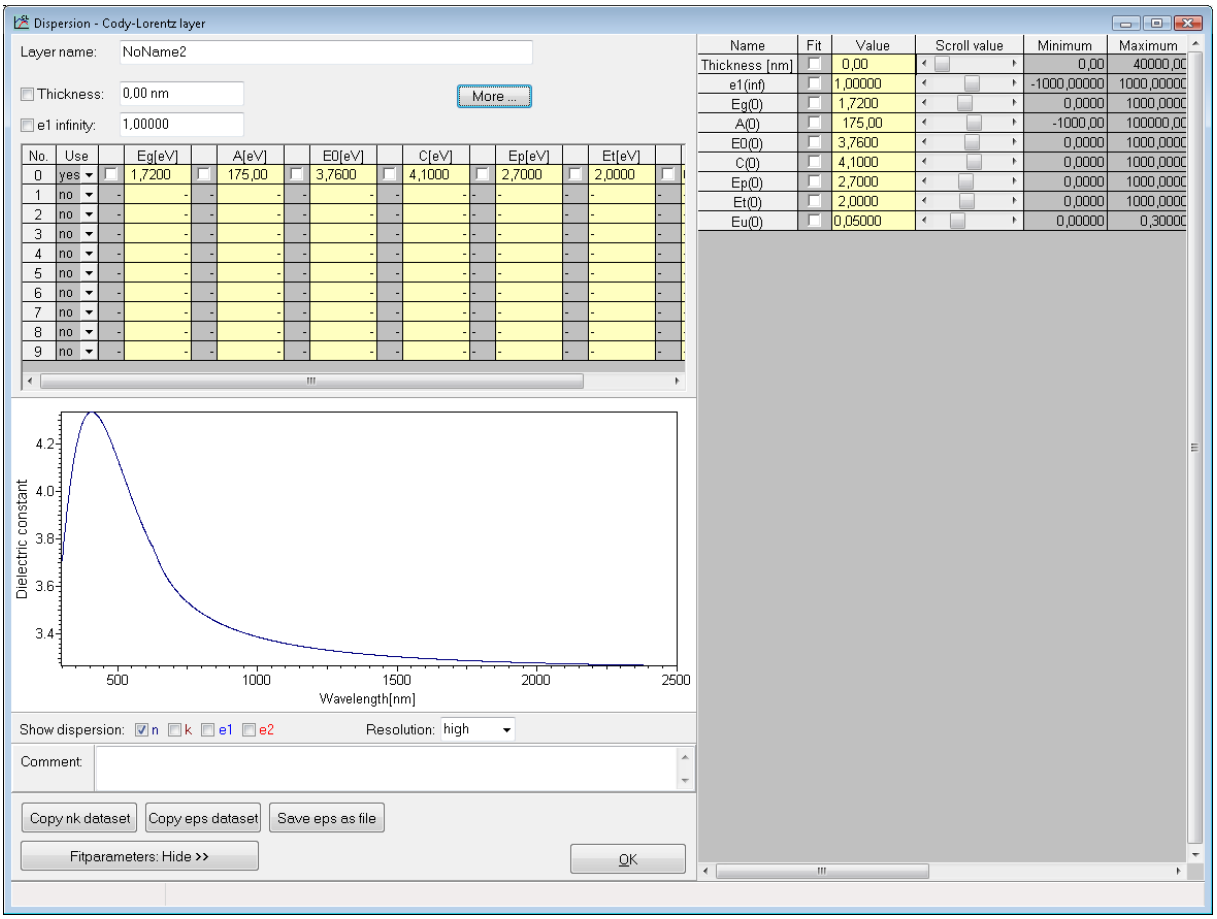


Fig. 5-61 Cody-Lorentz layer editor

Name	Fit	Value	Typ. Diff.	Minimum	Maximum	Reset Min.	Reset Max.	Accuracy
Thickness [nm]	0	0.0	20.00	0.0	40000	0.5	30000	0.1
E_g	0	1.720	0.100	0.0	100	0.1	8.0	0.001
A	0	175.0	10.00	-1000	100000	0.000	200	0.100
E_0	0	3.760	0.010	0.0	1000	0.100	8.0	0.001
C	0	4.100	0.010	0.0	1000	0.100	8.0	0.001
E_p	0	2.700	0.010	0.0	1000	0.100	8.0	0.001
E_t	0	2.000	0.010	0.0	1000	0.100	8.0	0.001
E_u	0	0.050	0.001	0.0	0.3	0.01	0.1	0.0001

Tab. 5-4 Default setup of fit parameters after a new Cody-Lorentz layer was created

Usually the maximum value of E_u should be limited near to 0.3 eV because for energies below E_u the absorption k increases again which is a non-physical behavior.
For the same reason the value of E_t should always be higher than or equal to E_g, because otherwise the Urbach tail will give non-physical solutions.

5.2.4.12 Drude-Lorentz oscillator layer

Theoretical assumptions:

The vibration of the molecules in a material may lead to resonances in the optical properties. For example the masses of the silicon atoms and the oxygen atoms in SiO_2 and their binding forces can be described by a mass-spring-system with resonances of certain frequency, strength and broadening. These resonance terms are also called oscillators.

The dielectric function can be described by a sum of Lorentz-oscillators, where $\boldsymbol{\Omega_p}$ gives the strength, $\boldsymbol{\Omega_0}$ gives the center frequency, and $\boldsymbol{\Omega_\tau}$ gives the damping of each resonance.

In addition the contribution of free charge carriers (for example electrons in a metal or in a doped semiconductor) can be described by a Drude-term, where $\boldsymbol{\omega_p}$ gives the strength and $\boldsymbol{\omega_\tau}$ gives the damping.

$$\boldsymbol{\varepsilon(\nu) = \varepsilon_1(\nu) + i\varepsilon_2(\nu) = \varepsilon_{1\infty} - \frac{\omega_p^2}{\omega^2 + i\omega_\tau \nu} + \sum_i \frac{\Omega_{p,i}^2}{\Omega_{0,i}^2 - \nu^2 - i\Omega_{\tau,i}\nu}}$$

As usual in infrared spectroscopy the wavenumbers $\boldsymbol{\nu}$ [cm^{-1}] are used for the spectral scale, and all parameters $\boldsymbol{\Omega_p}$, $\boldsymbol{\Omega_0}$, $\boldsymbol{\Omega_\tau}$, $\boldsymbol{\omega_p}$ and $\boldsymbol{\omega_\tau}$ are given in wavenumbers $\boldsymbol{\nu}$ [cm^{-1}] as well.

The spectroscopic values are connected with the values of the free charge carriers by the relations $\boldsymbol{\omega_p = \sqrt{\frac{Ne^2}{\varepsilon_0 m^*}}}$ and $\boldsymbol{\omega_\tau = \frac{e}{\mu m^*}}$ where **N** is the concentration, **μ** the mobility, **m*** the effective mass of the carriers and $\boldsymbol{\varepsilon_0}$ the permittivity of free space.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Drude-Lorentz oscillator layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for Drude-Lorentz oscillator layer is shown in Fig. 5-62. The example shown is typical for dielectric material with resonances the mid infrared spectral range. Every resonance is described by one oscillator with its 3 parameters.

The dielectric function of Gold in the mid infrared range is shown in Fig. 5-63 as another example. The Drude formula describes the metallic behavior.

The names $\boldsymbol{\Omega_p}$ etc. of the oscillator parameters are shown as Omega_p etc.
The names $\boldsymbol{\omega_p}$ etc. of the Drude parameters are shown as omega_tau_free_carriers etc.

Note: The editfield "e2 inf imag." should be set to zero at all times.

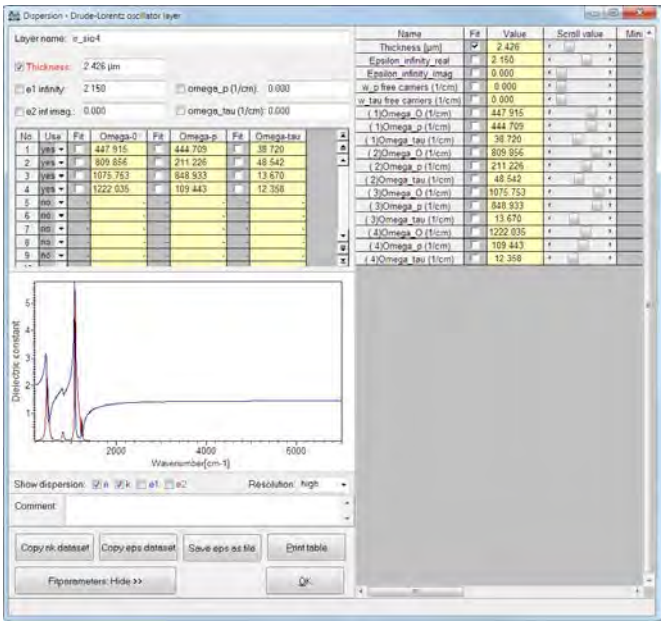


Fig. 5-62 Drude-Lorentz-oscillator layer editor for SiO_2 in the MIR

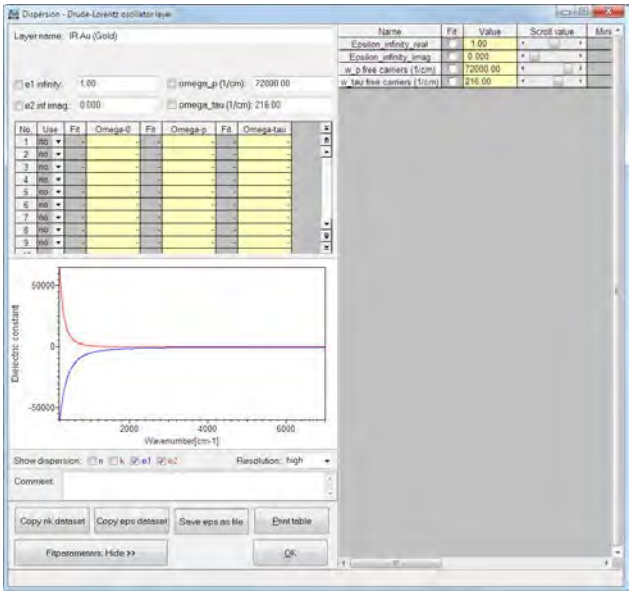


Fig. 5-63 Drude-Lorentz-oscillator layer editor for Au in the MIR

5.2.4.13 Drude-type 0 layer

Theoretical assumptions:

In addition to the Drude formula described in detail in chapter 5.2.4.12 similar formulas are used alternatively.

Drude type 0 layer:

$$\varepsilon_{Drude\_type0}(E) = \varepsilon_{1\infty} - \frac{Amp \cdot Br}{E^2 + i \cdot Br \cdot E} \qquad [\mathrm{E}] - \mathrm{eV},\ [Amp]\ - \mathrm{eV},\ [Br] - eV$$

Creating a new layer

A new Drude type0 layer is created by “File\New\Layer” and selecting the layer type “Drude type 0 layer”. This creates the new layer and opens the editor. The name of the new layer and its properties $\varepsilon_{1\infty}$, Amp and Br can be entered.

Editing the layer

The editor for the Drude type 0 layer is shown in Fig. 5-64. it gives an example for the dielectric function of gold in the mid infrared range. The Drude formula describes the metallic behavior.

The Drude type 0 layer can be used together with the 'Advanced combination layer' described in chapter 5.2.4.4 and the Lorentz layers described in chapter 5.2.4.23 because materials usually have one or more vibration bands that have to be described.

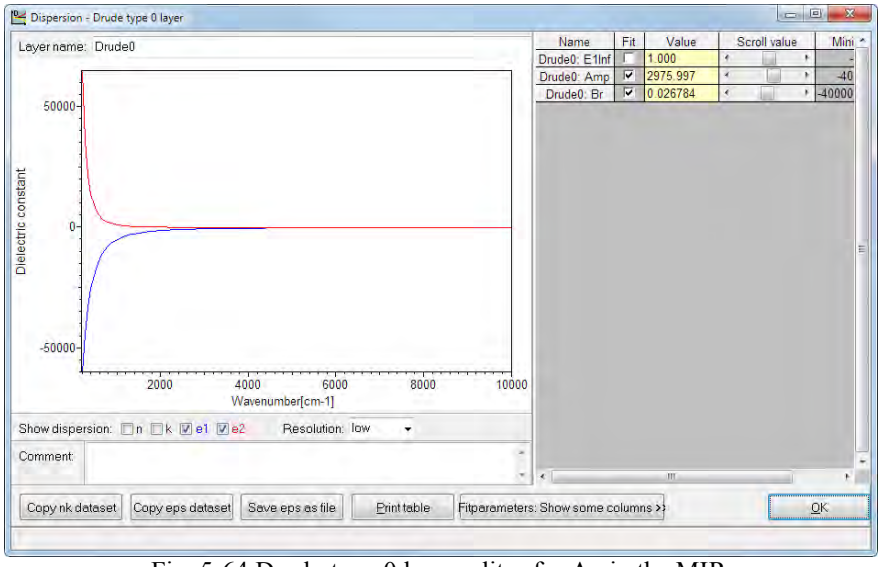


Fig. 5-64 Drude-type 0 layer editor for Au in the MIR

5.2.4.14 Effective medium layers

Theoretical assumptions

A material consisting of a host medium with inclusions of another medium can be described by a an 'effective medium approximation' which calculates a 'mixture' of the optical properties of both materials. The optical behavior of such EMA combinations is theoretically calculated by means of the effective medium approximation. These approximations can be Maxwell-Garnett, Lorentz-Lorenz, Bruggeman or chemical mixture.
The Maxwell-Garnett theory uses the inclusion in an infinite host medium. Therefore this should be used for small fractions of inclusions in the host medium (for example surface roughness).
If the fractions of the host and inclusion do not differ much the Bruggeman approximation should be used. You should use Bruggeman for layers consisting of components.
The chemical mixture approach is useful if the host and inclusions can't be treated as particles but as chemical compound. It averages the dielectric constants by the fractions of inclusions and host.

All theories have the same form

(1) $$\frac{\tilde{n}_e^2 - \tilde{n}_h^2}{\tilde{n}_e^2 + 2\tilde{n}_h^2} = \sum_{i=1}^{N} f_i \frac{\tilde{n}_i^2 - \tilde{n}_h^2}{\tilde{n}_i^2 + 2\tilde{n}_h^2}$$ N - number of constituents

where n_e, n_h, n_i are the complex refractive indices for the effective medium, the host medium and the inclusions. Note that we have not yet defined a "host" medium. The f_i represent the volume fractions of inclusions. We shall see the primary difference in Lorentz-Lorenz, Maxwell-Garnett and Bruggeman models is the choice of the host medium.
The underlying assumptions are spherical inclusion geometry and dipole interactions[6][7]. Although neither assumption is usually satisfied rigorously, these are standard first approximations that usually give good results.
The Lorentz-Lorenz approximation was developed to describe point polarizable entities embedded in vacuum. In this case n_h=1. The above equation becomes

(2) $$\frac{\tilde{n}_e^2 - 1}{\tilde{n}_e^2 + 2} = \sum_{i=1}^{N} f_i \frac{\tilde{n}_i^2 - 1}{\tilde{n}_i^2 + 2}$$ Lorentz-Lorenz model

For the roughness involved in island formation film growth, this is a reasonable approximation up to a volume fraction of about 20%[8].
The Maxwell-Garnett approximation corresponds to inclusions in a host background (other than vacuum) and the quantities in (1) have their obvious interpretations. In the case of a single inclusion n_1 in a single host n_h the equation becomes

(3) $$\frac{\tilde{n}_e^2 - \tilde{n}_h^2}{\tilde{n}_e^2 + 2\tilde{n}_h^2} = f_1 \frac{\tilde{n}_1^2 - \tilde{n}_h^2}{\tilde{n}_1^2 + 2\tilde{n}_h^2}$$ Maxwell-Garnett model

This degenerates to the Lorentz-Lorenz form, if the host happens to be vacuum or air. Again, this is not a bad approximation if the inclusions make up a small fraction of the total volume. Aspnes et al.[9] pointed out how this theory breaks down when using this model in rough surface applications or in other applications where there is about as much inclusion as there is a host. For a single type of inclusion, one calculates different values of n_e if the roles of host and inclusion are interchanged, even if the respective volume fractions stay the same.

[6] C.G.Grandqvist and O. Hunderi, Phys. Rev. B, 16, 3513 (1977)
[7] R. Landauer, in "Proceedings of the First Conference on Electrical Transport and Optical Properties of Inhomogeneous Media", edited by J. C. Garland and D.B. Tanner, AIP Conf. Proc. No. 40, AIP, New York (1978)
[8] Harland G. Tompkins, in „A User's Guide to Ellipsometry", Academic Press, New York (1993), p. 247
[9] D.E:Aspnes, J.B. Theeten, and F. Hottier, Phys. Rev. B, 20, 3292 (1979)

To deal with this matter, Bruggeman[10] suggested making the "host" the effective medium itself, i.e., making $n_h=n_e$. With this formulation, equation (1) becomes

(4) $$0=\sum_{i=1}^{N} f_i \frac{\tilde{n}_i^2-\tilde{n}_e^2}{\tilde{n}_i^2+2\tilde{n}_e^2}$$ Bruggeman model

The Maxwell-Garnett approximation covers therefore the Lorentz-Lorenz model and no special support is required for the latter model. If you want to use the Lorentz-Lorenz model use Maxwell-Garnett and ensure the inclusion to be vacuum. If you use index gradients you have to ensure the top medium to be air to use the Lorentz-Lorenz model.

SpectraRay supports a third type of EMA which is useful if the above condition of point entities is not applicable. This occurs when host and inclusion chemically react and create new combinations no longer having the volume dielectric function. The first approximation for this purpose is to average the dielectric constant ($\varepsilon=n^2$) with the volume fractions:

(5) $$\tilde{n}_e^2=\frac{\sum_{i=1}^{N} f_i \tilde{n}_i^2}{\sum_{i=1}^{N} f_i}$$ chemical mixture

Index Gradients

SpectraRay supports the above EMA models and the EMA layer uses these models in two forms. You can switch the EMA layer to act as an index gradient between two materials. If the layer thickness is z, the top and bottom refractive indices are n_t, n_b the index gradient is modeled by a series of N subsequent sub-layers, each of the thickness z/N having the refractive indices:

(6) $$n_i=n_b+\frac{2i-1}{2N}(n_t-n_b)$$ i = 1 ... N linear Gradient

(7) $$n_i=n_b+\frac{1}{2a}\left(\mathrm{a\,tan}\left(\frac{3\pi}{N}-\frac{3\pi}{2}\right)+a\right)(n_t-n_b)$$ arctan-Gradient

$$a=a\tan\left(\frac{3\pi}{2}\right)$$

The 0 -fraction and bottom of the layer is set to (-3/2Pi, ArcTan(-3/2Pi)) and the 1 fraction and top of the layer to (3/2Pi, ArcTan(3/2Pi)).

Creating a new layer

A new growing layer is created by "File\New\Layer" and selecting the layer type "Effective medium and index gradient layer". This creates the new layer and opens the editor. You should enter the name of the new layer and its properties.
A second step should specify the two materials used as host/inclusion or top/bottom. See Appendix D "Material name edit fields and buttons" for information on the functioning of the edit field and the associated button.

[10] D.A.G. Bruggeman, Ann. Phys. (leip.), 24, 636 (1935)

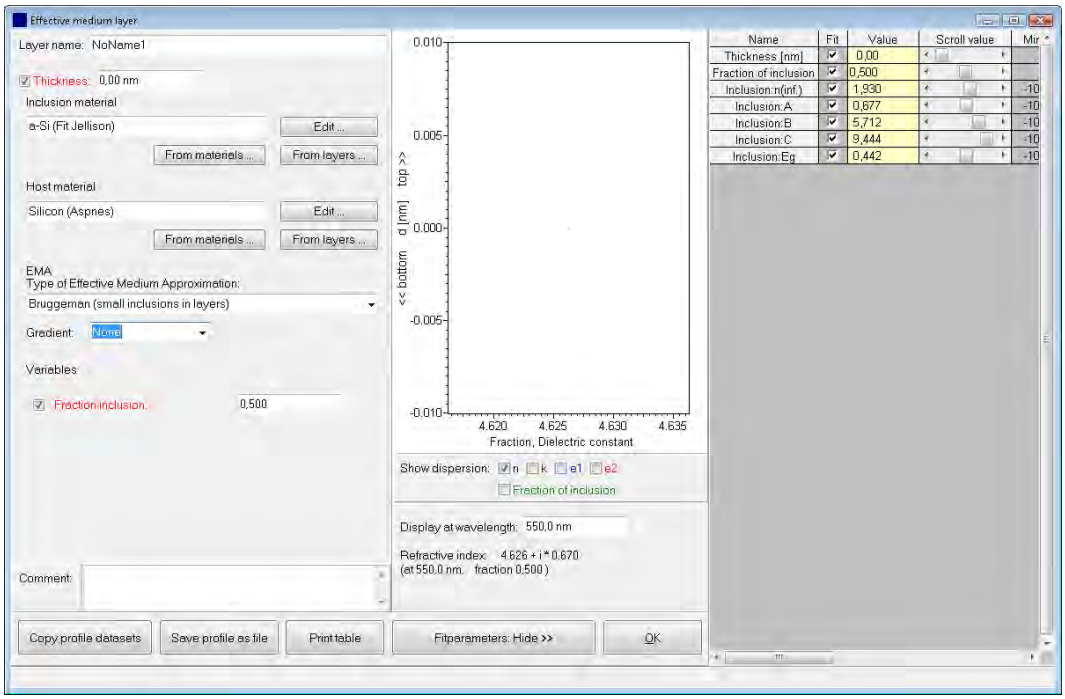


Fig. 5-65 EMA layer edit screen

An EMA layer has a name, a thickness, a host layer, an inclusion layer and the fraction of inclusions. The effective medium theory used is selected by a combobox.
Gradient layers: This layer type also can work as an index gradient layer if you select other gradient types as “none”. In this case the layer varies the fraction of the inclusion from 0 to 1 to create sublayers. These sublayers have a thickness of thickness/subdivision and a fraction of i/subdivision (linear gradient). The number of sublayers should be set in dependency from the environment: some cases work with 3 subdivisions well others require 100 or more. You can simply calculate curves with different values and use the smallest that produces no changes compared to higher values. For treating non-abrupt interfaces the ArcTan-gradient is introduced. Like the ArcTan-function this interface is smooth with no edges in the n(th)-curve.
Note, the index gradient is modeled by a series of sublayers with a varying refractive index. The “subdivision” sets the number of sublayers used. You should use a small number in all cases possible to reduce the calculation time.

Name	Fit	Value	Typ. Diff.	Min.	Maxi.	Reset Min.	Reset Max.	Accuracy
Thickness [nm]	0	1.0	20.0	0.0	400000.0	0.5	30000.0	0.1
bottom:N0	0	1.460	0.100	0.001	40.000	1.100	2.000	0.001
bottom:N1	0	0.000	100.000	0.000	4000.000	0.000	20.000	4.000
bottom:N2	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
bottom:K0	0	0.000	0.100	0.000	40.000	0.000	1.000	0.001
bottom:K1	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
bottom:K2	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
top:N0	0	1.465	0.100	0.001	40.000	1.100	2.000	0.001
top:N1	0	5.389	100.000	0.000	4000.000	0.000	20.000	4.000
top:N2	0	0.001	0.100	0.000	4000.000	0.000	20.000	4.000
top:K0	0	0.000	0.100	0.000	40.000	0.000	1.000	0.001
top:K1	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
top:K2	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000

Tab. 5-5 Index gradient: Default fit parameter setup with two Cauchy type materials used as top and bottom medium. The parameter of the index gradient layer is only the thickness. All others come from the “sub”-layers. The index gradient layer adds “bottom” and “top” for clearance to the parameter names.

Name	Fit	Value	Typ. Diff.	Min.	Maximum	Reset Min.	Reset Max.	Accuracy
Thickness [nm]	0	1.0	20.0	0.0	400000.0	0.5	30000.0	0.1
Medium fracti	0	0.500	0.100	0.000	1.000	0.100	0.900	0.001
host:N0	0	1.460	0.100	0.001	40.000	1.100	2.000	0.001
host:N1	0	0.000	100.000	0.000	4000.000	0.000	20.000	4.000
host:N2	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
host:K0	0	0.000	0.100	0.000	40.000	0.000	1.000	0.001
host:K1	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
host:K2	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
medium:N0	1	1.465	0.100	0.001	40.000	1.100	2.000	0.001
medium:N1	1	5.389	100.000	0.000	4000.000	0.000	20.000	4.000
medium:N2	1	0.001	0.100	0.000	4000.000	0.000	20.000	4.000
medium:K0	0	0.000	0.100	0.000	40.000	0.000	1.000	0.001
medium:K1	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000
medium:K2	0	0.000	0.100	0.000	4000.000	0.000	20.000	4.000

Tab. 5-6 EMA: Default fit parameter setup with two Cauchy type materials used as top and bottom medium. The parameter of the EMA layer is only the thickness. All others come from the “sub”-layers. The EMA layer adds “host” and “medium” for clearance to the parameter names.

5.2.4.15 File-Layer (splined table)

Theoretical assumptions

The dielectric function for most semiconductors is given in tables measured at clean and layer-free substrates in vacuum. The results are very precise but cannot be approximated by a single formula within the spectral range available. Because of the wide spectral range a series of different effects occur and such a formula would grow large. A computational efficient approach is to take the measured data tables and interpolate between the measured points.
The splined table layer uses a table of up to 8000 data pairs of (n, k) or (e1, e2). A special hashing algorithm improves access speed for spectrum calculations. Such a table may be non-evenly spaced as available data in literature are often non-evenly spaced.
During calculation of n and k data for display or fit the data between two tabulated points is interpolated by a spline function. For data outside the tabulated data range the lowest or highest available data is used.

Creating a new file layer

The basis of the file layer is a table. Therefore the table has to be imported from an existing text file or it must be entered manually in an editor. Select “File\New\Layer” and “File layer” from the list of available layers. The dialog box shown in Fig. 5-66 appears. Press 'yes' to import an existing table or 'no' to enter the data manually.

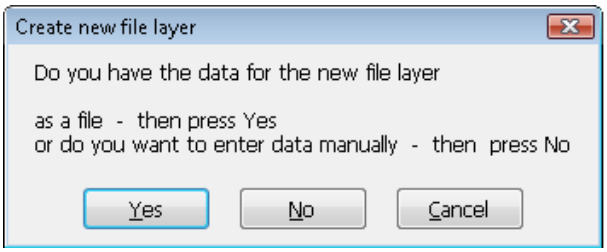


Fig. 5-66 Step 1: Creating a file layer

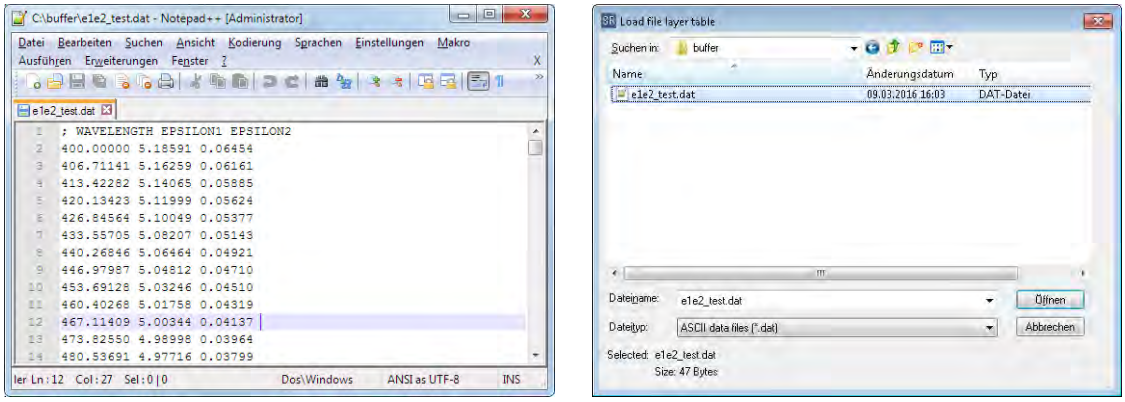


Fig. 5-67 Step 2a: Import from external epsilon data file

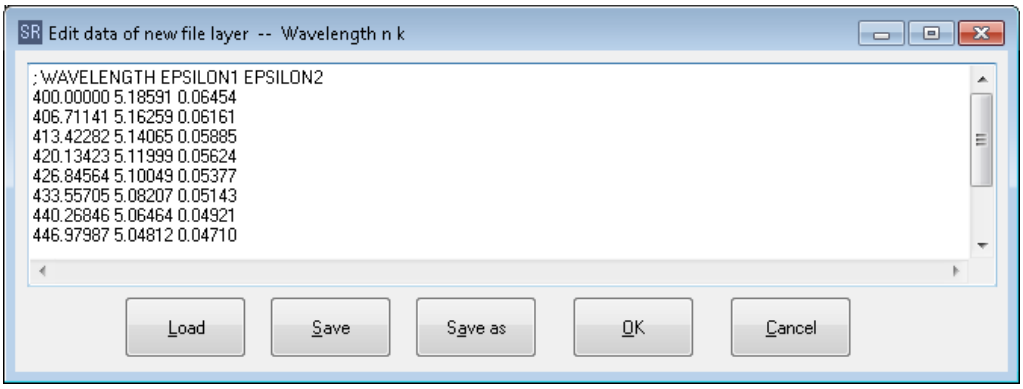


Fig. 5-68 Step2a: Check and edit imported epsilon data in the internal editor

An external file as shown in Fig. 5-67 can be imported in Steps 2a. It will appear in the internal editor shown in Fig. 5-68. The data may be edited within the editor - especially textlines may be deleted.

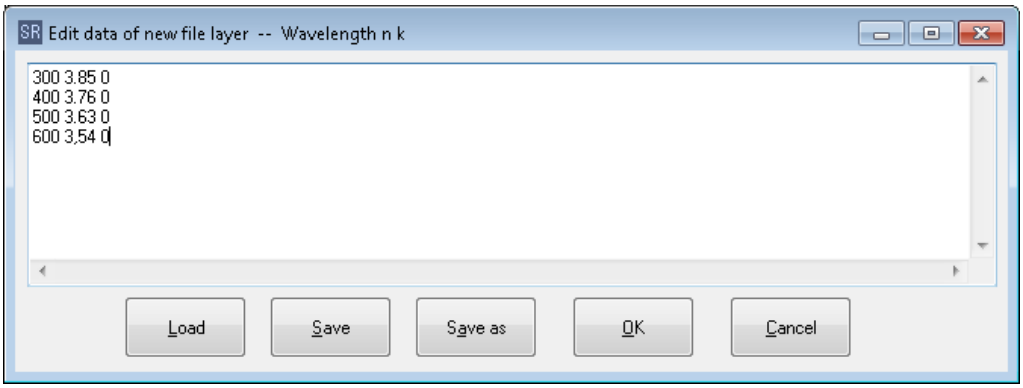


Fig. 5-69 Step 2b: Enter refractive index data into the internal editor

As Step 2b it is alternatively possible to enter all data manually into the editor as shown in Fig. 5-69.

The data format is identical to the rules described in chapter 5.5 (ASCII Data import). In this case two or three columns are needed. Two columns with “;Min =” and “;Max =” create evenly spaced data, three columns create a non-evenly spaced data set.
The last two columns can be pairs of (n, k) or (e1, e2). You can enter your numbers with a “.” for the decimal point or use the language dependent character defined in the Windows control panel.
The x-axis does not need to be specified because the third step opens the header page of the data editor. This allows you to import a broad range of data and to create material files. You can have your data in eV, nm, cm-1 and the data can be refractive indices, dielectric constants and measured (Ψ, Δ) values (at 70° angle of incidence !!!). If other angles are required use the data import, set up the correct angle in the title page of the data editor and convert the data to a file.

If you want to create a material file from a very large dataset (> 8000 spectral points) the editor for step 2 will not process this dataset (the load function takes only the first part of the file).

The file layer will be created from the data in the editor by pressing OK and a message shown in Fig. 5-70 should appear.

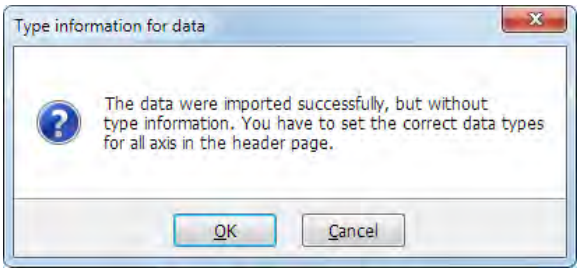


Fig. 5-70 Data import successful

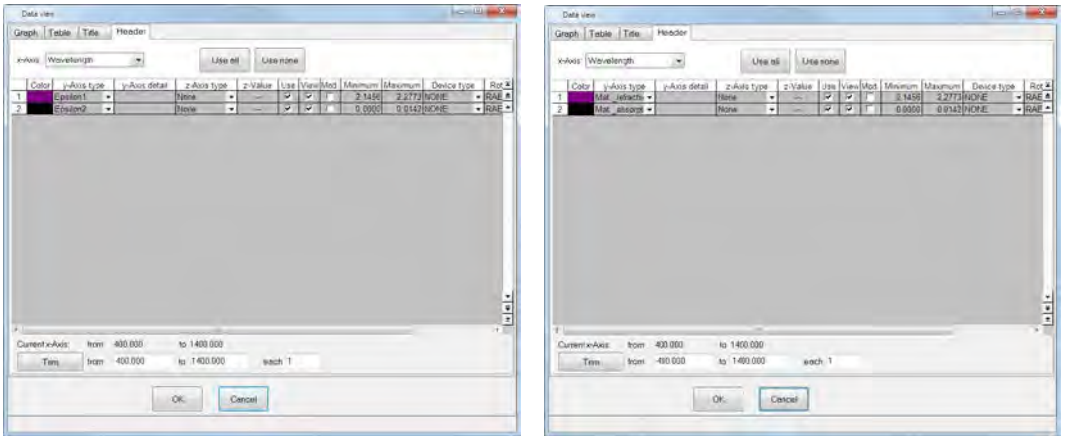


Fig. 5-71 Step 3: Determine type of imported data

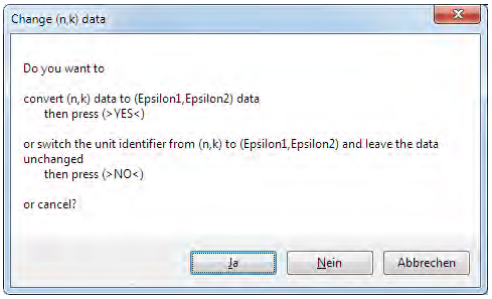


Fig. 5-72 Step 3: Determine type of imported data

As Step3 the type of data which has been imported has to be determined.
As shown in Fig. 5-71 the x-axis is be default set to 'wavelength'. The correct unit of the imported data has to be selected.
The y-axis of data column 1 and 2 is by default set to 'untyped'.
If the imported dataset contains refractive index data (n, k) select 'Mat_refractive_index' for column 1 and 'Mat_absorption' for column 2.
If the imported dataset contains dielectric function data (e1, e2) select 'Mat_refractive_index' for column 1 and 'Mat_absorption' for column 2.
As shown in Fig. 5-72 the change of the data type may happen with or without mathematical conversion between (n,k) and (e1,e2).

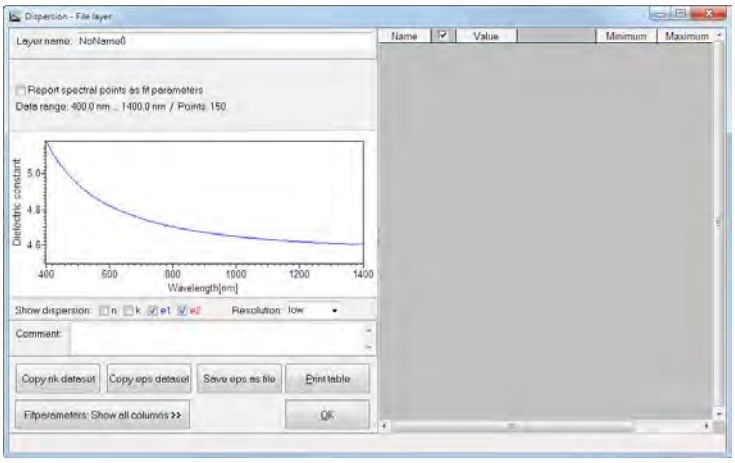


Fig. 5-73 Step 4: Check imported data in the file layer dialog

As Step 4 make sure the data is correctly imported and the types are correctly set by checking the diagram in the file layer as shown in Fig. 5-73.
Finally enter a suitable name for the created file layer.

Editing the layer

The editor for the table layer holds the dielectric function within the whole range of available data. For some semiconductors as c-Si the data are well known from the UV to the far infrared. Displaying the whole data range will not show UV specific data. Therefore the spectral range is limited by the spectral range defined within the environment. In this case a message “Display limited by environment settings” appears.

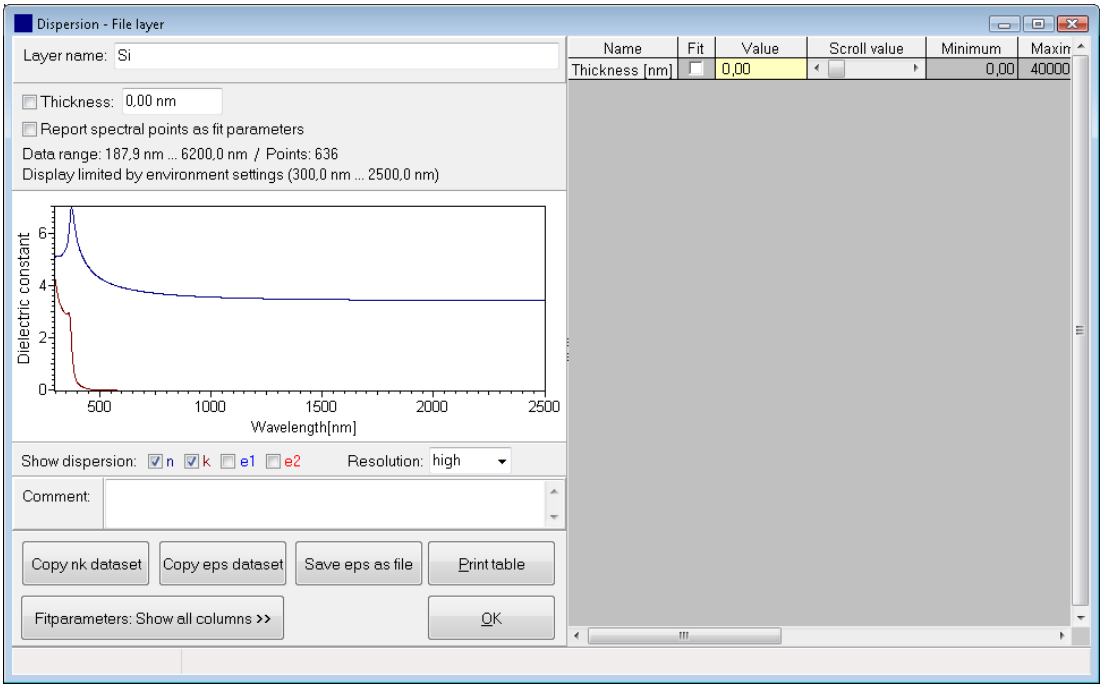


Fig. 5-74 Editor for file layers

The “Layer name” property sets the name of the layer listed within the model editors and within the material listbox. If the “thickness” property is visible the “layer” acts as a layer otherwise as a material.

An important flag is “Report spectral points as fit parameters”. If this flag is unchecked, the table stored within the layer is not available as fit parameter.

Checking this flag lets all table data added to the current set of fit parameters. This is useful for fitting an unknown dispersion function by a small (!!) number of points. If you have a tabular function consisting of many points it is strongly recommended to uncheck this flag to avoid time expansive handling of large sets of fit parameters and ambiguous solutions.

Name	Fit	Value	Typ. Diff.	Minimum	Maximum	Reset Min.	Reset Max.	Acc.
n298.9nm	0	4.992	0.100	0.001	400.000	0.500	3.000	0.001
k298.9nm	0	4.255	0.100	0.000	400.000	0.500	3.000	0.001
n302.6nm	0	5.020	0.100	0.001	400.000	0.500	3.000	0.001
k302.6nm	0	3.968	0.100	0.000	400.000	0.500	3.000	0.001
n306.5nm	0	5.019	0.100	0.001	400.000	0.500	3.000	0.001

Tab. 5-7 Default fit parameter settings for a file layer

Note that file layers are the basis of most material definitions and come from direct measurements on clean samples in vacuum without any layers and with reduced surface roughness. This importance of file layers is supported by directly converting measurements to file layers (*.spc, *.dob, *.dat to *.mat). See Appendix A “Drag&Drop overview” or the menu function reference for more information.

5.2.4.16 Formula layers

Theoretical assumptions

This most flexible type of layer allows using custom dispersion relations entered by the user. It requires a dispersion formula for the dielectric functions e1 and e2 or the complex refractive index n and k as a function of the wavelength (energy) and other parameters. The layer has predefined formulas for Cauchy, Fourohi-Bloomer, Schott, and Sellmeier and further formulas can be added.

A formula consists of user parameters and predefined symbols for wavelength, energy etc. See the editor description for a detailed description of these symbols. Hence, each formula must be unique, i.e. no sub-formulas are allowed. This requires to analytically expand formulas using other formulas involved.

The following formulas are used for standard applications and demonstration of the formula syntax:

Cauchy:

$$n(\lambda) = n_0 + n_1 \frac{10^2}{\lambda^2} + n_2 \frac{10^7}{\lambda^4}$$

$$k(\lambda) = k_0 + k_1 \frac{10^2}{\lambda^2} + k_2 \frac{10^7}{\lambda^4}$$

[λ]: nm, n_i, k_i : dimensionless

Forouhi-Bloomer:

$$n(E) = n(\infty) + \frac{B_0 E + C_0}{E^2 - BE + C}$$

$$k(E) = \frac{A(E - E_g)^2}{E^2 - BE + C}$$

$$Q = \frac{1}{2}\sqrt{4C - B^2} \qquad B_0 = \frac{-AB^2}{Q(2 + E_g B - E_g^2 + C)} \qquad C_0 = \frac{AB(E_g^2 + C)}{Q(2 - 2E_g C)}$$

[A] [$n(\infty)$] : dimensionless, [E], [B], [E_g]: eV, [C] : eV^2

Schott:

$$n^2 = A_0 + A_1\lambda^2 + \frac{A_2}{\lambda^2} + \frac{A_3}{\lambda^4} + \frac{A_4}{\lambda^6} + \frac{A_5}{\lambda^8}$$

$$k(\lambda) = 0$$

[λ]: µm [A0] -dim.-less, [A1] - μm^{-2} , [A2] - μm^2 , [A3] - μm^4 ,[A4] - μm^6 ,[A5] - μm^8

Sellmeier transparent:

$$n^2(\lambda) = 1 + \frac{A_1\lambda^2}{\lambda^2 - B_1} + \frac{A_2\lambda^2}{\lambda^2 - B_2} + \frac{A_3\lambda^2}{\lambda^2 - B_3}$$

$$k(\lambda) = 0$$

[λ]: µm [A_1], [A_2] , [A_3] : dimensionless, [B_1], [B_2], [B_3] : μm^2

Sellmeier absorbing with N=1

$$n^2 = 1 + \frac{A}{1 + \frac{B^2}{\lambda^2}}$$

$$k = \frac{C}{n \cdot D \cdot \lambda + \frac{F}{\lambda} + \frac{1}{\lambda^3}}$$

[λ]: nm [A], [C]:dimensionless, [B]:nm^2, [D]: nm^{-4}, [F]: nm^{-2}

These examples cover a broad range of applications, but you can expand the list of pre-defined dispersion relations to fulfill your own needs.

Creating a new layer

A new formula layer is created by "File\New\Layer" and selecting the layer type "Formula layer". This creates the new layer and opens the editor. The name of the new layer can be entered, the desired formula can be selected from the list select and the appropriate values for the parameters of this formula can be entered. If necessary a new formula can be entered and selected.

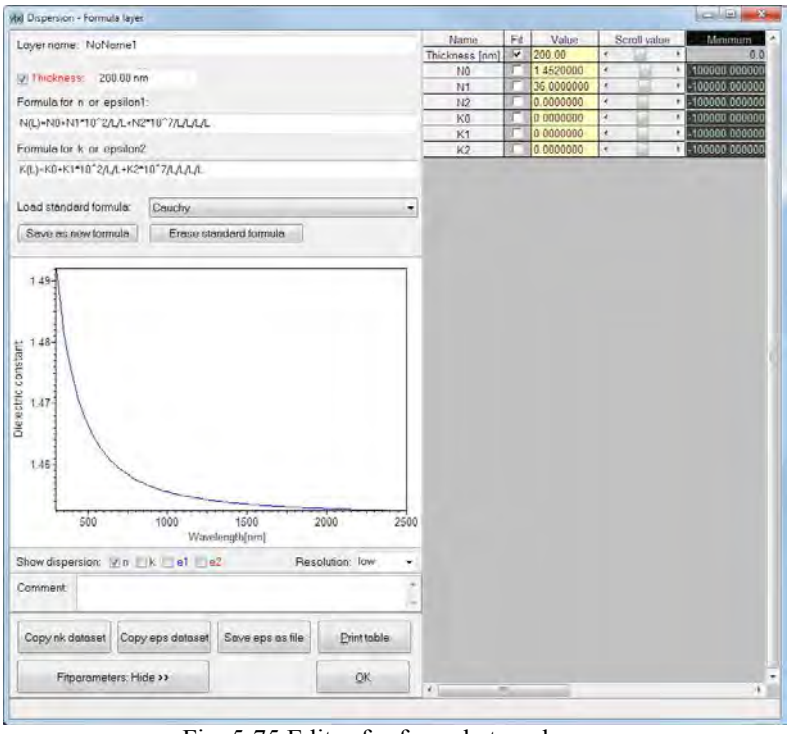


Fig. 5-75 Editor for formula type layers

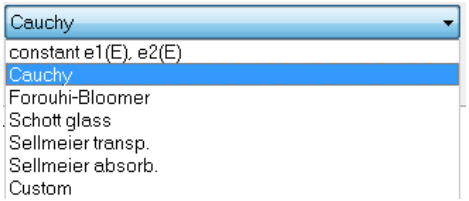


Fig. 5-76 Predefined formulas

Editor description

The central element of the formula layer is the built in expression parser. It evaluates entered formulas for correct semantic elements and structure. If a wrong formula is entered an error message is shown pointing to the wrong position and the type or error encountered.
Any formula entered must be like this

(8) $$y(x,y) = 1 + C0 / w$$

This expression is broken into tokens

y(..)	name of the function, “e1”, “e2”, “n” or “k” are allowed
x, y	one or multiple parameters, at least a single parameter required
=	assignment operator
1+...	expression used for evaluation
C0	user defined symbol
w	predefined symbol

The dielectric function can be defined either as $\tilde{\varepsilon}$ or $\tilde{n}$. The editor accepts the two formulas only if a pair of (“e1”, “e2”) or (“n”, “k”) is detected. The parameters can be any symbols, but at least one is required. The expression consists of operators, standard mathematical functions, predefined symbols and user symbols.
The difference between predefined and user symbols is the association of the values. For example the “w” symbol is associated to the wavenumber. This value automatically changes during calculation of a spectrum. A user symbol like “C0” in the above example always has a fixed value, but can be used as a fit parameter.

Category	Symbol	Description	Example
Relational operators	<	smaller	a<b
	>	larger	a>b
	<>	not equal	a<>b
	<=	smaller or equal	a<=b
	>=	larger or equal	a>=b
Adding operators	+	add	a+b
	or	logical or	a or b
	xor	logical exclusive or	a xor b
Multiplying operators	*	multiplication	a*b
	/	division	/
	and	logical and	a and b
	mod	logical modulo	a mod b
High priority operators	^	power operator	10^2
	not	logical not	not a
other symbols	(	opening parenthesis	(a+b)
	,	colon	y(x,y)
	)	closing parenthesis	(a+b)
	pi	3.1415926	1+pi
	e	2.7182818	e^2
functions	exp	powers of e	exp(x)
	ln	logarithm to basis e	ln(x)
	neg	negative value	Neg(x)=-x
	log	logarithm	log(a,b)
	sin	trig. sinus in radiants	sin(x)
	cos	trig. cosine in radiants	cos(x)
	tan	trig. tangent in radiants	tan(x)
	sec	trig. secans in radiants	sec(x)
	sqrt	square root	sqrt(x)
	abs	absolute value	abs(x)
predefined symbols	eV	energy [eV]	1+eV
	l	wavelength [nm]	1/l
	w	wavenumber [cm^{-1}]	w-w0
	Phi	angle of incidence [°]	sin(phi*pi/180)
	Theta	rotation of sample [°]	theta/2/pi
	T	temperature [°C]	T/1000
	Ti	process time [s]	Ti/60

Tab. 5-8 Symbol reference for formula expressions

Tab. 5-8 gives the available symbols recognized by the expression parser. All elements which do not appear in the table and consist of alphanumeric characters are treated as user symbols and extracted to the user symbol table on the right hand side.

On the left hand side the editor consists of two sections. The upper part contains all elements of formula handling. The combobox lists all formulas which are predefined. These split up into two groups. The first group consists of the documented set of formulas for fixed ε, Cauchy, Forouhi-Bloomer, Schott glass and Sellmeier. The second group is the set of formulas added by the user.

If you want to add a formula enter your formulas for (n, k) or (e1, e2) and press “Save as new formula”. A new name for the formula has to be entered and the new dispersion is added to the list of available formulas. The opposite function is performed by “Erase type” which deletes the selected formula name. The built-in formulas cannot be changed and cannot be erased.

The lower part displays the actual dielectric function in the spectral range defined within the environment. The four checkboxes allow to display the spectral dependence of n, k, e1 and e2.

When the formula is changed the expressions are evaluated and all user symbols are displayed with default values in the symbol table. If one of the formulas contains errors the last valid formula is used.

After the formula is set up the further value for each fit parameter (like minimum, maximum etc.) should also be set up. For example the Cauchy formula uses a refractive index style symbol “N0”. The typical difference default value is 1. Refractive indices should be set up with values of 0.1 or 0.05. Similar changes suitable to the individual parameters should be applied for a new formula. All user symbols have the same default parameters, which should be adapted. The thickness parameter is set up correctly.

The graphical display changes on each change of data or formula immediately and allows evaluating the formula and parameters.

Error handling: The evaluation of (n, k) or (e1, e2) gives default values of n=1, k=0 for any error during calculating the formulas (such as “1/0”, “sqrt(-1)”, “ln(-1)” etc.).

Name	Fit	Value	Typ. Diff.	Min.	Max.	Reset Min.	Reset Max.	Accuracy
Thickness [nm]	0	0.0	20.0	0.0	40000	0.5	30000.0	0.1
NU	0	1.6419	0.100	-10000	10000	0.000	10.000	0.001
A	0	0.2177	0.100	-100000	10000	0.000	10.000	0.001
C	0	12.711	0.100	-100000	10000	0.000	10.000	0.001
B	0	5.2326	0.100	-100000	10000	0.000	10.000	0.001
EG	0	0.5071	0.100	-100000	10000	0.000	10.000	0.001

Tab. 5-9 Default fit parameter setup for a Forouhi-Bloomer formula layer

5.2.4.17 Forouhi Bloomer layer

Theoretical assumptions:

The Forouhi Bloomer relation was developed to model the dielectric function of amorphous semiconductors [Reitano et al. "Spectroscopic ellipsometry of a-Si" Thin solid films, 233 (1993) 203-206], [G.E. Jellison, Thin solid films, 234 (1993), 416]. A typical example of this material is a-Si. The dispersion uses five parameters for n and k in the following formulas:

$$n(E) = n(\infty) + \frac{B_0 E + C_0}{E^2 - BE + C}, \qquad k(E) = \frac{A\left(E - E_g\right)^2}{E^2 - BE + C},$$

$$Q = \frac{1}{2}\sqrt{4C - B^2}, \qquad B_0 = \frac{-AB^2}{Q\left(2 + E_g B - E_g^2 + C\right)}, \qquad C_0 = \frac{AB\left(E_g^2 + C\right)}{Q\left(2 - 2E_g C\right)}.$$

[A] [$n(\infty)$] - dimensionless, [B] , [E_g] - eV, [C] - eV^2

Creating a new layer

A new layer is created by "File\New\Layer" and selecting the layer type "Forouhi Bloomer layer". This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

Fig. 5-77 gives an example for a Forouhi-Bloomer layer according to the data for Kr^+-doped a-Si found in the above mentioned article from Reitano et.al.

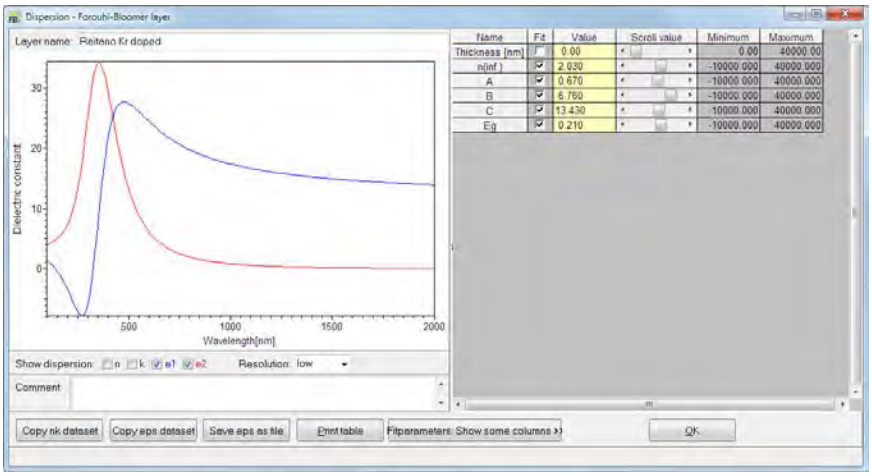


Fig. 5-77 Example for Forouhi-Bloomer layer

5.2.4.18 Harmonic oscillator layer

Theoretical assumptions:

Similar to - but different from - the Lorentz oscillator described in chapter 5.2.4.12 is the formula for the harmonic oscillator layer.

The dielectric function can be described by a sum of Harmonic-oscillators, where $\boldsymbol{\Omega_p}$ gives the strength, $\boldsymbol{\Omega_0}$ gives the center frequency, and $\boldsymbol{\Omega_\tau}$ gives the damping of each resonance.

$$\boldsymbol{\varepsilon(\nu) = \varepsilon_1(\nu) + i\varepsilon_2(\nu) = \varepsilon_{1\infty} + \sum_i \frac{\Omega_{p,i}^2}{\Omega_{0,i}^2 - \nu^2 + \frac{1}{4}\Omega_{\tau,i}^2 - i\Omega_{\tau,i}\nu}}$$

As usual in infrared spectroscopy the wavenumbers $\boldsymbol{\nu}$ [cm^{-1}] are used for the spectral scale, and all parameters $\boldsymbol{\Omega_p}$, $\boldsymbol{\Omega_0}$, $\boldsymbol{\Omega_\tau}$, are given in wavenumbers $\boldsymbol{\nu}$ [cm^{-1}] as well.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Harmonic oscillator layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for Harmonic oscillator layers is shown in Fig. 5-78.

The names $\boldsymbol{\Omega_p}$ etc. of the oscillator parameters are shown as Omega_p etc.

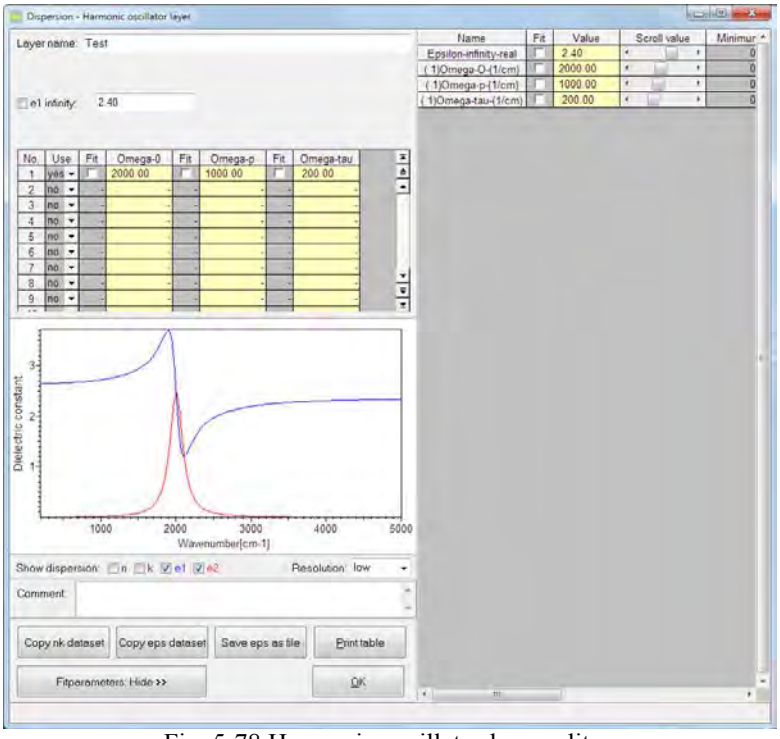


Fig. 5-78 Harmonic-oscillator layer editor

5.2.4.19 Homogeneous growing layer

Theoretical assumptions

A growing layer is simply any layer type put together with an initial thickness and growth rate. The initial thickness d_0 is the thickness at process time less or equal the beginning of the growth t_{min}. The growth rate g introduces the time dependency of the thickness. If the process time is greater than the end time of the growth t_{end} the layer has a fixed final thickness. Between both times the thickness d grows linearly from the initial thickness to the end thickness displayed.

$$d(d_{star}, G, t, t_{Start}, t_{End}) = \begin{cases} d_{start} & if \quad t < t_{start} \\ d_{start} + G\dfrac{(t - t_{start})^2}{t_{end} - t_{start}} & if \quad t \in [t_{start}, t_{end}] \\ d_{start} + G(t - t_{start}) & if \quad t > t_{end} \end{cases} \tag{9}$$

The application of time intervals allows separating the growth of several layers within one dataset.

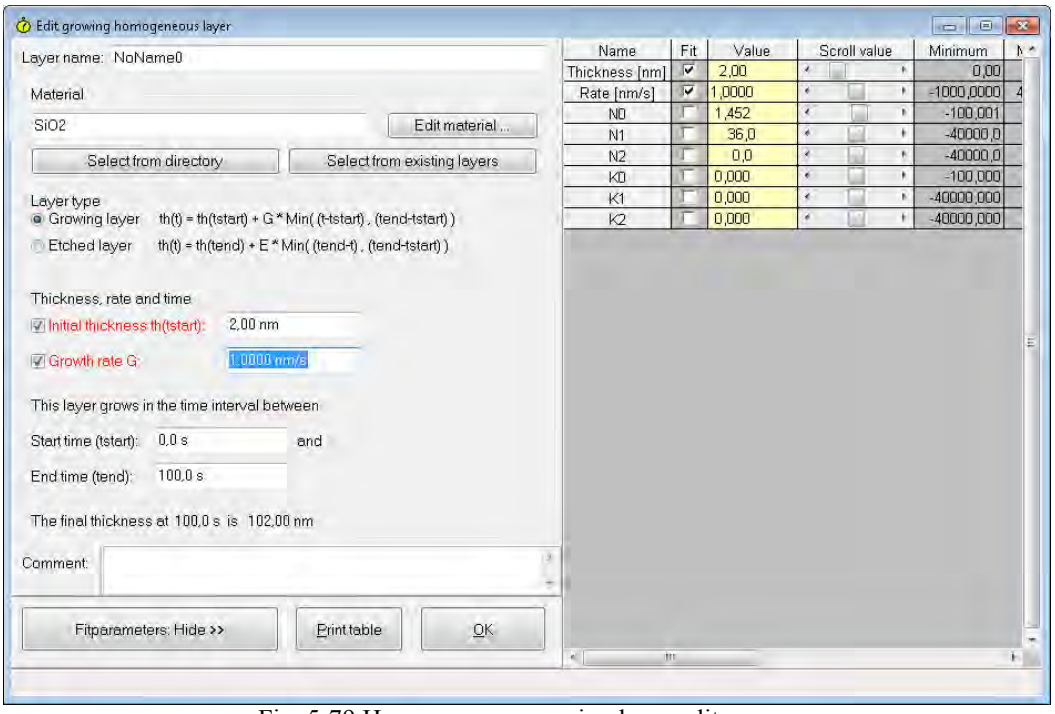


Fig. 5-79 Homogeneous growing layer edit screen

Creating a new layer

A new growing layer is created by “File\New\Layer” and selecting the layer type “Homogeneous growing layer”. This creates the new layer and opens the editor. You should enter the name of the new layer and its properties th_{start}, G, t_{start}, t_{end}.
A second step should specify the growing material. See Appendix D “Material name edit fields and buttons” for information on the functioning of the edit field and the associated button.

Editor description

The “Layer name” property is associated to a material. Changing of these materials is supported as documented in Appendix D “Material name edit fields and buttons”.
Initial thickness is useful for any types of layers deposited on silicon or similar semiconductors having a native oxide. The growth rate applies only between the start and end time. The thickness, growth rate and the two time

edit fields are edit fields for physical numbers. See Appendix D “Physical number edit fields” for more information.
Short reference on selecting the material: The behavior of the material button is as follows. If the name field is empty it opens a material select file box. If the name exists in the model such named layer is selected and edited.

Name	Fit	Value	Typ. Diff.	Min.	Max.	Reset Min.	Reset Max.	Accuracy
Initial Thickness [nm]	0	0.0	20.0	0	400000	0.5	30000	0.1
Growth rate [nm/s]	0	1.000	5.0000	-1000	40000	1.1000	200	0.0100
N0	1	1.465	0.100	0.001	40	1.100	2.000	0.001
N1	1	5.389	100.000	0	4000	0.000	20.000	4.000
N2	1	0.001	0.100	0	4000	0.000	20.000	4.000
K0	0	0.000	0.100	0	40	0.000	1.000	0.001
K1	0	0.000	0.100	0	4000	0.000	20.000	4.000
K2	0	0.000	0.100	0.000	4000	0.000	20.000	4.000

Tab. 5-10 Default fit parameter setup for a homogeneously growing layer. The last six parameters belong to a Cauchy-type layer.

5.2.4.20 ITO Hamberg layer

Theoretical assumptions:

Transparent conducting oxides (for example ZnO:Al or ITO) can be described by an oscillator approach for the UV-VIS range and a Drude approach for the NIR range. Looking more precisely the Drude approach can be improved by advanced dispersion theories named after Hamberg and Sernelius. ['Optical characterization of aluminium-doped Zinc oxide films by advanced dispersion theories', A. Pflug, V. Sittinger, F. Ruske, B. Szyszka, G. Dittmar, Thin Solid Films 455-456 (2004), pp.201-206].

For the Hamberg model a frequency- and wavenumber-dependent dielectric function $\varepsilon(k,\omega)$ based on a Lindhard function with a Hubbard correction is introduced. A dynamic resistivity $\rho(\omega)$ and a corresponding dielectric function $\varepsilon(\omega)$ is obtained as follows:

$$\varepsilon = \varepsilon_\infty + \varepsilon_{IR}$$

$$\varepsilon_{IR}(\omega) = \frac{i}{\varepsilon_0(\omega)\left(\rho(\omega) - \frac{i\omega}{\varepsilon_0 {\omega_p}^2}\right)}$$

$${\omega_p}^2 = \frac{n_e e^2}{\varepsilon_0 m_c^*}$$

$$\rho(\omega) = i\frac{Z^2 n_i}{6\pi^2 \varepsilon_0 {n_e}^2 \omega}\int_0^\infty k^2 dk\left[\frac{1}{\varepsilon(k,\omega)} - \frac{1}{\varepsilon(k,0)}\right]$$

Standard values for the parameters and their meaning are:

Parameter	Default value	Description	Unit
Epsilon-infinity	3.29	ε_∞	dimensionless
Effective electron mass (relative)	0.21	m_c^*	dimensionless
Epsilon background	1.266	ε_0	dimensionless
Charge number	0.111	Z	dimensionless
Free carrier density	0.252	n_e	10^{21} / cm^3
Impurity density	5.579	n_i	10^{21} / cm^3

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “ITO Hamberg layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

An example for the ITO Hamberg layer is given in Fig. 5-80.

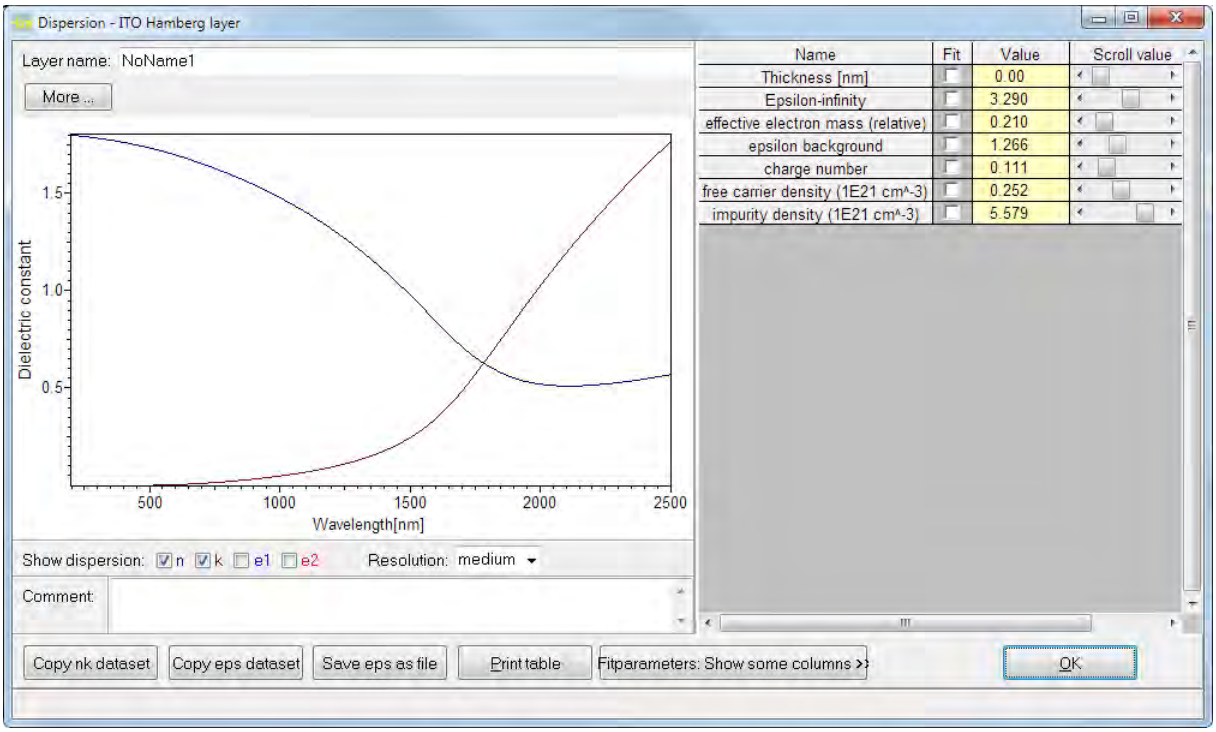


Fig. 5-80 Example for ITO Hamberg layer

5.2.4.21 ITO Sernelius layer

Theoretical assumptions:

Transparent conducting oxides (for example ZnO:Al or ITO) can be described by an oscillator approach for the UV-VIS range and a Drude approach for the NIR range. Looking more precisely the Drude approach can be improved by advanced dispersion theories named after Hamberg and Sernelius. ['Optical characterization of aluminium-doped Zinc oxide films by advanced dispersion theories', A. Pflug, V. Sittinger, F. Ruske, B. Szyszka, G. Dittmar, Thin Solid Films 455-456 (2004), pp.201-206].

For the Sernelius model a frequency-dependent damping $\omega_\tau(\omega)$ is introduced into a Drude formula.

$$\varepsilon = \varepsilon_\infty + \varepsilon_{IR}$$

$$\varepsilon_{IR}(\omega) = -\frac{{\omega_p}^2}{\omega^2 + i\omega \cdot \omega_\tau(\omega)}$$

$$\omega_\tau(E) = f(E)\cdot(\omega_{\tau 0} - \omega_{\tau.ph}(E)) + (1 - f(E))\cdot(\omega_{\tau 0} + \omega_{\tau 1})\left(\frac{E}{E_{tr}}\right)^{-\frac{3}{2}}$$

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_{tr}}{\sigma}\right)}$$

Standard values for the parameters and their meaning are:

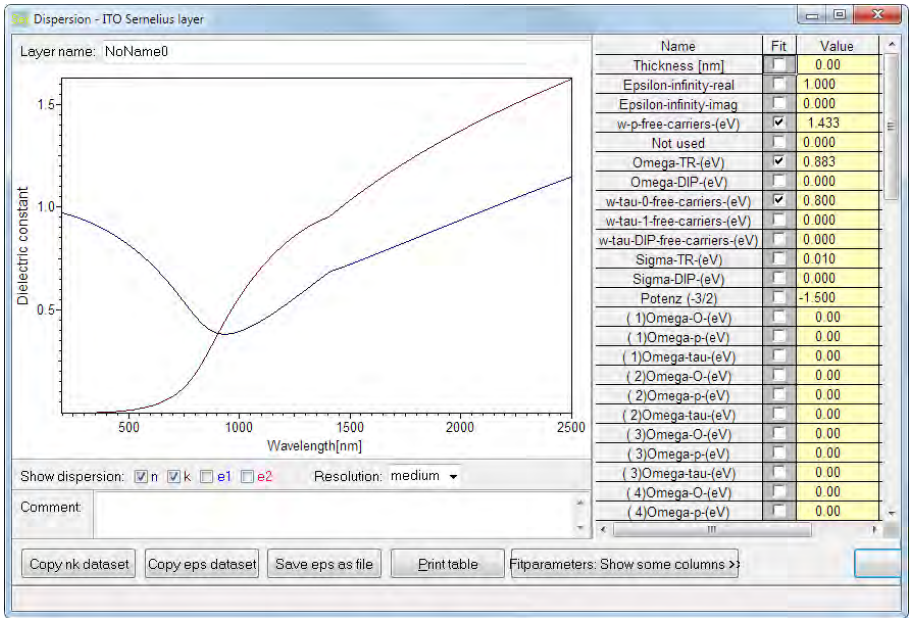
Parameter	Default value	Description	Unit
Epsilon-inifinity-real	1	ε_∞	dimensionless
Epsilon-inifinity-real	0.0	Should always be 0	dimensionless
w-p-free-carriers	1.433	ω_p	eV
Omega-TR	0.883	E_{tr}	eV
Omega-DIP	0	Not used, should always be 0	dimensionless
w-tau-0-free-carriers	0.8	$\omega_{\tau 0}$	eV
w-tau-1-free-carriers	0.12	$\omega_{\tau 1}$	eV
w-tau-DIP-free-carriers	0	Not used, should always be 0	eV
Sigma-TR	0.01	σ	eV
Sigma-DIP	0	Not used, should be 0	eV
Potenz	-1.5	Exponent of expression (E/E_{tr})	dimensionless
Omega-0	0	Position of additional Lorentz oscillator	eV
Omega-p	0	Strength of additional Lorentz oscillator	eV
Omega-tau	0	Damping of additional Lorentz oscillator	eV

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “ITO Sernelius layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

An example for the ITO Sernelius layer is given in Fig. 5-81.



Name	Fit	Value
Thickness [nm]	☐	0.00
Epsilon-infinity-real	☐	1.000
Epsilon-infinity-imag	☐	0.000
w-p-free-carriers-(eV)	☑	1.433
Not used	☐	0.000
Omega-TR-(eV)	☑	0.883
Omega-DIP-(eV)	☐	0.000
w-tau-0-free-carriers-(eV)	☑	0.800
w-tau-1-free-carriers-(eV)	☐	0.000
w-tau-DIP-free-carriers-(eV)	☐	0.000
Sigma-TR-(eV)	☐	0.010
Sigma-DIP-(eV)	☐	0.000
Potenz (-3/2)	☐	-1.500
(1)Omega-O-(eV)	☐	0.00
(1)Omega-p-(eV)	☐	0.00
(1)Omega-tau-(eV)	☐	0.00
(2)Omega-O-(eV)	☐	0.00
(2)Omega-p-(eV)	☐	0.00
(2)Omega-tau-(eV)	☐	0.00
(3)Omega-O-(eV)	☐	0.00
(3)Omega-p-(eV)	☐	0.00
(3)Omega-tau-(eV)	☐	0.00
(4)Omega-O-(eV)	☐	0.00
(4)Omega-p-(eV)	☐	0.00

Fig. 5-81 Example for ITO Sernelius layer

5.2.4.22 Leng oscillator layer

Theoretical assumptions:

A damped oscillator model has been developed by Leng et al ['Analytic representations of the dielectric functions of materials for device and structural modelling.' J. Leng et. al. , Thin Solid Films 313-314 (1998) pp. 133-136].
The formula has been expanded by Sentech by a non-constant offset in the real part and a constant offset in the imaginary part of the dielectric function.

The formula can be used for crystalline semiconductors and alloys.

$$\varepsilon(E) = \varepsilon_\infty + \sum_{i=1}^{N}\left[\frac{C_{0_i}}{E^2}\left[e^{j\beta_i}(E_{g_i} - E - j\Gamma_i)^{\mu_i} + e^{-j\beta_i}(E_{g_i} + E + j\Gamma_i)^{\mu_i} - 2\,\mathrm{Re}\left[e^{-j\beta_i}(E_{g_i} + j\Gamma_i)^{\mu_i}\right] - 2j\mu_i \cdot E \cdot \mathrm{Im}\left[e^{-j\beta_i}(E_{g_i} + j\Gamma_i)^{\mu_i - 1}\right]\right]\right] + m_0 E^{x_0} + jk_0$$

$[\varepsilon_\infty],[\beta_i],[\mu_i],[x_0],[k_0]$: dimensionless

$[E],[E_g],[\Gamma_i]$: eV

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Leng oscillator layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

An example is given in Fig. 5-82 showing n and k of silicon.

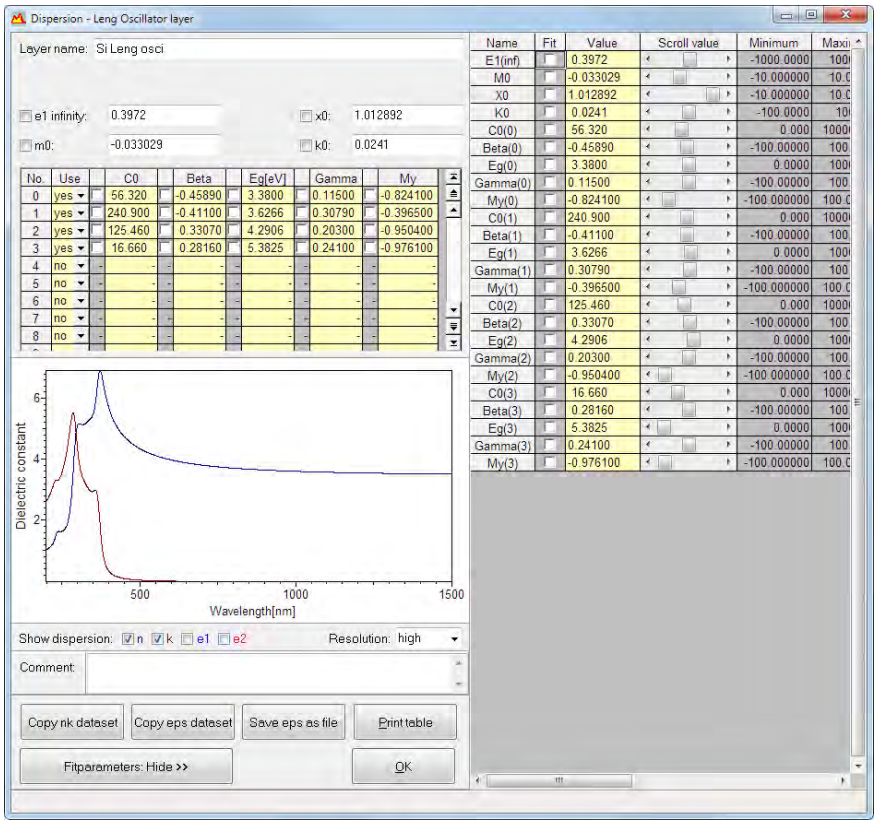


Fig. 5-82 Example for a Leng oscillator layer (silicon)

5.2.4.23 Lorentz type 0 and Lorentz type 1 oscillator layer

Theoretical assumptions:

In addition to the Lorentz oscillator formula described in detail in chapter 5.2.4.12 ('Drude-Lorentz oscillator') similar formulas are used alternatively.

Lorentz type 0 layer:

$$\varepsilon_{Lor\_type0}(E) = \varepsilon_{1\infty} - \frac{A \cdot B_r \cdot E_n}{E_n^{\,2} - E^2 - i \cdot B_r \cdot E}$$

[E], [E_n], [B_r] – eV, [A] dimensionless

Lorentz type 1 layer:

$$\varepsilon_{Lor\_type1}(E) = \varepsilon_{1\infty} - \frac{A \cdot E_n}{E_n^{\,2} - E^2 - i \cdot B_r \cdot E}$$

[E], [E_n], [B_r], [A] – eV

Creating a new layer

A new Lorentz layer is created by “File\New\Layer” and selecting the layer type “Lorentz oscillator type 0” etc. This creates the new layer and opens the editor. The name of the new layer and its properties A, En and Br can be entered.

Editing the layer

The editor for the Lorentz type 0 layer is shown in Fig. 5-83. The editor for the Lorentz type 1 layer is shown in Fig. 5-84.

The Lorentz type 0 layer and the Lorentz type 1 layer only hold one oscillator. They can be used together with the 'Advanced combination layer' described in chapter 5.2.4.4 because materials usually have more than one vibration band that has to be described.

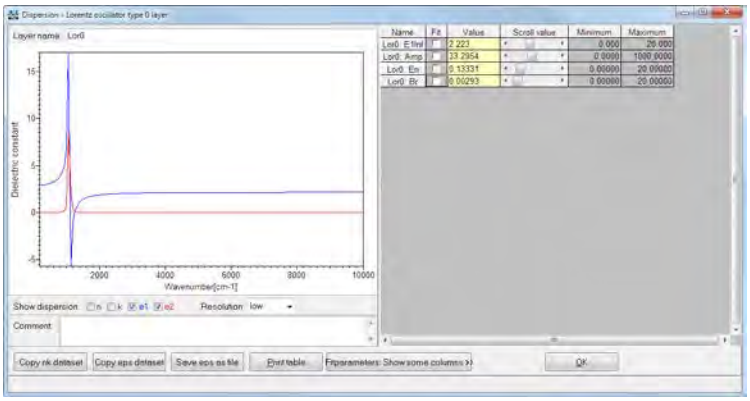


Fig. 5-83 Lorentz type 0 editor

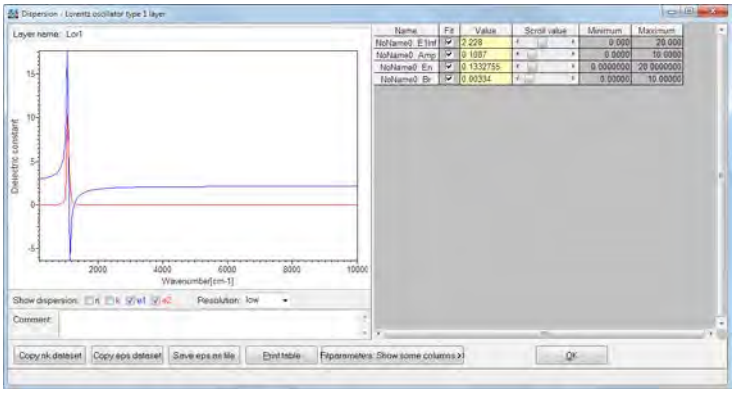


Fig. 5-84 Lorentz type 1 editor

5.2.4.24 NK-Layer: Fixed refractive index and absorption

Theoretical assumptions:

The simplest form of a dielectric function is a constant value independent from any other parameter. This model is suitable for air (no high or low pressures), vacuum or for any measurement with single wavelength devices. Since at a fixed wavelength the dielectric function degrades to a dielectric constant

$$\tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2 \qquad \tilde{n} = n + ik \qquad \tilde{\varepsilon} = \tilde{n}^2$$

This layer type has only 2 constants: refractive index and extinction (real and imaginary part of the complex refractive index). If a conversion to ε is required, use the simulation.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “NK layer”. The name and the properties of the new layer can be entered.

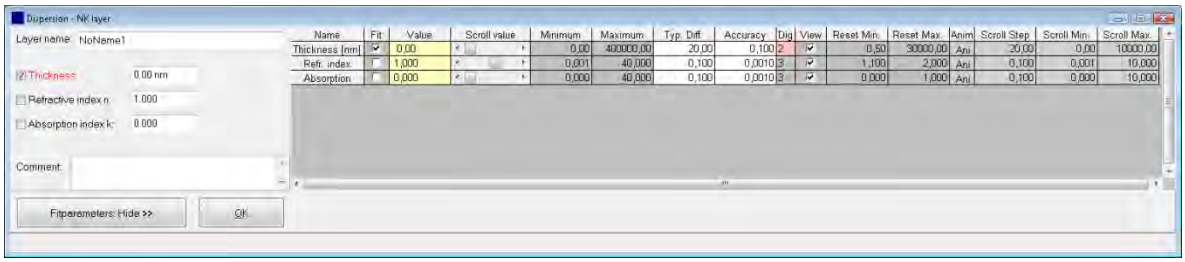


Fig. 5-85 NK layer editor

Editing the layer

The editor sets the above mentioned values. If the checkbox at the left side of each value is checked the text is shown in red color. This indicates the selection for fit as you can also see in the more detailed list on the right hand side. The checked parameters are fitted.

Typical values for n and k at 633 nm wavelength for a large number of materials are shown in Tab. 5-11. They can be used for single wavelength optical devices.

Name	n	k
Air or vacuum	1	0
Ag - Silber [Palik: Handbook of opt. const.]	0.13	3.99
Ag - Silber [Itakura: J.Vac.Sci. A 1991]	0.13	3.49
Al - Aluminium [Palik: Handbook of opt. const.]	1.3745	7.6134
Al - Aluminium [Palik: Handbook of opt. const.]	1.49	7.34
Al2O3 - Aluminiumoxid [Palik: Handbook of opt. const. II]	1.77	0
Al2O3 - Alumiunimoxid sputt. [Richter]	1.62	0
AlAs - Aluminiumarsenid [Palik: Handbook of opt. const. II]	3.11	0
AlON - Aluminiumoxynitrid [Palik: Handbook of opt. const. II]	1.79	0
Au - Gold [Palik: Handbook of opt. const.]	0.18	3.10
AlGaAs - Aluminium Gallium Arsenid x=0.1	3.8025	0.1551
AlGaAs - Aluminium Gallium Arsenid x=0.2	3.7354	0.1064
AlGaAs - Aluminium Gallium Arsenid x=0.3	3.6722	0.1323
AlGaAs - Aluminium Gallium Arsenid x=0.4	3.6236	0.0052
AlGaAs - Aluminium Gallium Arsenid x=0.5	3.5220	0.0030
AlGaAs - Aluminium Gallium Arsenid x=0.6	3.4402	0.0012
AlGaAs - Aluminium Gallium Arsenid x=0.7	3.3374	0.0000
AlGaAs - Aluminium Gallium Arsenid x=0.8	3.2600	0.0000
Be - Beryllium [Palik: Handbook of opt. const. II]	3.46	3.19

Bi - Wismut [Atkinson: Thin solid films 1985]	1.8	4.0
Bi2O3 - Wismutoxid [Atkinson: Thin solid films 1985]	2.6	0
BK7 - Glas	1.510	0
CaF2 - Calciumfluorid [Palik: Handbook of opt. const. II]	1.43	0
CdS - Cadiumsulfid [Palik: Handbook of opt. const. II]	2.38	0.52
CdSe - Cadmiumselenid [Palik: Handbook of opt. const. II]	2.74	0.27
CdTe - Cadmiumtellurid	2.9810	0.3472
Co - Kobalt [Palik: Handbook of opt. const. II]	2.21	4.17
Co - Kobalt [Palik: Handbook of opt. const. II]		1.96
Cr - Chrom	3.1365	3.3118
Cr - Chrom [Palik: Handbook of opt. const. II]	3.58	4.36
CsJ - Cäsiumjodid [Palik: Handbook of opt. const. II]	1.78	0
Cu - Kupfer	0.1337	3.8182
Cu - Kupfer [Palik: Handbook of opt. const. II]	0.25	3.41
Cu2O - Kupferoxid [Palik: Handbook of opt. const. II]	2.94	0.11
C - Diamant [Palik: Handbook of opt. const.]	2.4094	0.0000
Fe - Eisen [Zakroczymski: J. Electrochem.Soc. 1985]	2.43	3.3
GaAs - Galliumarsenid [Palik: Handbook of opt. const. II]	3.86	0.20
GaP- Galliumphosphid	3.3174	0.0000
Ge - Germanium	5.4727	0.5670
H2O- Wasser [Palik: Handbook of opt. const. II]	1.3315	0.0000
Hg - Quecksilber [Palik: Handbook of opt. const. II]	1.99	5.24
InAs - Indiumarsenid [Palik: Handbook of opt. const. II]	3.9621	0.6059
InGaAs - Indiumgalliumarsenid	3.9898	0.3796
InP - Indiumphosphid [Palik: Handbook of opt. const.]	3.54	0.31
InP - Indiumphosphid [X. Liu: J. Electrochem. Soc. 1990]	3.52	0.30
InP - Indiumphosphid [Scheps: J. Electrochem. Soc. 1984]	3.47	0.45
InP - Indiumphosphid [SOPRA]	3.5364	0.0000
InSb - Indiumantimonid [Palik: Handbook of opt. const.]	4.2544	1.8014
Ir - Iridium [Palik: Handbook of opt. const.]	2.53	4.61
Ir - Iridium [J. Ord: J. Electrochem. Soc. 1982]	2.52	5.09
K - Kalium [Palik: Handbook of opt. const. II]	0.05	1.75
KBr - Kaliumbromid [Palik: Handbook of opt. const. II]	1.56	0
KCl - Kaliumchlorid [Palik: Handbook of opt. const.]	1.49	0.00
LiF - Lithiumflourid [Palik: Handbook of opt. const.]	1.40	0.00
MgO - Magnesiumoxid [Palik: Handbook of opt. const. II]	1.735	0
Mo - Molybdän [Palik: Handbook of opt. const.]	3.70	3.54
Mo - Molybdän [De Smet: J. Electrochem. Soc. 1976]	4.01	3.86
Mo - Molybdän [SOPRA]	3.5800	3.7035
Na - Natrium [Palik: Handbook of opt. const. II]	0.05	2.64
NaCl - Natriumchlorid [Palik: Handbook of opt. const.]	1.542	0
NaF - Natriumfluorid [Palik: Handbook of opt. const. II]	1.325	0
Nb - Niobium [Palik: Handbook of opt. const. II]	2.83	2.86
Nb - Niobium [J. Ord: J. Electrochem. Soc. 1972]		
Ni - Nickel [Palik: Handbook of opt. const.]	1.97	3.72
Ni - Nickel [SOPRA]	2.0671	3.8945
Os - Osmium [Palik: Handbook of opt. const.]	3.90	1.66
PbS - Bleisulfid [Palik: Handbook of opt. const.]	4.338	1.444
PbSe - Bleiselenid [Palik: Handbook of opt. const.]	3.97	3.032
PbSe - Bleiselenid [SOPRA]	3.7458	2.8851
PbTe - Bleitellurid [Palik: Handbook of opt. const.]	6.352	4.060
Pd - Palladium [Palik: Handbook of opt. const. II]	1.77	4.29
Pt - Platin [Palik: Handbook of opt. const. II]	2.33	4.15
Rh - Rhenium [Palik: Handbook of opt. const. II]	2.15	5.61
SiC - Siliziumcarbid [Palik: Handbook of opt. const.]	2.632	0
SiC - Siliziumcarbid [Palik: Handbook of opt. const. II]	2.66	0
Si3N4 - Siliziumnitrid	2.021	0.0000
SiO2 - Siliziumdioxid therm.	1.462	0
SiO - Siliziumoxid [Palik: Handbook of opt. const.]	1.965	0.010
a-SiO2 - amorphes Siliziumdioxid [Palik: Handbook of opt. const.]	1.542	0
c-SiO2 - kristallines Siliziumdioxid [Palik: Handb. of opt. const.]	1.457	0
a-Si - Polysilicon	3.95	0.04
a-Si - amorphes Silizium [Palik: Handbook of opt. const.]	4.206	0.422
a-Si - amorphes Silizium [SOPRA]	4.5164	0.2367

c-Si - Silizium	3.858	0.018
c-Si - Silizium [Palik: Handbook of opt. const.]	3.882	0.019
SnTe - Zinntellurid [Palik: Handbook of opt. const. II]	3.257	5.311
SrTiO - Strontiumtitanat	2.409	0
Ta - Tantal [Palik: Handbook of opt. const. II]	1.72	2.09
Ta - Tantal [Leslie: J. Electrochem. Soc. 1974]	2.3	2.6
Ta - Tantal [J. Ord: J. Electrochem. Soc. 1972]	3.02	2.57
TaO2 - Tantaldioxid [Leslie: J. Electrochem. Soc. 1974]	2.22	0
Ti - Titan [J. Ord: J. Electrochem. Soc. 1989]	3.23	3.62
Ti:W - Titan/Wolfram [Tompkins: J. Appl. Phys. 1988]	2.84	3.08
Ti:W ox. - Ti:W Oxyd [Tompkins: J. Appl. Phys. 1988]	2.25	0.12
TiN - Titannitrid [Tompkins: J. Appl. Phys. 1991]	1.39	1.76
TiO2 - Titandioxid [Tompkins: J. Appl. Phys. 1991]	2.2	0
V - Vanadium [Palik: Handbook of opt. const. II]	3.53	2.95
V - Vanadium [J. Ord: J. Electrochem. Soc. 1991]	3.637	3.334
V - Vanadium [J. Clayton: J. Electrochem. Soc. 1976]	3.838	3.56
W - Wolfram [Palik: Handbook of opt. const.]	3.64	2.91
W - Wolfram [J. Ord: J. Electrochem. Soc. 1972]	4.3	3.1
WSi - Wolfram/Si(2.2) Leg. [Thompkins: Thin solid films 1985]	4.25	1.37
Xe - Xenon [Itakura: J. Vac. Sci 1991]	1.48	0
ZnTe - Zinktellurid [Palik: Handbook of opt. const. II]	2.98	0.075
Zr - Zirkonium [Hopper: J. Electrochem. Soc. 1977]	2.21	3.04
ZrO - Zirkoniumoxid [Hopper: J. Electrochem. Soc. 1977]	2.17	0.033

Tab. 5-11 Set of refractive indices at 633 nm wavelength (for SE400adv and most single wavelength ellipsometers).

5.2.4.25 Nuclei growth

Theoretical assumptions

The growth of surfacing layers is more complicated than at homogeneous layers. You have to combine thickness growth, effective medium theory and coalescence. For this reason a layer type with growing semi spheres is used. As shown in the sketch below the basic model assumes a basic cell of tetragonal type (hexagonal type is reserved for future support).

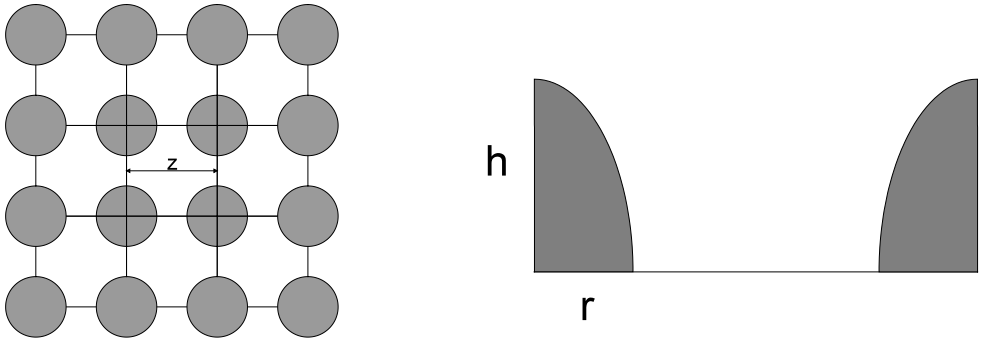


Fig. 5-86 Tetragonal lattice with ellipsoidal nuclei (z-cell width): left top view, right cell view

Each edge of this basic cell is center of a growing semi sphere. These spherical islands have a radius and height. Both follow an exponent rule and have independent parameters to switch between horizontal and height growth continuously. By introducing independent growth rates this layer covers a broad range of applications. The usage of the time window for growth is the same as for a homogeneous layer, see there for more information.

(10) $$\mathrm{R}(t) = \mathrm{A}t^{a} + \mathrm{R}_0 \qquad h(t) = Bt^{b} + \mathrm{th}_{\mathrm{start}}$$

(11) $$d(t) = \begin{cases} \mathrm{th}_{\mathrm{start}} & if \quad t < t_{start} \\ \mathrm{th}_{\mathrm{start}} + h(t - t_{start}) & if \quad t \in [t_{start}, t_{end}] \\ \mathrm{th}_{\mathrm{start}} + h(t_{end} - t_{start}) & if \quad t > t_{end} \end{cases}$$ d- thickness

If the semi spheres grow the radii become larger than the half cell width. The resulting overlap is correctly treated. There are two points were the horizontal growth causes “edges” in the calculated data. The first point is when the radius is the half of the cell width. The second point is reached when the radius is the half of the cells diagonal. If the radius becomes infinite this approach reaches to compact layer model.

Creating a new layer

A new growing layer is created by “File\New\Layer” and selecting the layer type “Nucleus growing layer”. This creates the new layer and opens the editor. You should enter the name of the new layer and its properties $\mathrm{th}_{\mathrm{start}}$, B, b, A, a, R_0, z, start and end time of growth.
A second step should specify the growing materials “nuclei” and “filling”. See Appendix D “Material name edit fields and buttons” for information on the functioning of the edit fields and the associated buttons.

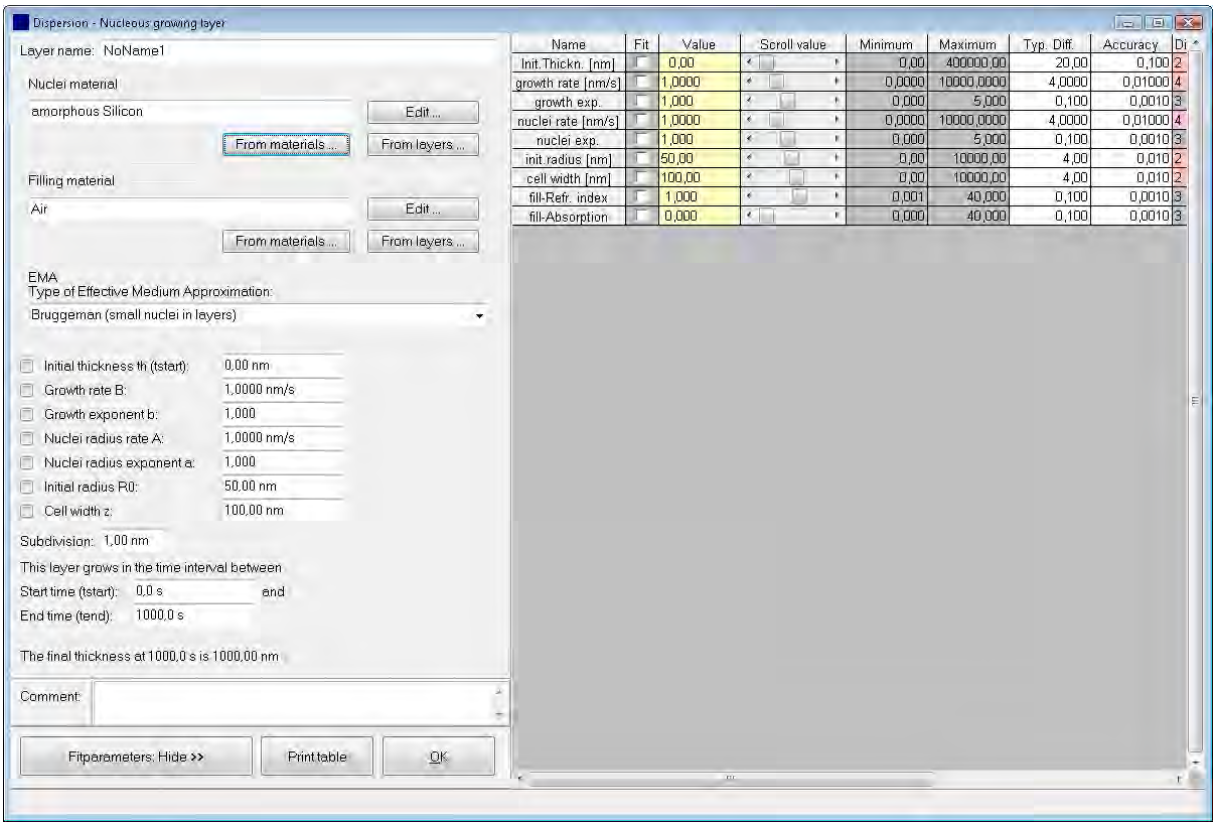


Fig. 5-87 Nuclei layer edit screen

Editor description

The th_{start}, B, b, A, a, R_0, z, start and end time edit fields handle physical numbers. See Appendix D “Physical number edit fields” for more information. The “Filling material” and “Nuclei material” name edits have special functionality (see Appendix D “Material name edit fields and buttons”). For effective medium models see the description of the EMA layer.

Name	Fit	Value	Typ. Diff.	Min.	Max.	Reset Min.	Reset Max.	Accuracy
init. thickn. [nm]	0	0	20.0	0	400000	0.5	30000.0	0.1
growth rate [nm/s]	0	1	4.0000	0	10000	0.1	200.0000	0.0100
growth exp.	0	1	0.100	0	5	0.1	1.000	0.001
nuclei rate [nm/s]	0	1	4.0000	0	10000	0.1	200.0000	0.0100
nuclei exp.	0	1	0.100	0	5	0.1	1.000	0.001
init. radius [nm]	0	50.0	4.0	0.0	10000	0.1	200.0	0.0
cell width [nm]	0	100.0	4.0	0.0	10000	0.1	200.0	0.0

Tab. 5-12 Default parameters of the nuclei growth layer. The parameters of the sublayers are not listed in this table.

5.2.4.26 Parametric file (2D) layer

Theoretical assumptions:

The spectral dielectric function of materials usually changes with temperature or other external parameters. In a similar way the dielectric function of alloys changes with the composition.
These dependencies can be handled by the parametric file (2D) layer. Measured spectral data are stored in the layer depending on the temperature, composition etc.

Creating a new layer

A new Cauchy layer is created by “File\New\Layer” and selecting the layer type “Parametric file (2D) layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for the periodical layer is shown in Fig. 5-88Fig. 5-89.

An example is given for the System $Al_xGa_{(1-x)}As$. The parameter is the fraction x of the composition. When measured data are compared to the dielectric functions in the 2D layer it is possible to determine the composition of the measured sample.

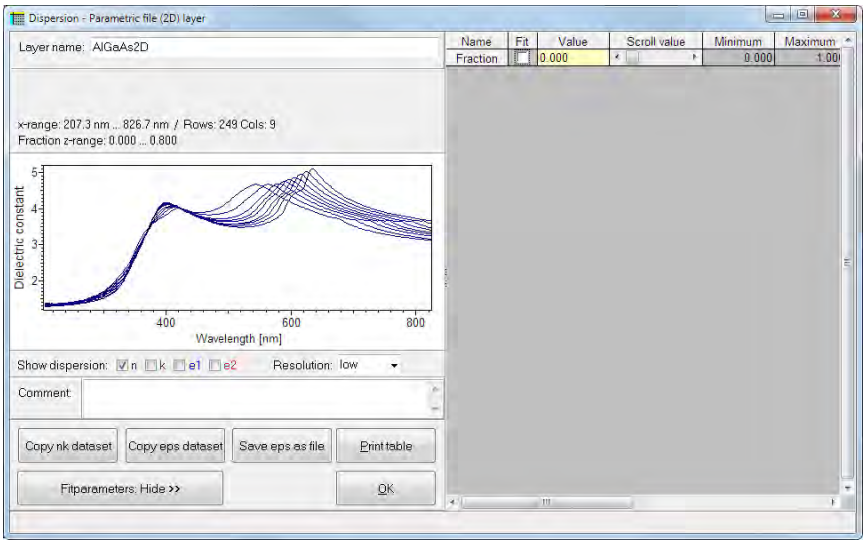


Fig. 5-88 Parametric file (2D) layer editor

5.2.4.27 Periodical layer

Theoretical assumptions:

For functional layer stacks it is often necessary to use periodical structures consisting of 2 or more layers that are alternated periodically. The periodical layer can describe these multilayer stacks.

Creating a new layer

A new Cauchy layer is created by “File\New\Layer” and selecting the layer type “Periodical layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for the periodical layer is shown in Fig. 5-89. A typical example is given with 2 alternating sublayers (SiO_2 and TiO_2)

The sublayers can be added or inserted to the list on the left side of the editor either from a material library ('Add material' / 'Insert material') or from the already existing layers in the main layer stack ('Add layer' / 'Insert layer'). The selected sublayer can be edited or deleted.

The diagram shows the refractive index versus thickness of the periodical layer. The thickness must be greater than 0 for a reasonable display. The example shows the change of n between the SiO_2 and the TiO_2 layer at the wavelength selected below the diagram.

The thickness of the periodical layer can be defined by

- total thickness or
- a number of complete periods.

The total thickness will usually lead to a 'broken' period at the top of the layer and can be used to model the situation during the coating process.
The number of complete periods is usually used to model the ideal situation in order to design a suitable layer stack.

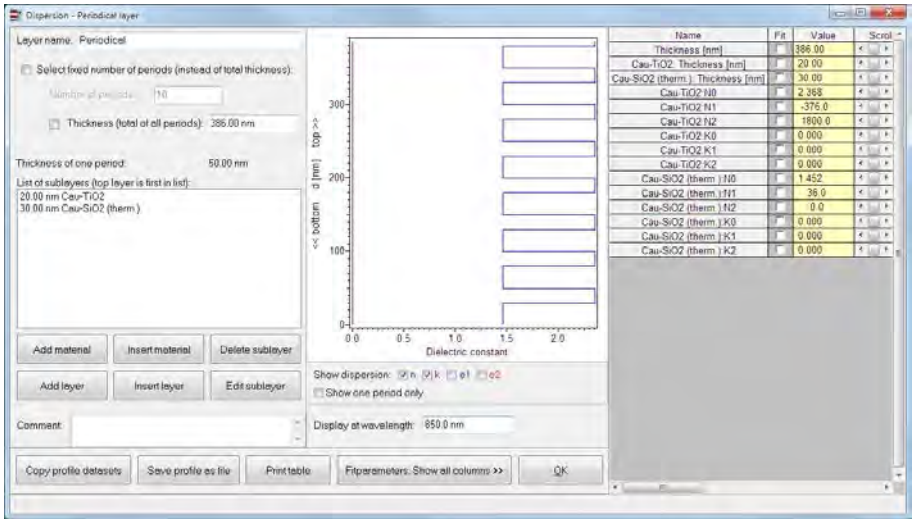


Fig. 5-89 Periodical layer editor with example of 2 sublayers

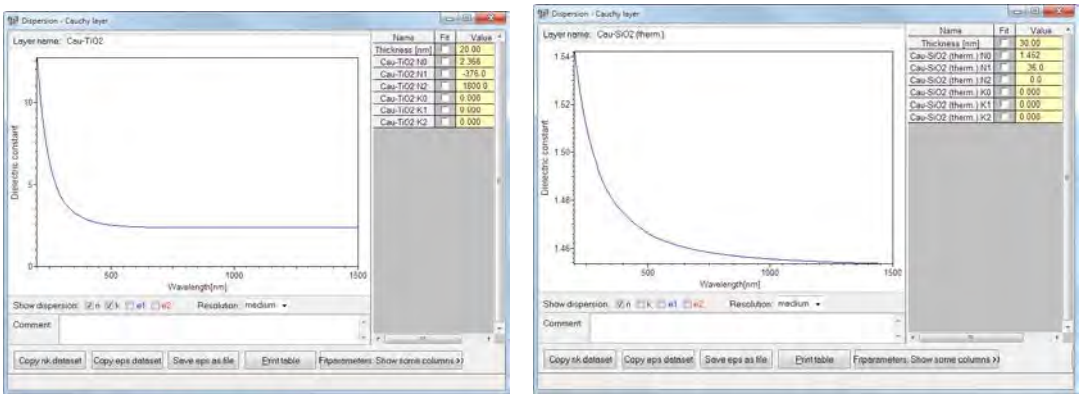


Fig. 5-90 Alternating sublayers

A simulation of the example shown in Fig. 5-91 with the total thickness of the periodical layer as curve parameter as shown in Fig. 5-92 leads to the dependence of Ψ and Δ from the thickness as shown in Fig. 5-93.

Title	Thickness	State	Layer Type	Info [633.0 nm]
Air			NK layer	n=1.0000
Periodical	386.00 nm		Periodical layer	
Cau-TiO2	20.00 nm		Cauchy layer	n=2.3863
Cau-SiO2 (therm.)	30.00 nm		Cauchy layer	n=1.4610
Si DUV-NIR			File layer	n=3.8736 k=0.01455

Fig. 5-91 Layer stack including a periodical layer

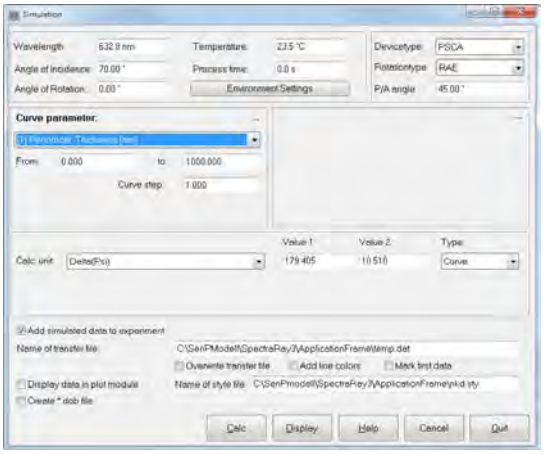


Fig. 5-92 Simulation with thickness as curve parameter

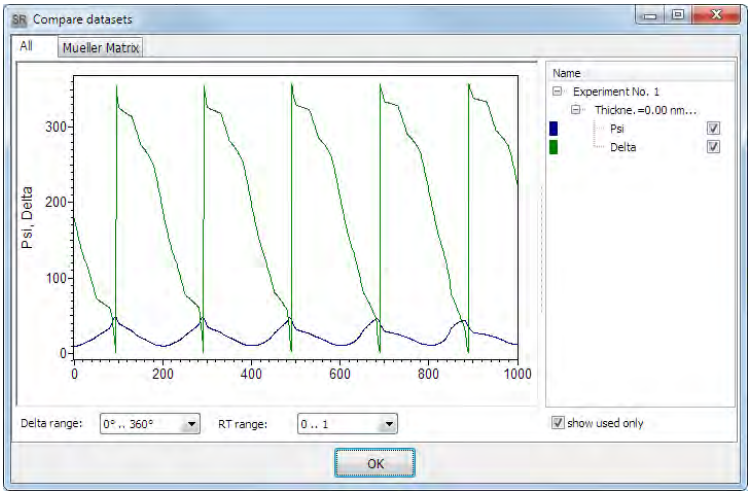


Fig. 5-93 Resulting dependence of Ψ and Δ from total thickness.

5.2.4.28 Polynomial-Layer

Theoretical assumptions:

A general polynomial approach is used for the description of n and k.

$$n(\lambda) = \sum_{i=0}^{9} \frac{n_i}{\lambda^i} \qquad [n_i]: \text{nm}^i$$

$$k(\lambda) = \sum_{i=0}^{9} \frac{k_i}{\lambda^i} \qquad [\lambda_i]: \text{nm}^i$$

Creating a new layer

A new Cauchy layer is created by “File\New\Layer” and selecting the layer type “Polynomial layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for Cauchy layers is shown in Fig. 5-94Fig. 5-95.

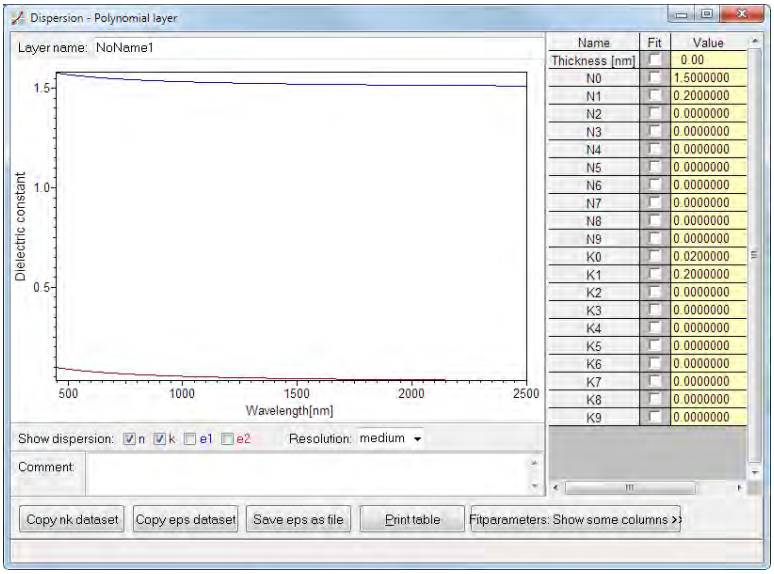


Fig. 5-94 Polynomial layer editor

5.2.4.29 Schott-Layer

Theoretical assumptions:

The following formula allows to model the refractive index of Schott glass materials by means of six parameters:

$$n^2(\lambda) = A_0 + A_1\lambda^2 + \frac{A_2}{\lambda^2} + \frac{A_3}{\lambda^4} + \frac{A_4}{\lambda^6} + \frac{A_5}{\lambda^8}$$

$$k(\lambda) = 0$$

[A0] -dimensionless, [A1] - μm^{-2} , [A2] - μm^2 , [A3] - μm^4 ,[A4] - μm^6 ,[A5] - μm^8

Creating a new layer

A new Cauchy layer is created by “File\New\Layer” and selecting the layer type “Schott layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor for Cauchy layers is shown in Fig. 5-95.

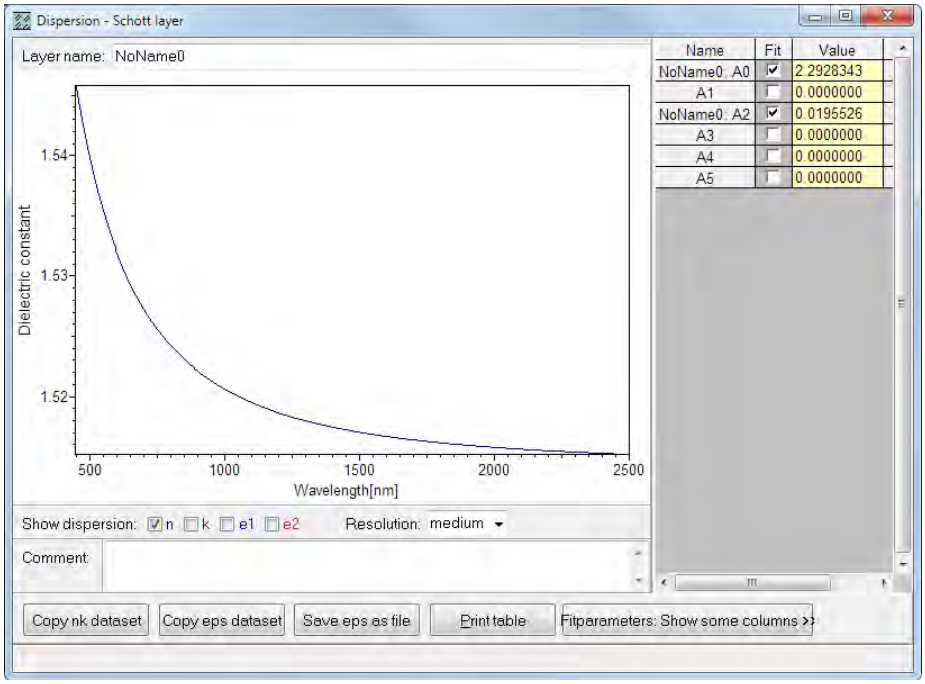


Fig. 5-95 Schott layer editor

5.2.4.30 Sellmeier layer

Theoretical assumptions:

The Sellmeier-equation is an empiric description of the dispersion of transparent media developed by Wolfgang Sellmeier in 1871. It is most useful for the precise description of the dispersion of glasses and other window materials in the visible and near infrared spectral range.

The formula uses an approximation for the refractive index. As the description is used for transparent materials the absorption is not considered.

$$n^2(\lambda) = 1 + \frac{A_1\lambda^2}{\lambda^2 - B_1} + \frac{A_2\lambda^2}{\lambda^2 - B_2} + \frac{A_3\lambda^2}{\lambda^2 - B_3}$$

$$k(\lambda) = 0$$

[λ] - µm $\quad [A_1, A_2, A_3]$: dimensionless $\quad [B_1, B_2, B_3]$ - µm^2

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Sellmeier layer”. This creates the new layer and opens the editor. The name of the new layer and its properties A_1, A_2, A_3, B_1, B_2 and B_3 can be entered.

Editing the layer

The editor for is shown in Fig. 5-96 with a typical example for the dispersion of CaF_2. The settings can be made as explained in chapter 5.2.4.3.
Note that data from literature sometimes use values for the coefficients B_i as B_i^2.

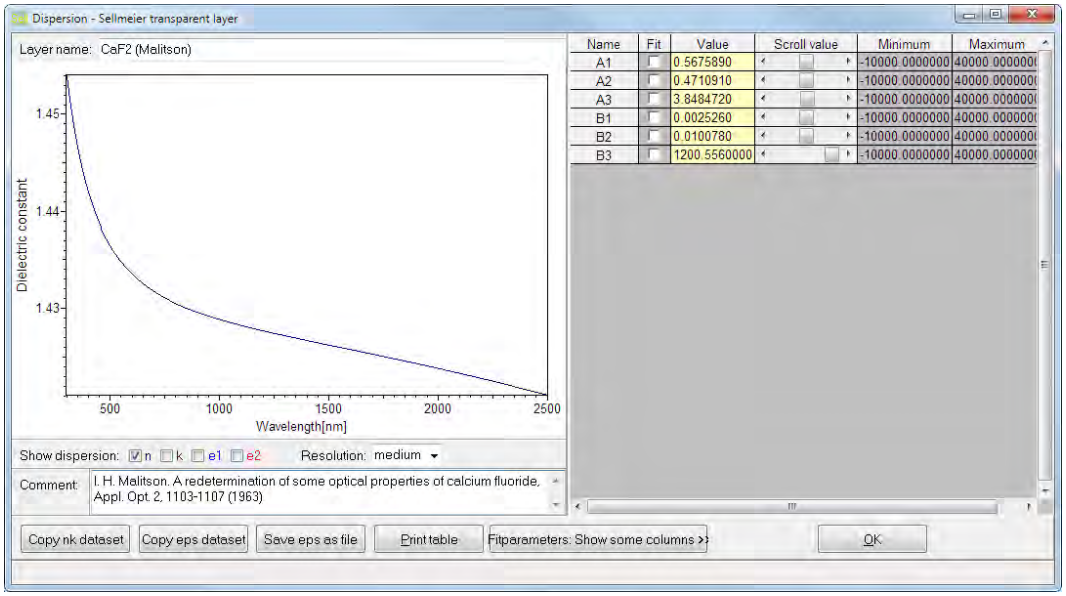


Fig. 5-96 Sellmeier layer editor

A comparison between the Cauchy formula and the Sellmeier formula is shown in Fig. 5-97 for BK7 glass. The values of both formulas agree well in the visible range. Therefore the simpler Cauchy model is usually sufficient in the visisble range. But in the near infrared range the Sellmeier formula offers a better description.

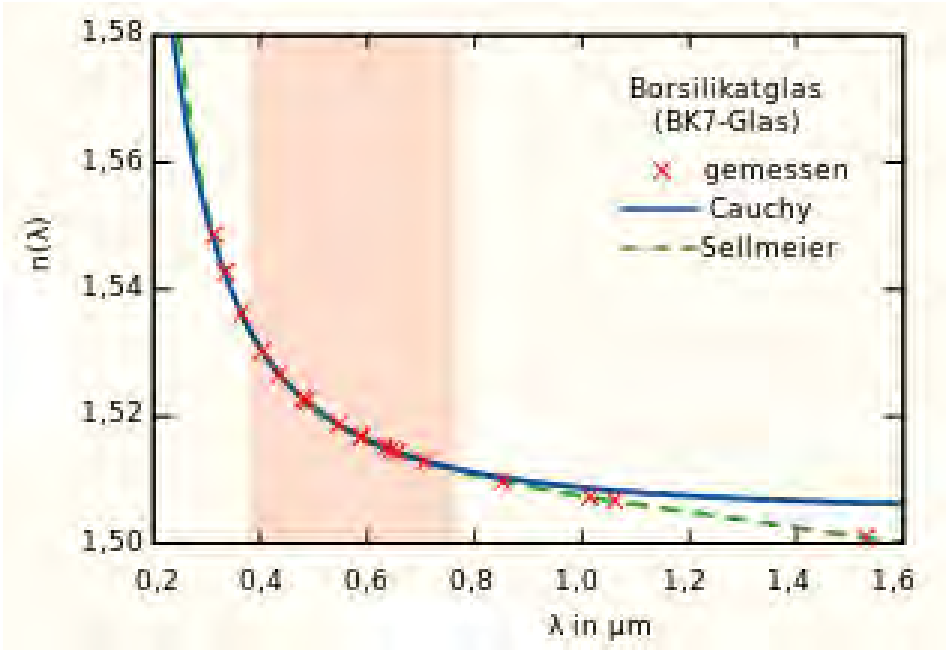


Fig. 5-97 Comparison of Cauchy and Sellmeier dispersion

5.2.4.31 Silicon epitaxial layer

Theoretical assumptions:

The optical properties of a layer stack consisting of silicon of different levels of doping can be described with the silicon epitaxial layer. This layer has to be placed between two Drude-Lorentz oscillator layers described in 5.2.4.12 which describe Silicon with different doping levels. The Drude terms in both layers are obviously most important here.

A gradient type and number of sublayers can be selected. According to the gradient the concentration of free carriers is calculated from each sublayer and the optical properties can be calculated using this stack of sublayers.

Creating a new layer

A new Cauchy layer is created by “File\New\Layer” and selecting the layer type “Silicon epitaxial layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Usually the message shown in Fig. 5-98 will appear. It states that the silicon epitaxial layer works with a Drude-Lorentz layer above and below only.

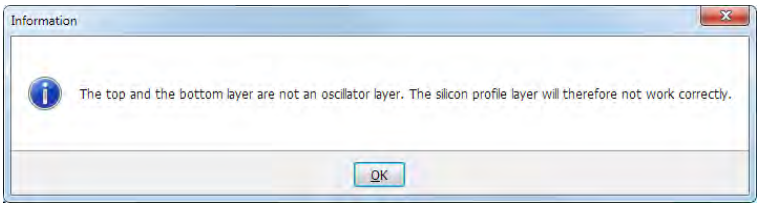


Fig. 5-98 Silicon epitaxial layer warning

Editing the layer

The editor for Silicon epitaxial layers is shown in Fig. 5-99.

A layer stack has to be set up similar to the one shown in Fig. 5-100 with the two Drude-Lorentz layers at the top and the bottom as shown in Fig. 5-101. These layers have to be defined in the edit fields 'Top material' and 'Bottom material'. This can be done by loading the material from a material library ('From materials...') or from the already existing layers in the main layer stack ('From layers...').

The type of gradient and the number of steps can be chosen in the list shown in Fig. 5-102.
The fraction of the top material can be shown in the diagram. It corresponds to the selection of the gradient type.

The diagram shows n, k, e1 or e2 versus thickness of the layer. The wavelength for the display of the refractive index can be chosen below the diagram.

For a reasonable display in the diagram the thickness must be higher than 0.

The effective mass can be set. The default value of 0.26 will be fine in many cases.

The list of fit parameters contains the effective mass and the parameters of the bottom and the top layer.

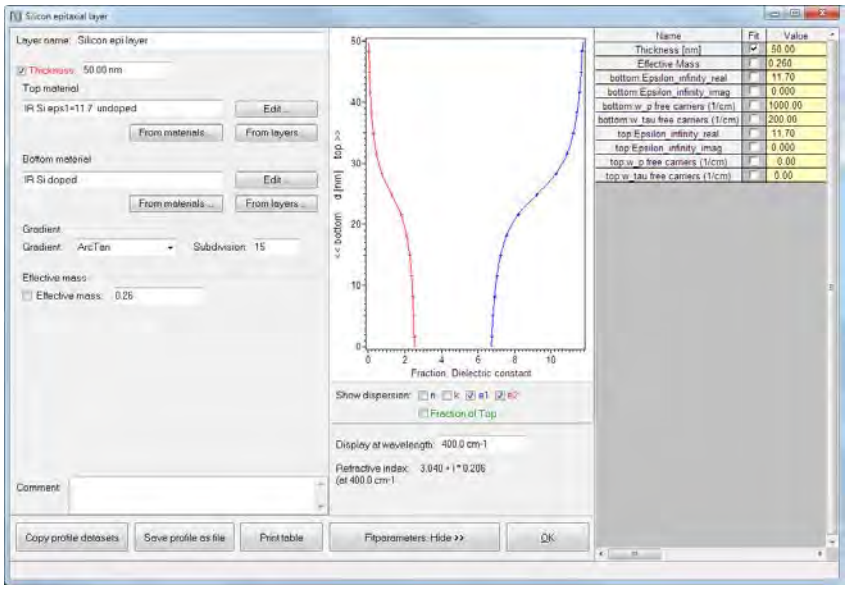


Fig. 5-99 Silicon epitaxial layer editor

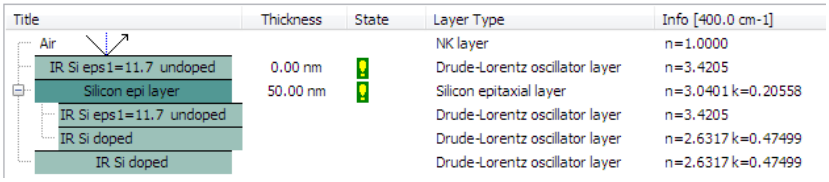


Fig. 5-100 Silicon epitaxial layer stack

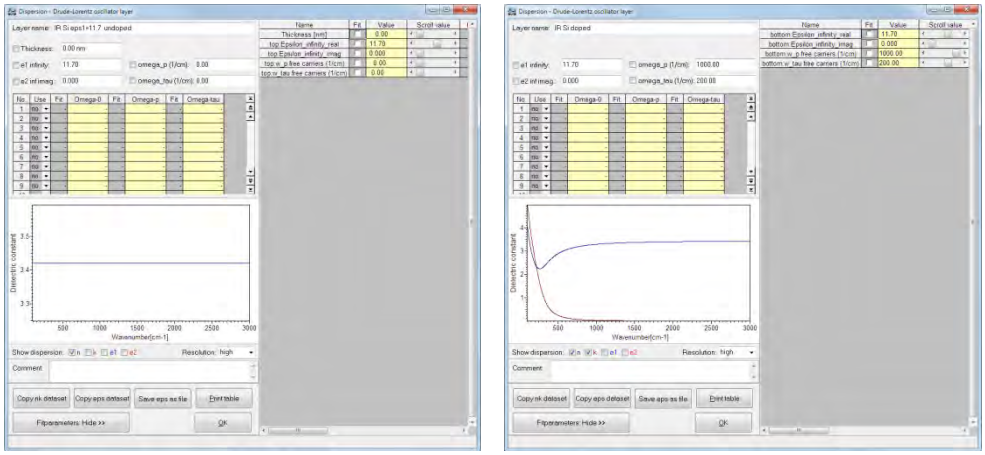


Fig. 5-101 Top and bottom layer

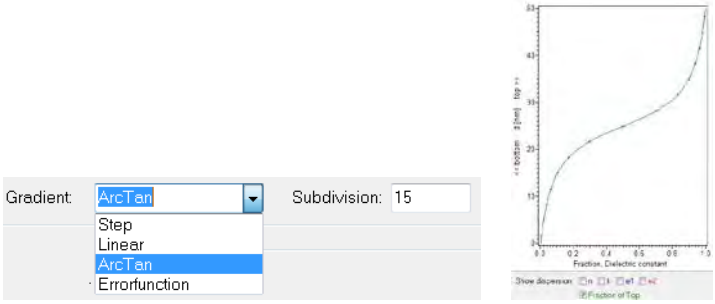


Fig. 5-102 Gradient type, number of steps and resulting fraction versus thickness

5.2.4.32 Spectral combination layer

An improved version of this layer type is the Advanced combination layer described in chapter 5.2.4.4. For new models it is recommended to use the new version.

Theoretical assumptions:

Dispersion relations of materials can in many cases be described by model functions. But these model functions usually give a good description in a certain spectral range only.

For example a transparent conducting material may be described by a Tauc-Lorentz model in the visible range where it is highly transparent and a Drude model for the infrared range where the conductivity leads to a 'partially metallic' behavior of the material.

The combination of these contributions allows to setup a combined model for the dispersion in the whole spectral range.
The combination has to be done in terms of the complex dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2$. The contributions to ε are added to give the resulting dielectric function.

$$\boldsymbol{\varepsilon = \varepsilon_1 + i\varepsilon_2 = \varepsilon_{1\infty} + \sum_{c=1}^{c\_max} (\varepsilon_{1,c} - \varepsilon_{1\infty,c}) + i \sum_{c=1}^{c\_max} \varepsilon_{2,c}}$$

The constant part $\varepsilon_{1\infty}$ has to be treated in a special way. If the individual contributions have their own $\varepsilon_{1\infty,c}$ this value has to be subtracted. In addition one common final $\varepsilon_{1\infty}$ for the resulting dispersion is added. This procedure avoids multiple ambiguous fit parameters.
This procedure works for all contributions that have their own $\varepsilon_{1\infty}$ in their formulas. This is the case for example in the Drude-, Lorentz-, Cody-Lorentz-, Harmonic-, Leng-, Tauc-Lorentz, Hamberg- and Sernelius-formulas.
In other contributions a separate $\varepsilon_{1\infty,c}$ is not available, for example in Cauchy-, Forouhi-Bloomer-, Schott-, Sellmeier-, Tanguy-formulas and in the File-layer. In these cases no subtraction of $\varepsilon_{1\infty,c}$ should take place and the resulting $\varepsilon_{1\infty}$ should be set to 0.

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Spectral combination layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The editor is shown in Fig. 5-103 with a typical example for the dispersion of TCO. The individual contributions for this example are a Tauc-Lorentz and a Drude term. They are shown in Fig. 5-104. In the experiment view the combination layer appears together with the contributions as shown in Fig. 5-105.

The diagram of the spectral combination layers shows the combined dielectric function as continuous line and the individual contributions as broken or dotted line.

The contributions can be loaded from a directory with material files or from the already existing layers in the layer stack using the related buttons.

The checkboxes 'Subtract e1 infinity' allow to subtract the individual $\varepsilon_{1\infty,c}$ terms as discussed above.

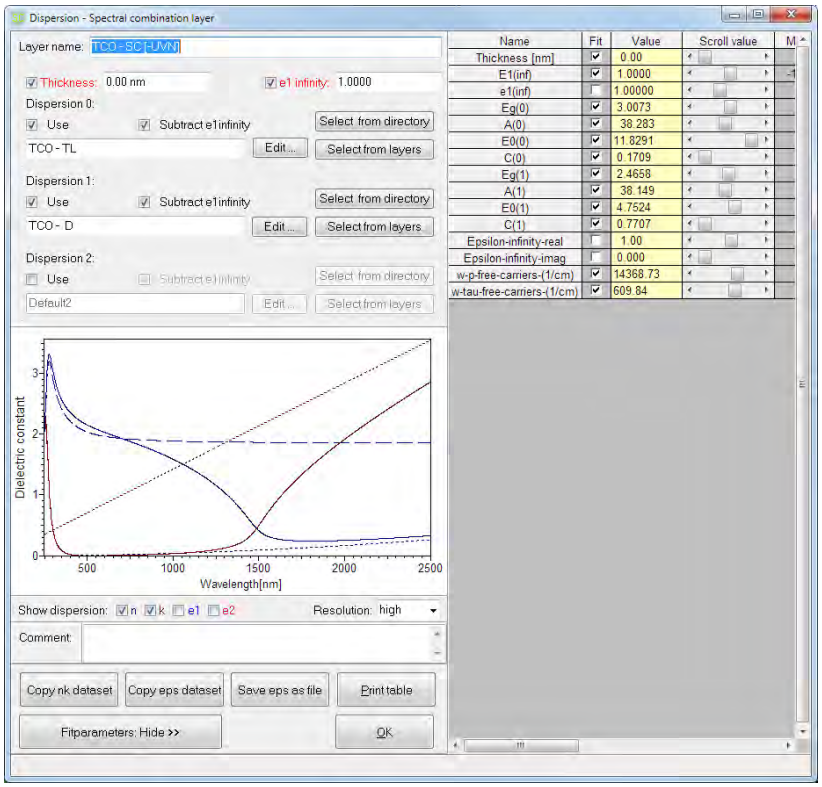


Fig. 5-103 Spectral combination layer editor

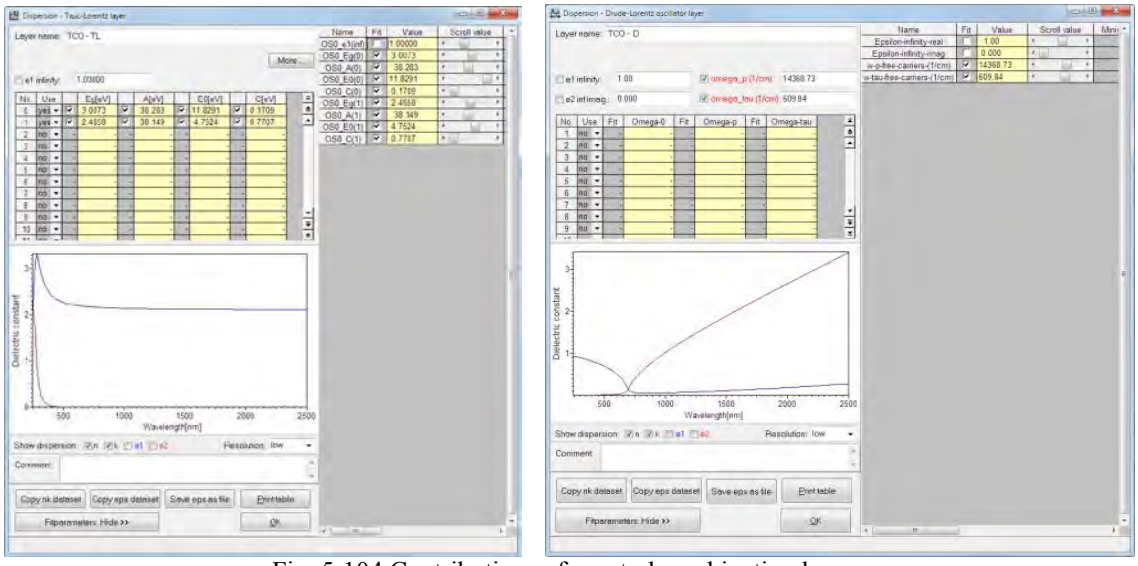


Fig. 5-104 Contributions of spectral combination layer

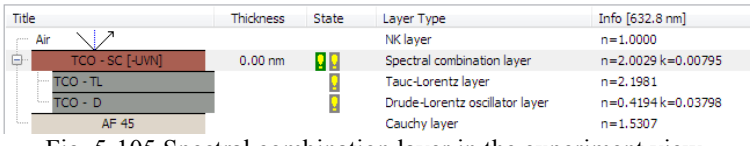


Fig. 5-105 Spectral combination layer in the experiment view

5.2.4.33 Tanguy layer

Theoretical assumptions:

For the description of III-V semiconductors like GaAs Tanguy has developed formulas for the dielectric function using Wannier excitions. The implementation in SpectrRay is based on the articles of Christian Tanguy [IEEE Journal of Quantum Electronics, Vol. 32, No. 10, Oct. 1996, p.1746 // Physical Review Letters 11/1995; 75(22):4090-4093 // J. Appl.Phys. B2(2), 15 July 1997, p.798]
The formula gives the complex dielectric constant of Wannier excitons, which includes exactly the contributions of all bound and unbound states. It allows an improved description of the excitonic influence on the optical properties of semiconductors near the band gap, especially with respect to dispersion effects.

$$\varepsilon(E) = 1 + \frac{a}{b - E^2} + \frac{CA\sqrt{R}}{(E + i\Gamma)^2}\left\{g\left[\xi\left(E + i\Gamma\right)\right] + g\left[\xi\left(-E - i\Gamma\right)\right] - 2g\left[\xi(0)\right]\right\}$$

$$\xi(z) = \sqrt{\frac{R}{E_g - z}} \qquad g(\xi) = 2Ln(\xi) - 2\pi Cot(\pi\xi) - 2\psi(\xi) - \frac{1}{\xi}$$

$$\psi(z) = \frac{d}{dz} Ln\left[\Gamma(z)\right]$$

The function ψ is the so called diagamma function with complex arguments (in Mathematica it is called PolyGamma(0,z)).

The refractive index is calculated using the simple formula n=Re(ε) but the absorption is expanded by a second order polynomial above the band gap:

$$k = \mathrm{Im}[\varepsilon] \qquad if\ E < E_g$$

$$k = \mathrm{Im}[\varepsilon] + c(E - E_g) + d(E - E_g)^2 \qquad if\ E \geq E_g$$

Standard values for the parameters and their meaning are:

Parameter	Default value	Description	Unit
Eg	1.425	Direct band gap energy	eV
R	0.0034	Binding energy of exciton, typically a few meV	eV^2
Gamma	0.0045	Broadening of energy levels, typically 0-25 meV	eV
CA	2	Proportional to the square of the Kane momentum	eV
a	117.1	Corresponds to the height of the absorption peak	eV^2
b	12.4	Corresponds to the position of the absorption peak	eV^2
c	0.154	Linear factor for k above the band gap	eV^{-1}
d	0.15	Second order factor for k above the band gap	eV^{-2}

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Tanguy layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

An example is given in Fig. 5-106and Fig. 5-107 showing n and k respectively.

Note: The dispersion relation is defined near the band gap only. The energy range should be limited to approx. 0.5...2 eV.

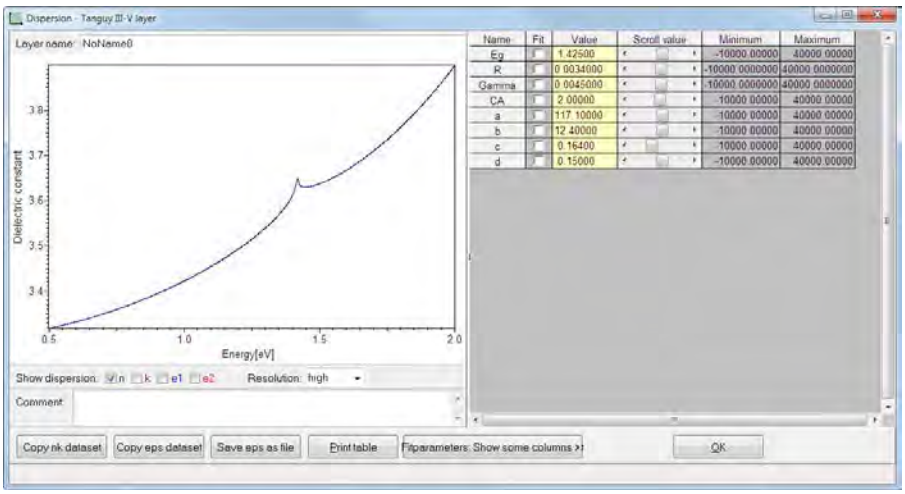


Fig. 5-106 Example for a Tanguy layer (n)

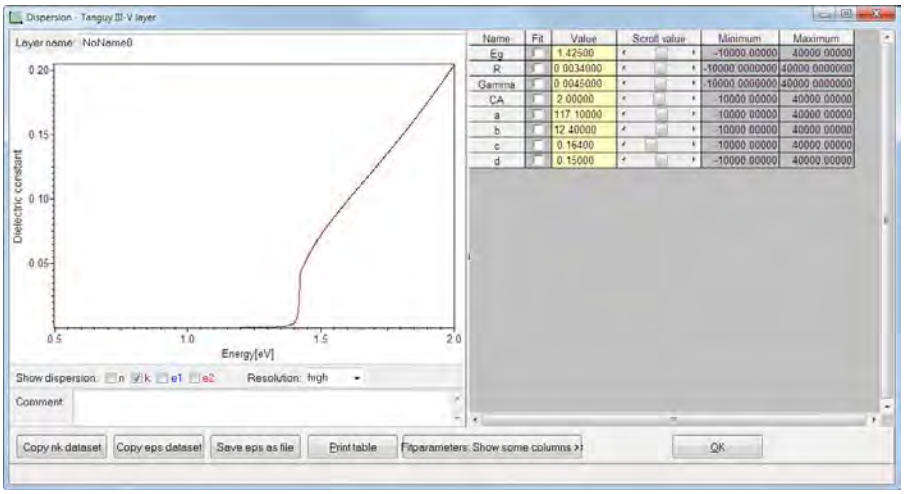


Fig. 5-107 Example for a Tanguy layer (k)

A comparsion for GaAs between the Tanguy layer and the Afromovitz layer (see chapter 5.2.4.5) shows that the Tanguy layer can describe the material more precise.

5.2.4.34 Tauc-Lorentz oscillator layer

Theoretical assumptions:

The Jellison-Modine model [G.E.Jellison Jr., F.A.Modine, P. Doshi, A.Rohatgi" Spectroscopic ellipsometry characterization of thin-film silicon nitride", Thin Solid Films 313-314 (1998) 193-197] uses the Tauc-Lorentz formula. It has been developed for Silicon nitride and amorphous semiconductors. It is based on an oscillator expression for ε_2 and the Kramers-Kronig integral is used to obtain ε_1.

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0C(E-E_g)^2}{(E^2-E_0^2)^2+C^2E^2}\frac{1}{E} & E > E_g \\ 0 & E \le E_g \end{cases}$$

$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{x\varepsilon_2(x)}{x^2 - E^2} dx$$

The formula is given for a single oscillator but the software supports multiple oscillators. The layer type has 4N+1 constants if N is the number of oscillators ($\varepsilon_1(\infty)$ is typically fixed at near 1).

The parameters have the following meaning which is also shown in Fig. 5-108:

E_g	Bandgap: Onset of the absorption given in photon energy [eV].
A	Strength of the oscillator (amplitude) [eV]
E_o	Resonance frequency [eV] Approximate (for small C values) position of the turning point of k (here outside the spectral range)
C	Broadening of the oscillator [eV] Small (C < 1.0) values will give sharp oscillators High (C >> 1.0) will create broad oscillators

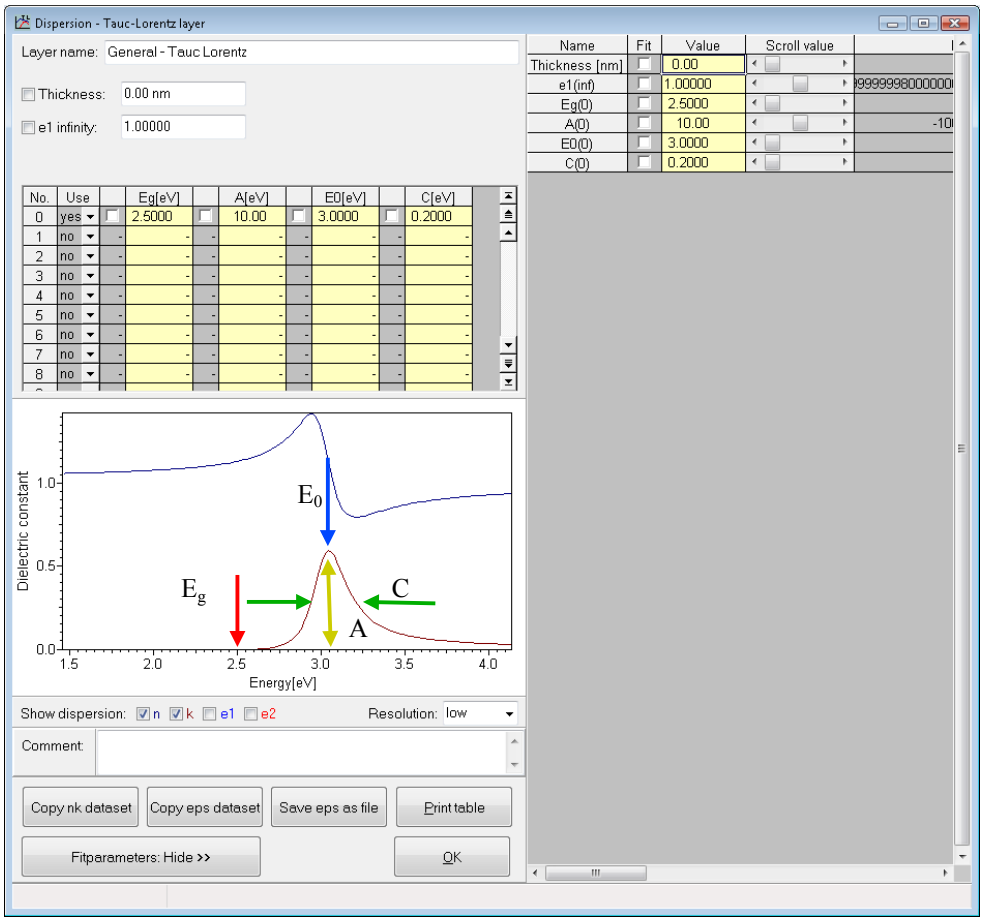


Fig. 5-108 Example of the Tauc-Lorentz-oscillator with effects of the parameters

Creating a new layer

A new layer is created by “File\New\Layer” and selecting the layer type “Tauc-Lorentz layer”. This creates the new layer and opens the editor. The name of the new layer and its properties can be entered.

Editing the layer

The Tauc-Lorentz oscillator dispersion formula is mainly used to describe transparent dielectric materials with absorption in the short-wavelength range. It can also be used to describe the dispersion of:

- absorption bands in polymers (like conjugated polymers in OLED applications)
- amorphous semiconductors like a-Si
- amorphous carbon

As an example for materials which absorbs in the short wavelength range Fig. 5-109and Fig. 5-110 show the dispersion of n and k of Si rich Nitride described by a Tauc-Lorentz oscillator.

The parameters of the TL-oscillator have the unit eV. Therefore it is useful to change the units of the wavelength scale from nm to photon energy (eV).

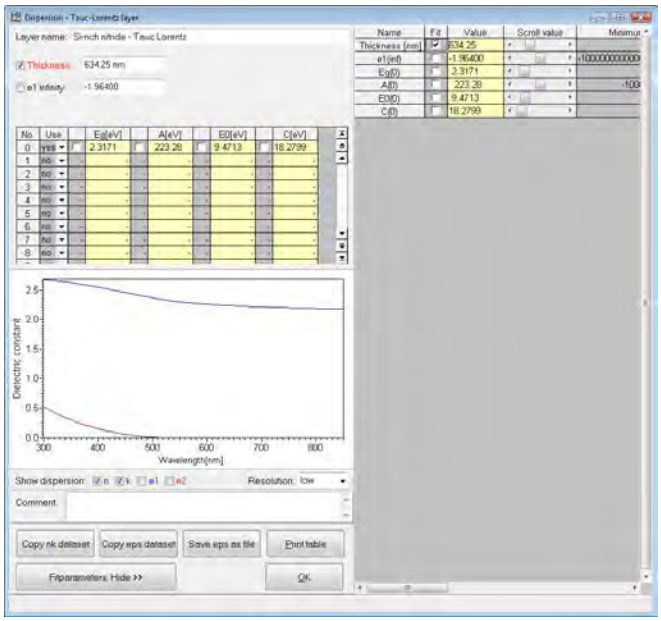


Fig. 5-109 Example for a Tauc-Lorentz layer (x-axis: wavelength / nm)

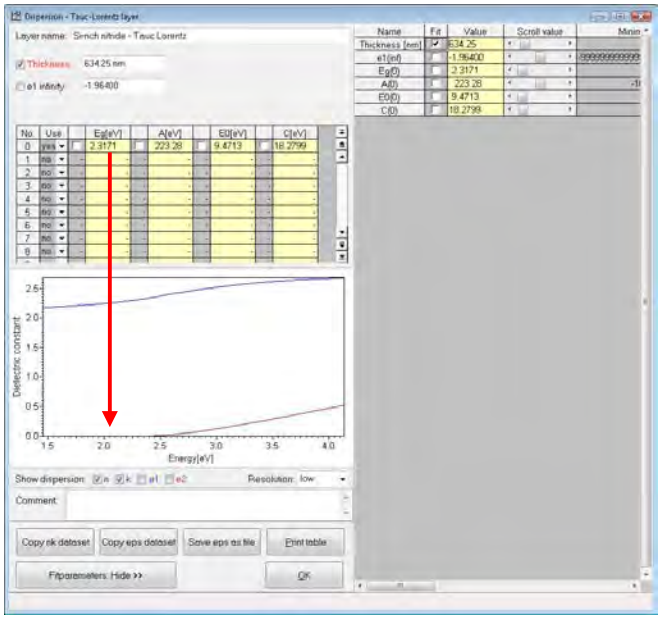


Fig. 5-110 Example for a Tauc-Lorentz layer (x-axis: photon energy / eV)

5.2.4.35 Uniaxial anisotropic layer

This layer deals with uniaxial anisotropic materials only. More general biaxial materials and arbitrary rotations of coordinate systems can be handled with the Biaxial anisotropic layer described in chapter 5.2.4.7.

Theoretical assumptions

A series of layers is anisotropic depending on temperature, pressure and some materials even show anisotropy at laboratory conditions. Anisotropy can be classified in two categories: Uniaxial has one axis of the dielectric tensor parallel and the second normal to surface of the material while the biaxial material introduces a third axis in the layers surface plane. This layer type covers uniaxial anisotropic layers.
The special case of interest is that in which the optical axis of the uniaxial film is perpendicular to its boundaries with the ambient and substrate. This condition is encountered, for example, when Langmuir-Blodgett layers (which are monomolecular layers of well-oriented molecules) are deposited on isotropic substrates, or when thin vacuum-deposited films have island like structures.
Because of the symmetry, when the incident wave in the ambient is either p or s polarized, the excited waves in the uniaxial film and in the isotropic substrate will possess the same polarization, i.e., p or s, respectively. This is equivalent to $R_{ps}=R_{sp}=0$ while R_{pp} and R_{ss} (the Fresnel coefficients) have different expressions (the following set of formulas applies for simplicity to the special case of a single uniaxial layer on an isotropic substrate):

$$(12) \qquad R_{pp} = \frac{r_{01pp} + r_{12pp} e^{-2i\beta_p}}{1 + r_{01pp} r_{12pp} e^{-2i\beta_p}} \qquad R_{ss} = \frac{r_{01ss} + r_{12ss} e^{-2i\beta_s}}{1 + r_{01ss} r_{12ss} e^{-2i\beta_s}}$$

In the above equations r_{01pp}, r_{12pp} and r_{01ss}, r_{12ss} are the reflection coefficients at ambient-film (0-1) and film-substrate (1-2) interfaces for the p- and s- polarization, respectively. They are related to the refractive indices and angle of incidence as follows:

$$(13) \qquad r_{01pp} = \frac{n_{1o} n_{1e} \cos\varphi_0 - n_0 \sqrt{n_{1e}^2 - n_0^2 \sin^2\varphi_0}}{n_{1o} n_{1e} \cos\varphi_0 + n_0 \sqrt{n_{1e}^2 - n_0^2 \sin^2\varphi_0}}$$

$$(14) \qquad r_{12pp} = \frac{-n_{1o} n_{1e} \cos\varphi_2 - n_2 \sqrt{n_{1e}^2 - n_2^2 \sin^2\varphi_2}}{n_{1o} n_{1e} \cos\varphi_2 + n_2 \sqrt{n_{1e}^2 - n_2^2 \sin^2\varphi_2}}$$

$$(15) \qquad r_{01ss} = \frac{n_0 \cos\varphi_0 - \sqrt{n_{1o}^2 - n_0^2 \sin^2\varphi_0}}{n_0 \cos\varphi_0 + \sqrt{n_{1o}^2 - n_0^2 \sin^2\varphi_0}}$$

$$(16) \qquad r_{12ss} = \frac{-n_2 \cos\varphi_2 - \sqrt{n_{1o}^2 - n_2^2 \sin^2\varphi_2}}{n_2 \cos\varphi_2 + \sqrt{n_{1o}^2 - n_2^2 \sin^2\varphi_2}}$$

where n_0, n_2 are the refractive indices of the isotropic ambient and substrate and n_{1o}, n_{1e} are the ordinary and extraordinary refractive indices of the uniaxial film. ϕ_0 is the angle of incidence in the ambient, ϕ_2 is the angle of refraction in the substrate and these two angles are interrelated by Snell's law

$$(17) \qquad n_0 \sin\varphi_0 = n_2 \sin\varphi_2$$

The phase thicknesses β_p and β_s for the p- and s-polarizations that appear in the above equations are given by

$$(18) \qquad \beta_p = 2\pi \frac{d_1}{\lambda} \frac{n_{1o}}{n_{1e}} \sqrt{n_{1e}^2 - n_0^2 \sin^2\varphi_0}$$

$$(19) \qquad \beta_s = 2\pi \frac{d_1}{\lambda} \sqrt{n_{1o}^2 - n_0^2 \sin^2\varphi_0}$$

where d_1 is the film thickness and λ is the free-space wavelength of light. The SpectraRay definition of n_{1e} and n_{1o} uses two different materials which can follow any dispersion rule. The anisotropic layer type consist therefore of two materials and a thickness.

Creating a new layer

A new uniaxial anisotropic layer is created by "File\New\Layer" and selecting the layer type "Uniaxial anisotropic layer". This creates the new layer and opens the editor. You should enter the name of the new layer and its properties.
A second step should specify the two materials used as ordinary/extraordinary dielectric function definition. See Appendix D "Material name edit fields and buttons" for information on the functioning of the edit field and the associated button.

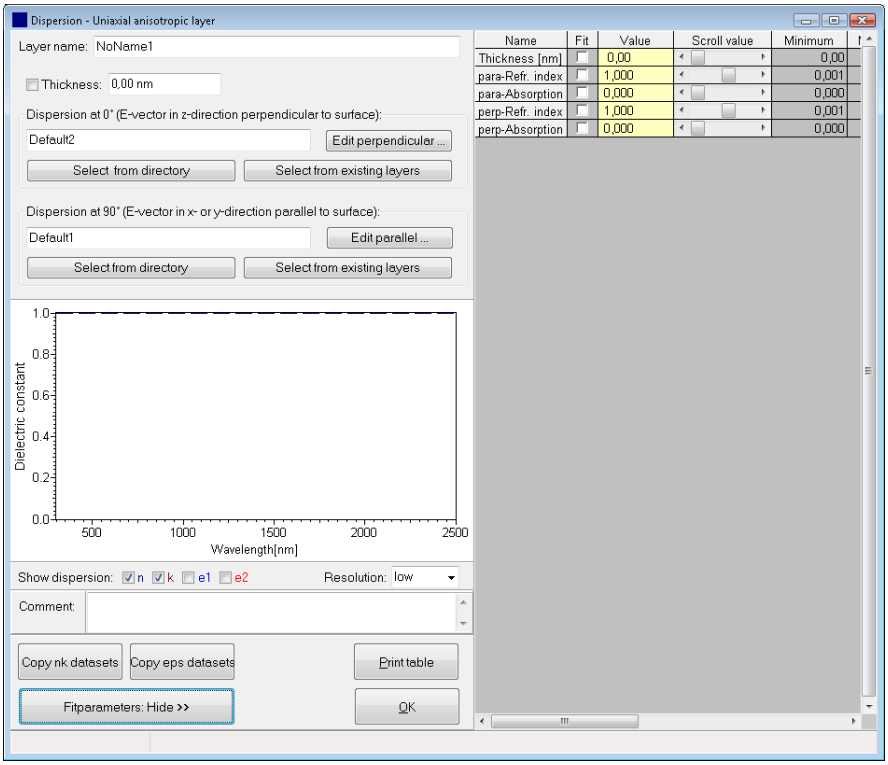


Fig. 5-111 Editor of uniaxial anisotropic layer

Editor description

The editor defines the materials used for the ordinary axis dielectric function (active at 0° angle of incidence) and for the extraordinary dielectric function (active at 90° angle of incidence) by two edit field - button combinations. See Appendix D "Material name edit fields and buttons for more information". The thickness field works as a physical number edit (see Appendix D: Physical number edit fields).

Name	Fit	Value	Typ. Diff.	Min.	Max.	Reset Min.	Reset Max.	Accuracy
thickness [nm]	0	0	20.0	0	400000	0.5	30000.0	0.1

Tab. 5-13 Default fit parameters for the uniaxial anisotropic layer (sublayer parameters are not listed in this table)

5.2.5 Creating and editing models

A model is the theoretical description of your sample. SpectraRay supports stacks of layers and can simulate non-ideal effects. A Sample description consists of a stack of layers, where the top is the ambient medium and the bottom is the substrate (or the backside ambient if transparent substrate mode is used). Furthermore a set of information is included describing the special properties of certain layers, non-ideal effects and settings required for display and fit control. This set of information is called the environment (see chapter 5.2.6).
The following explains handling of materials and layers: Loading, saving, replacing, creating and editing of layers. Certain functions are often used and available in the menu as well as in the speedbar (see Appendix B). Moving layers is easily performed by using drag&drop (see Appendix A). So the user interface is very fast and convenient.

A **new model** is created by selecting the "File/New/Model" menu or dragging all layers from the model listbox and dropping them on the material file listbox, on the recycle bin or any free space in the program window. A new model shows an empty (model-) listbox and has default parameters (when using "File/New/Model").
After you have initialized the model you can build up your new stack of layers. You have the following set of basic operations with layers and materials:

Adding a layer

You can add a layer by dragging the material name from the material listbox to the model listbox and dropping it on the insert/append position in the model listbox you want. This allows you easily loading material files to desired positions in the layer stack.
Another way to add a layer is to choose "File/Load" with *.mat. This allows loading materials from any directory, while the above methods operate on the current material directory path (see menu command reference File/Directories for more information).

Removing a layer

A layer contained in the model listbox can be removed by dragging it to the material listbox, the recycle bin or any free space in the program window and dropping it. This function does not save the layer! The same function is available by the "Remove" button .

Saving a layer

If you finished your modeling and fit the result in many cases a new material definition is contained in the layer parameters. You can save any layer to a material file by pressing the "Save" button 

in the upper left corner or right above the model listbox in the upper right corner  . This opens a file dialog box where you can enter the material file name. You should use the extension *.mat because only these files are listed in the material listboxes. The same function is performed when you choose "File/Save as" with *.mat and a layer is selected within the model listbox.

Exchanging layers

A special combination of removing and loading layers is the exchange function. This function is useful to check a series of materials when fitting data. Its special enhancement is to save the thickness of the layer removed and set the thickness of the layer inserted at the same place to the same value just by dragging a new material and dropping it onto the old material.

Creating new layers

SpectraRay comes with a large collection of material definitions. But your own samples may require adding new layers different from the original. You have two ways to get a new layer: The first method loads an original layer near to the layer you want to create. The second method is to create a new layer based on the available layer

types in memory and to save it to a material file as described above. If you choose “File/New/Layer” or click on the “Add” button + you open the selection box of basic layer types.

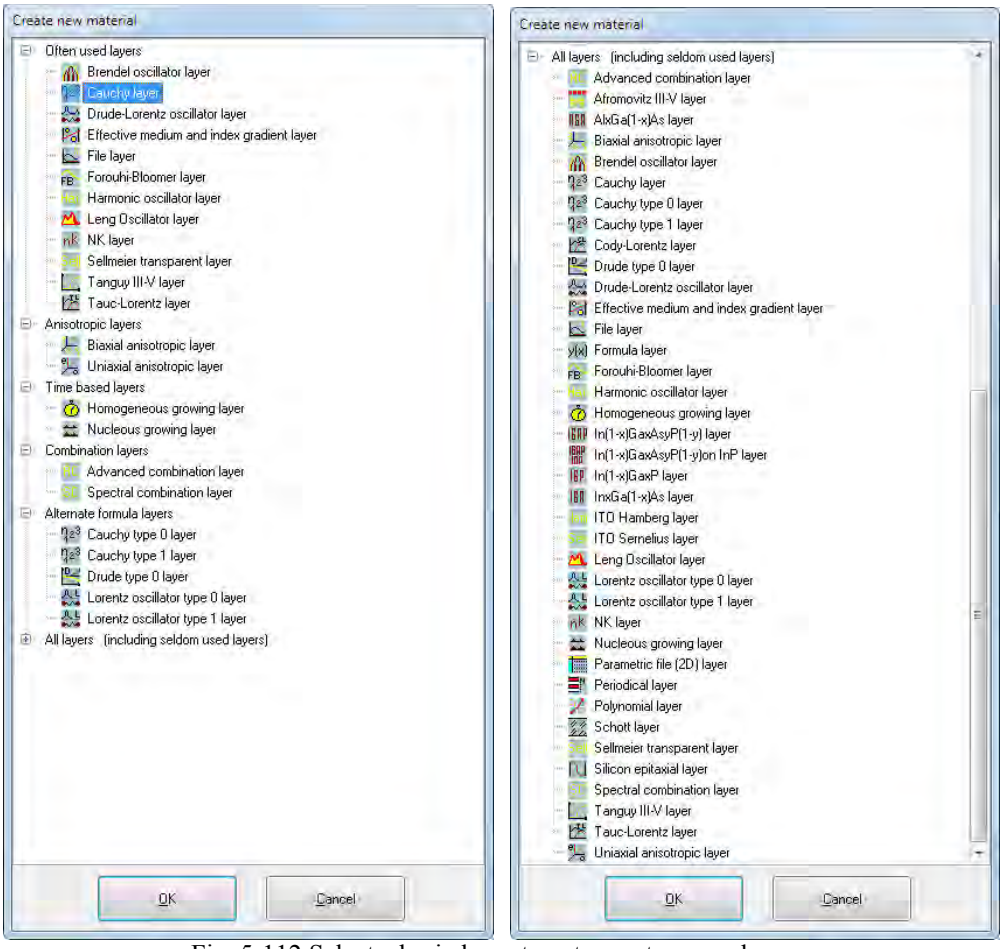


Fig. 5-112 Select a basic layer type to create a new layer

After selecting the new layer type a series of steps is performed. If additional steps are needed you find it documented in chapter 5.2.4 specific for each layer type. The result of this procedure is a new layer added to the model. If you use this layer for improving your fit you don’t need to save the layer, because saving the experiment (actual model plus actual data sets) affects all layers. Just the opposite applies if you intend to create a new material file *.mat. In this case you must save the layer to a file and remove it from the model because it is no longer needed.

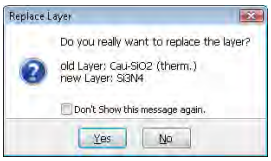
Editing layers

Each layer consists of a lot of settings and parameters. During a fitting session you have to edit these data repetitively. The editor related to a layer depends on the layer type. You can click on to edit the layer selected within the model listbox. If no layer is selected nothing happens. A more straightforward way is to double-click the layer. The editors dialog box opens and you can enter or change the settings. See chapter 5.2.4 for more information on layer specific editors.
After editing a layer you may have the parameters changed. If this occurs you should save the layer to a material file to save these settings (only if it was proven to be a good material definition).

Moving/Replace layers

The editing facilities of the model editor include the drag&drop support for sorting the layers. If you want to move the top layer to the button simply use drag and drop. The result is displayed immediately. You should keep in mind that the first and last layers are used as semi-infinite media. If you move a layer from the middle to the top it loses its thickness information while the old top layer gets the thickness property. The effect is visible in

the list of fit-parameters (see chapter 5.6.2). If you drop a layer onto an existing layer you replace this layer by the new one. A message box will appear for confirming the replacement.



Pressing the CTRL-key of your keyboard while dragging a layer of the model will create a copy of the dragged layer after dropping it at any place inside the model. This copy will have the same name and parameters. If you change any parameter of the copied (or original) layer the parameters of the original (or copied) layer will be changed too. The layers will always have the same parameters.

Pressing the CTRL- and SHIFT-key of your keyboard while dragging a layer of the model will create a new layer with the same parameters but different name after dropping it at any place inside the model. If you now change any parameter of the copied (or original) layer the parameters of the original (or copied) layer will not be affected.

After the model was created or edited the model listbox shows the description of the layer stack. The first line in the listbox defines the top ambient and the last line the bottom ambient (in most cases the substrate). Each line consists of three topics:

<Title> <Thickness> <State> <Layer Type> <Info>

The thickness is displayed in the physical unit selected for thicknesses within the environment (page units, see chapter 5.2.6). The state shows if the layer reports any parameters to be fitted or nothing if the parameter set of the layer is fixed. Info displays the refractive index for the wavelength selected within the environment (page values, see chapter 5.2.6).

Clicking on 

opens a graph for displaying the refractive index in dependence of the wavelength.

5.2.6 Environment

The environment is an abbreviation for the set of parameters not stored within the models layer stack and not stored within the data sets. There is a broad range of settings defined within the environment: Actual wavelength, angle of incidence etc. for simulations, physical units for default display of parameters, actual parameter ranges and non-ideal effects. This makes the environment the control panel for nearly every function.
The environment is stored within model description file *.mod, experiments *.exp and recipes *.rcp. So you have the possibility to recover the whole setup of the program by loading a single file. The environment editor is split into several pages:

1. Values: Wavelength, Angle etc. used for simulations and related settings
2. Ranges: The wavelength, angle, temperature and time range used for fits
3. Units: selection of default units for wavelength, thicknesses etc.
4. Substrate: settings needed for handling transparent substrates
5. Inhomog.: resolution effects for wavelength, angle and thickness

The following section describes the pages of the environment in detail. The theoretical description of non-ideal effects is in chapter 5.2.7.

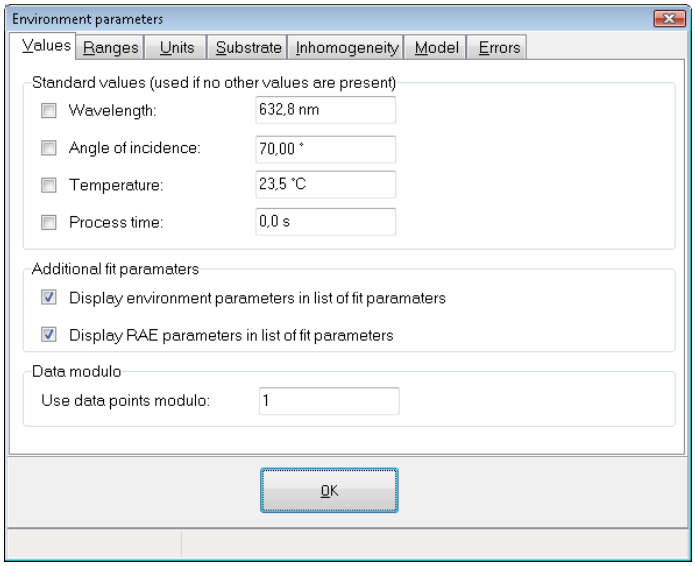


Fig. 5-113 The page “Values” of the environment

“Values”-page

The first page of the environment sets the values of wavelength, angle of incidence, temperature and process time used for simulations. If you intend to calculate a spectrum of (ψ, Δ) at 70° angle of incidence the wavelength is varied within the simulation but the angle has to be set within the environment.
The second function of these values is to be fit parameters if the checkbox is checked (see Appendix D “physical number edit fields” p. 424).
The page contains a set of checkboxes representing internal flags. The flag “Display environment parameters in list of fit parameters” is used to report the environment parameters to the lists of fit parameters. A typical application is to fit the angle of incidence at in-situ ellipsometers. You should load data without a z-value to activate the angle of incidence in the environment (otherwise the measurement condition “angle” overwrites the angle within the environment), select the angle as fit parameter and run a fit including the angle of incidence.
Very important is the value of “Use data points modulo”. Measurements with spectroscopic ellipsometers with diode arrays or FTIR modules generate large data sets of several thousand data points. In many cases this amount of data is not needed for getting the first approximations of a sample model. For reducing the calculation time you can use only every second, third or tenth point. The “each” is setup by the modulo: A data point is used within the FOM (figure of merit).

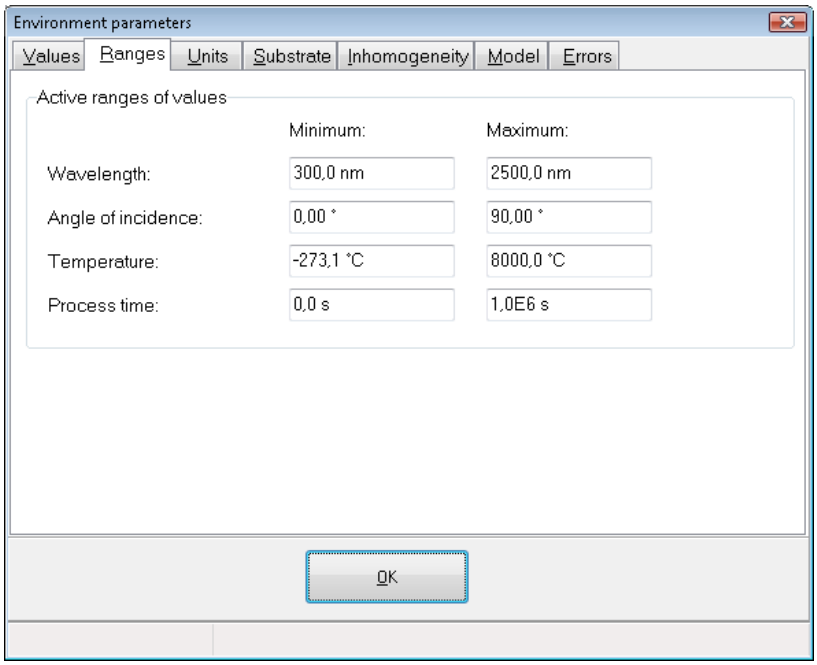


Fig. 5-114 The page "Ranges" of the environment

"Ranges" page

This page is used most during fitting sessions. If you have samples with unknown layers it may be difficult to fit the whole spectrum. For instance if a spectrum contains intervals of absorbance and transparency the interpretation of the whole spectrum requires a more complicated model than the transparency region.
Because of the above considerations it is very useful to setup the data interval you want to use without changing the data sets (i.e. trimming of files). The related functionality driven by this dialog covers the following things:

1. Limiting the data used for calculation of the FOM to the intervals set up here (this applies for wavelength to this wavelength range, for angles to this range of angles ...)
2. Limiting the display of curves during fits to the intervals defined here
3. Limiting the output of calculated curves and data curves of the fitting dialog to these ranges.

You have the possibility to define individual ranges for the four basic parameters wavelength (energy, wavenumbers,...), angle of incidence, temperature and process time. A range is a set of values for minimum and maximum. It doesn't matter if "minimum" is smaller than "maximum", both values are sorted anyway. All edit fields can process physical units (see Appendix E "physical number edit fields").

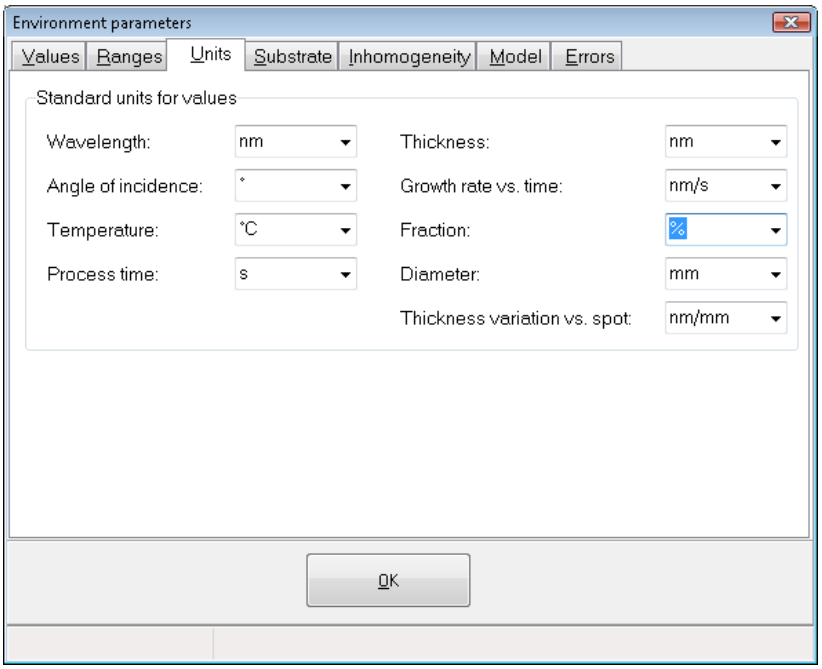


Fig. 5-115 The page “Units” of the environment

“Units” page

The third page of the environment contains the settings for support of physical numbers. See Appendix D “physical number edit fields” on page 424 for more information on the functioning of these fields.
This dialog sets the units used for default output of data:

1. Parameters in layer editors
2. Parameters in fit-lists
3. Conversion of x-axis for fit-display
4. Conversion of x-axis in plots of (n, k) in layer editors

These settings are used for the programs *default* output. Anyway you can enter the data in the units you prefer as far as the unit is correct. A complete list of unit types and supported units is given in Appendix C.

“Substrate” page

The settings for transparent substrates are located on the “substrate” page of the environment. Transparent or weekly absorbing substrates differ from conventional substrates as silicon in the backside reflections modifying the measuring beam. The backside reflections have to be taken into account each time a substrate is measured in a spectral range of transparency or week absorbance. If this is the case the substrate acts as a non-coherent (i.e. thick) layer.
SpectraRay allows you to use one thick layer with two piles of films on the top and on the backside. The substrate is by definition the thickest layer of all layers. The special treatment of transparent substrates includes the calculation of the Stokes vectors of all partial beams used. Partial beams are used to add the influence of the backside. The number of multiple reflections on the substrate backside is identical to the number of beams entering the detector aperture. So the selection for transparent substrate mode is done by entering the number of backside reflections. If this value is zero, the bottom layer of the stack is used as the semi-infinite bottom ambient. Setting a non-zero count of backside reflections enables the transparent substrate mode. The top and bottom layer are still the semi-infinite media but the thickest layer between them is treated as the incoherent layer. The layers on the top of this “substrate” create the top pile and the layers below the “substrate” create the bottom pile. The calculation of the interference in the intensity space requires additional information on the separation of the partial beams caused by the path through the thick “substrate”. The superposition of partial beams bases on the superposition of illuminated circles and uses the beam diameter, the substrate thickness and the diameter of the aperture. For a detailed description see chapter 5.2.7.

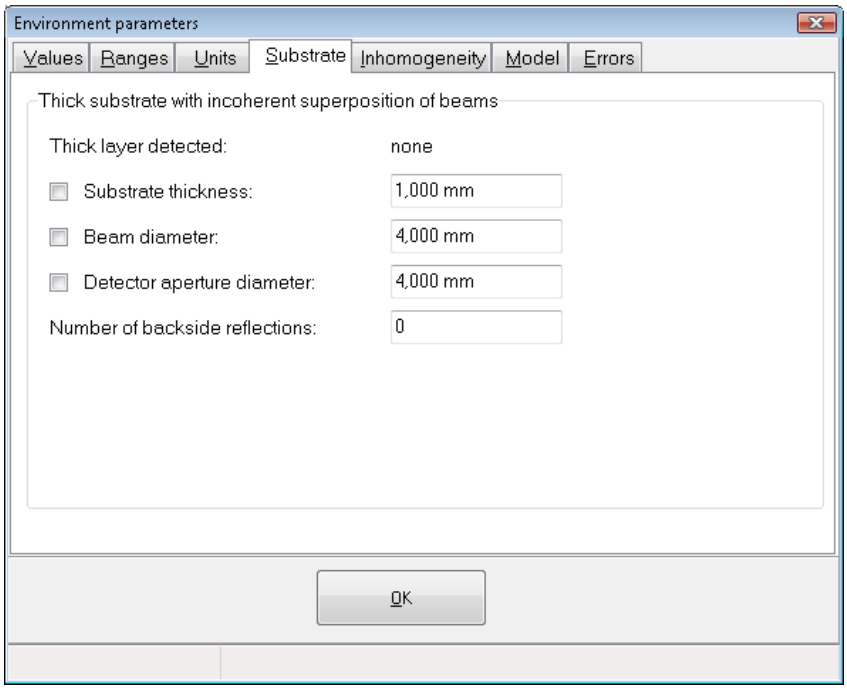


Fig. 5-116 The page “Substrate” of the environment

“Inhomogeneity” page

The real measurement differs from the ideal by the device capabilities. The set of these capabilities are set up on the “inhomogeneity” page of the environment. The non-ideal effects of a measurement device supported are

1. thickness variations within the measurement spot
2. limited wavelength resolution
3. influence of focused measurement beams (µ-Spot, FTIR-add-ons)

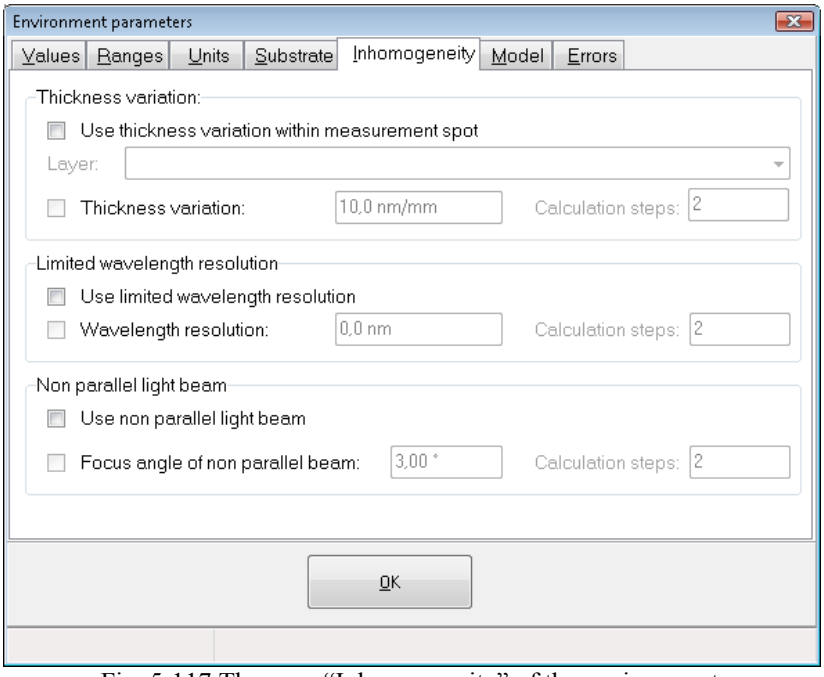


Fig. 5-117 The page “Inhomogeneity” of the environment

All three effects are driven by a flag and some parameters. The flag always indicates whether the effect is in use or not. The “steps” define the number of steps left and right from the center value calculated for numerical integration of the curves s_1 and s_2 (afterwards ψ and Δ or R or T).
The thickness variation uses a combobox to select the layer which should cause the thickness non-uniformity. The thickness gradient is entered within the edit field.
Each spectroscopic device has a limited wavelength resolution which could soften peak structures. A successful fit is only possible, if no differences in the peaks remain after plain portions of the spectrum were fitted. If you use this feature you have to enter the spectral resolution you use (e.g. 4.5 nm for a SER 800 with photodiode array, 0.1 nm for example for a monochromator or 2 cm^{-1} for the NIR portion of a SER 850).
The third effect is the influence of non-parallel beams. Such beams are caused by focusing lenses used in microspots or focusing mirrors in FTIR devices. You should enter the opening angle.
It should be mentioned that all number edit fields (except the “steps”) process physical units (see Appendix D “physical number edit fields”).

“Model” page

The flag “Reverse layer stack” is used to reverse the stack defined in the model listbox for simulating measurements on the backside of a sample. This requires the mode for transparent substrates.

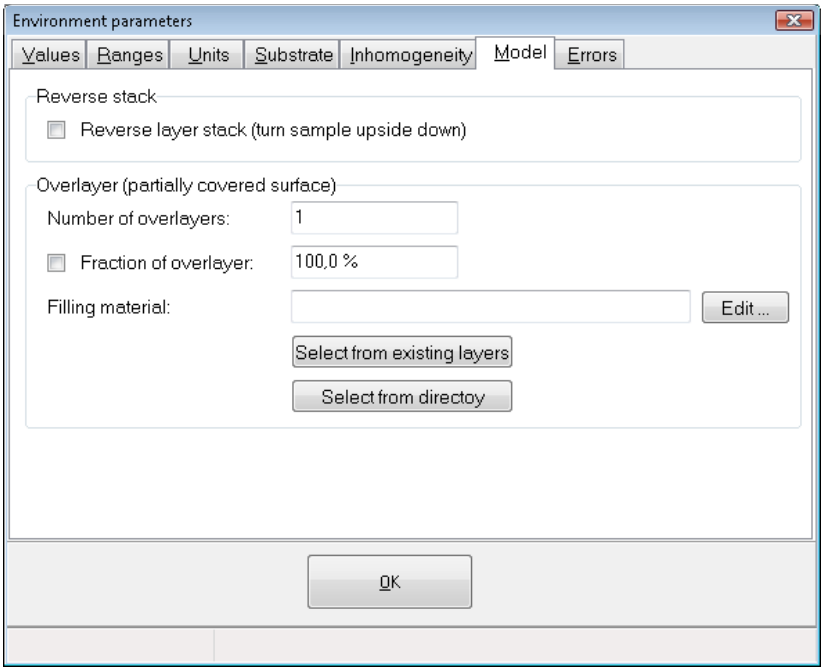


Fig. 5-118 The page “Model” of the environment

“Errors” page

This page contains the settings for the error calculation. You can select how the errors are calculated and which precisions of the measured data are used for the error calculation.

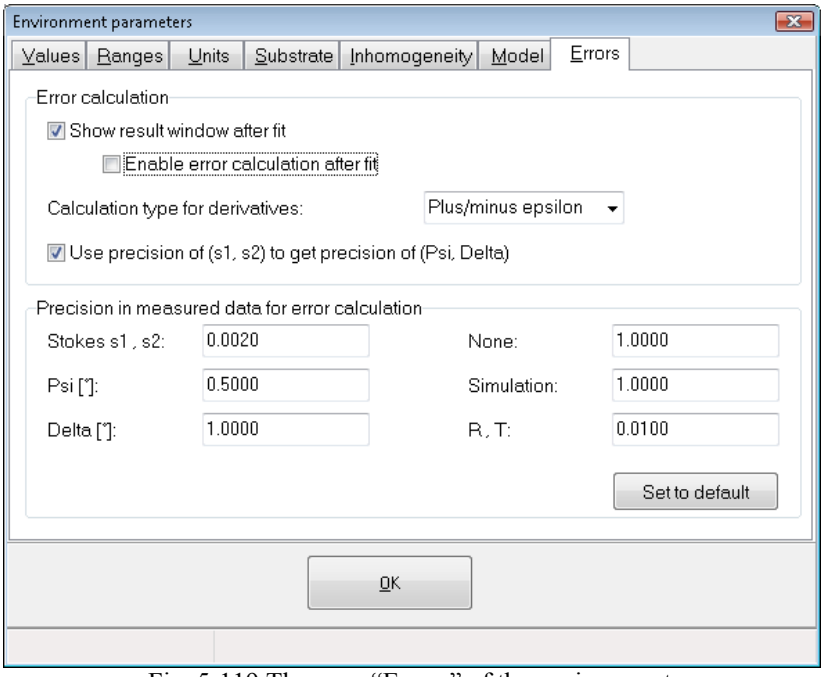


Fig. 5-119 The page “Errors” of the environment

5.2.7 Non-ideal effects

The practical application of ellipsometry, reflectance or transmittance measurements considers non-ideal samples and uses non-ideal devices. The samples may have non-abrupt interfaces, may create stray light or may be inhomogeneous. All these effects are introduced into SpectraRay by basic layer types.
The device dependent part is defined by the environment. This covers transparent substrates, wavelength resolution effects and focusing beams. The following sections describe in detail who these effects are modeled and which parameters are introduced.

5.2.7.1 Limited wavelength resolution

Spectroscopic ellipsometers or spectrometers using photodiode arrays, monochromators or interferometers all have the limited spectral resolution in common. Spectral resolution means that the information taken at a certain wavelength always contains information on a small range left and right from the so called center wavelength. Everything you measure is the weighted sum of information of all points in such intervals. If a monochromatic beam of light λ_0 is measured, you get a spectrum $U(\lambda)=G(\lambda-\lambda_0)$, where U is the voltage output from the detection system and G is the shape of monochromatic light of the wavelength λ_0. When you illuminate a detection system with a spectrum $\Phi(\lambda)$, you measure the convolution of G with F:

$$U(\lambda) = \int_0^\infty \Phi(\lambda) \cdot G(\lambda - x)\,dx = \Phi * G \tag{20}$$

The numerical integration of this convolution assumes a Gaussian profile for G:

$$G(\lambda) = e^{-\left[a(\lambda-\lambda_0)\right]^2} \tag{21}$$

The half width is defined by a value of $G(\lambda)=½$. From the above equation the relation between a and the half width h follows:

$$h = 2\left(\lambda_{1/2} - \lambda_0\right) = \frac{2\sqrt{\ln(2)}}{a} \tag{22}$$

Most spectrometers are specified by their resolution which is the half width in many cases. The half width h is used to specify the spectral resolution. Some typical resolutions are:

SER 800 with photodiode array: 4.5 nm
SER 850 NIR portion: 2 cm^{-1}

The numerical calculation converts the above integral into a sum

$$U\left(\lambda_0\right) = \sum_{\lambda=\lambda_0-kz}^{\lambda=\lambda_0+kz} \Phi(\lambda) e^{-(akz)^2} \tag{23}$$

where λ_0 is the wavelength U has to be calculated at. The value a is calculated from the half width as shown above. The integer k makes the above integral to a sum. You should keep in mind that values of k cause additional 2k calculations at each wavelength. Therefore steps of 2...5 are recommended.

5.2.7.2 Use of a microspot focus

A microspot or mirror can focus the light beam. This removes the assumption of a parallel beam made during the modeling. The calculation has to introduce and averaging scheme able to handle the mixture of different partial beams. We consider the beam as a series of stripes of a circle, each stripe at its own angle of incidence. It is very important to average again in the intensity space (no simple ψ or Δ averaging). If we compare the areas of each individual stripe with the area of the beam (diameter!), the weights w for the intensity averaging can be calculated:

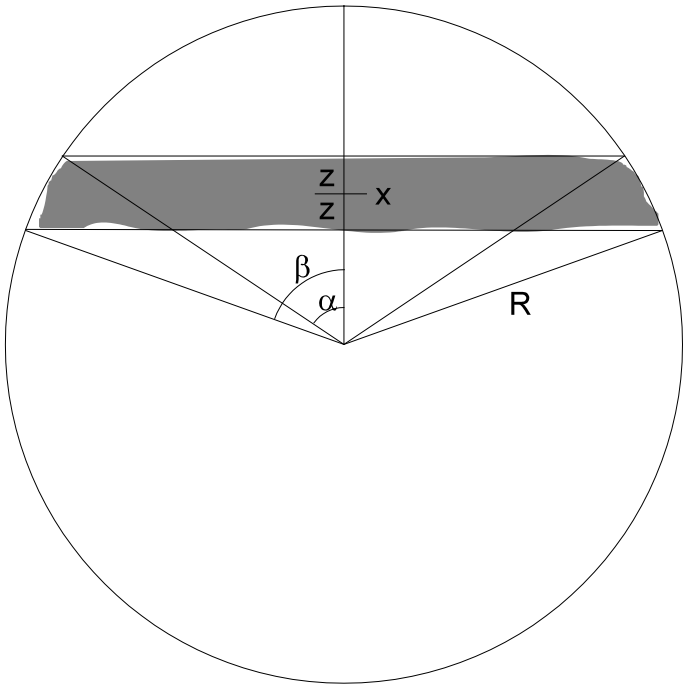


Fig. 5-120 Stripe definition for focus effect

The radius R is the half of the beam diameter. A stripe of the width 2z at the position x creates an area A, which is the difference between the two pies defined by 2α and 2β. These angles have to be calculated first:

(24) $$\tan\alpha = \sqrt{\frac{R^2 - (x+z)^2}{R^2}} \qquad \tan\beta = \sqrt{\frac{R^2 - (x-z)^2}{R^2}}$$

From these angles the area of the pies is calculated:

(25) $$A(\beta) = 2\pi R^2 \beta \qquad A(\alpha) = 2\pi R^2 \alpha$$

The area of the stripe becomes

(26) $$A_{Stripe} = A(\alpha) - A(\beta)$$

and the weight for this individual stripe will be

(27) $$w(x) = \frac{A_{Stripe}}{A_{Circle}} = \frac{A(\alpha) - A(\beta)}{\pi R^2} = 2(\beta - \alpha) \qquad \beta=\beta(x),\ \alpha=\alpha(x)$$

Obviously the weight is independent from the actual beam diameter. Now we have the weights and have to use them to average the intensities. This requires going from the beams cross section to the focusing plane.

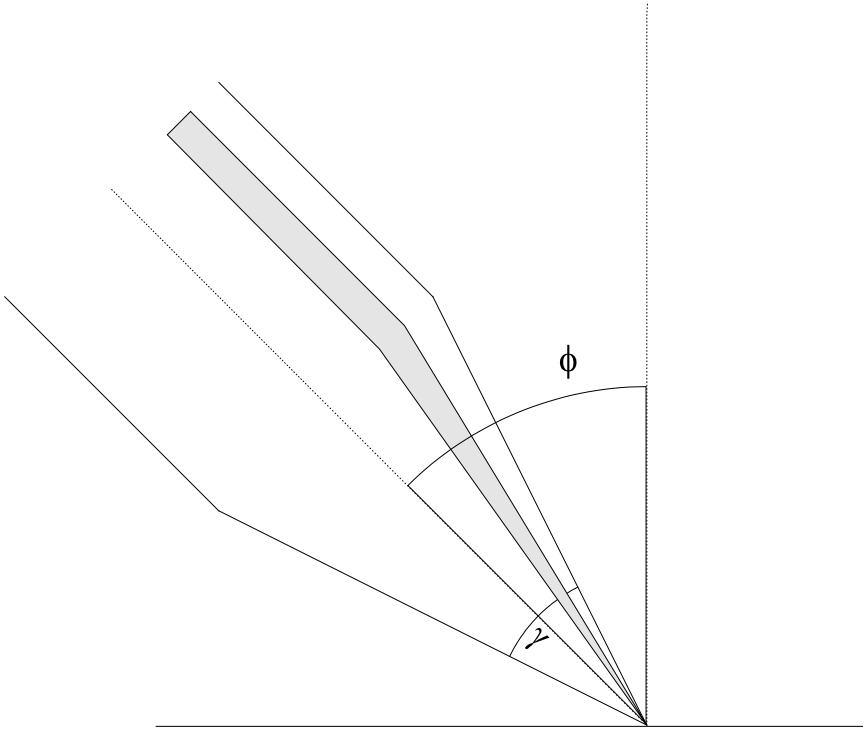


Fig. 5-121 The individual angle of a cross sectional stripe

The opening angle γ creates a set of angles of incidence around the primary angle of incidence ϕ_0. Now the integral could be written as:

$$U(\varphi_0) = \frac{\int_{\varphi_0-\gamma/2}^{\varphi_0+\gamma/2} w(\varphi-\varphi_0)U(\varphi)d\varphi}{\int_{\varphi_0-\gamma/2}^{\varphi_0+\gamma/2} w(\varphi-\varphi_0)d\varphi} \quad (28)$$

There is a slightly different formula for the weight in the argument. The expression above uses x and an angle is needed. If the focusing length is f the relation needed becomes:

$$\varphi-\varphi_0 = \arctan\frac{x}{f} \xrightarrow{f>>x} x = \frac{2(\varphi-\varphi_0)}{\gamma} \quad (29)$$

Numerical integrations require converting the above integral into a sum. The number of stripes is set from infinity to 2N+1 and we get the sum expression:

$$U(\varphi_0) = \frac{\sum_{i=-N}^{N} w\left(\frac{2iR}{N}\right)U\left(\varphi_0+\frac{2i\gamma}{N}\right)}{\sum_{i=-N}^{N} w\left(\frac{2iR}{N}\right)} \quad (30)$$

The value for N should be set in the range 2...5, to reduce calculation time (using this feature adds 2N+1 calculations at each measurement point).

5.2.7.3 Transparent substrates

The classical understanding of a substrate in ellipsometry is only a special case of the more general model of transparent substrates. The main difference between both models is the handling of backside reflections. The classical model does not care for backside reflections and is valid only for absorbing materials with thicknesses large enough that any reflections occurring are damped enough not to influence the intensity measurement.

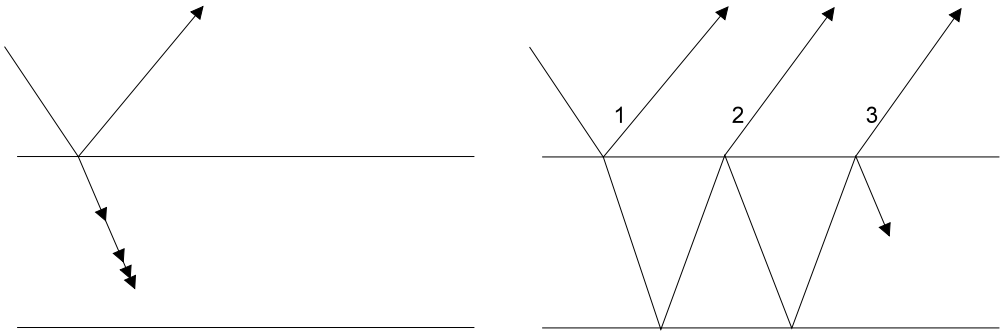


Fig. 5-122 The classical substrate model (left) and the transparent substrate (right)

The “transparent” substrate handles multiple reflections within the substrate and assumes the substrate to act as an incoherent medium (that means the coherent interferences are not resolved or do not exist). Obviously this model works for transparent materials as well as for absorbing materials. This is necessary for measurement of colored glasses in the UV. A second example is the use of standard silicon wafers (backside polished) in the UV/Infrared. Such spectra contain as well absorbance as transparency intervals. For all these reasons the “transparent” substrate is the choice for many applications. The term “transparent” grew in history from the problem of measuring glasses. The same procedure applies for many other applications but the name is still the same.

The special treatment of backside reflections must operate with intensities because this is what the detector of each device measures. Just the opposite is what you measure with ellipsometers: A complex ratio of reflectance, both independent from the absolute intensity. How is the way out?
A light beam is characterized in its intensity and polarization by a vector of 4 numbers forming the so called stokes vector. The interaction of such light beams with optical elements or samples is described by so called Mueller matrices. When calculating the reflection of a beam at a transparent substrate the Stokes vector must be multiplied with all components’ Mueller matrices. These components are:

1. Top pile of layers (R, T)
2. substrate (T)
3. Bottom pile of layers (R, T)

As described in chapter 5.2.6 SpectraRay divides two whole stacks of layers into the above triple of components. The change of the Stokes vector is calculated for the number of partial beams required and all these resulting Stokes vectors have to be added with appropriate weights.
The problem of weights is a difference in certain software implementations, but SpectraRay has the most general approach. Why using weights? You see from the picture above that there is a separation of the partial beams which is of the order of the substrate thickness. This thickness is about one or more millimeters in contrast to the separation of partial beams for multiple reflections in deposited layers (less 10 microns). Since the beam diameters and detector entry apertures have comparable diameters errors could occur if the separation is not handled properly.
As Fig. 5-122 shows, the separation is dependent from the angle of incidence. The overlap of the spots can be treated in the model of overlapping circles. The data you need to calculate such overlaps are

- substrate thickness
- beam diameter
- detector aperture diameter
- number of secondary beams involved
- R, T matrices of the components

The latter item is defined by the layer structure. The thickest layer is assumed the substrate; the others create the top and bottom pile. Some environment parameters are needed to calculate the separation (angle of incidence). Calculating the overlap requires additionally the beam and detector aperture diameter.
It should be mentioned, that the superposition is performed by using stokes vectors. Any physical can be calculated from this vector: ψ, Δ, R, T and more. This method is more precise than other models

- incoherent matrix model (no beam separation treatment)[11]
- effective fraction model (beam separation is not angle dependent)[12]

The next question arising is how these numbers are measured. The beam diameter and aperture diameter do not play a totally different role and do not need to be determined to their absolute value.
If a device uses fibers to transport light, the meaning of "aperture" is changed. The aperture is in these cases the whole optical focusing system, picturing the beam onto the core of the fiber. To avoid the demand for such device data the easier way is calibration.

Calibrating the aperture diameter and beam diameter

The following instructions assume the substrate thickness measured by means of a micrometer screw or known. Before making a calibration measurement the sample has to be placed on the sample stage.
The backside of the sample must contact air, in no case the surface of the sample stage. An arrangement like in the picture below can be achieved by using to sticks of the same thickness or a carrier plate with a center hole of a diameter larger than the beam.

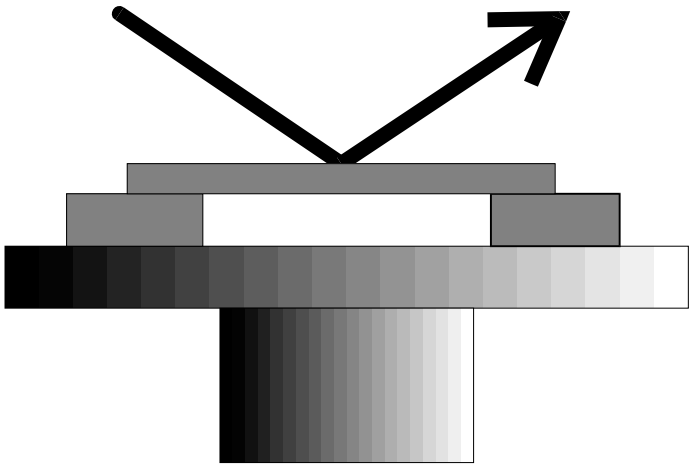


Fig. 5-123 Sample positioning for transparent substrates

A multiple angle measurement should be performed on the free substrate (no layers!!!) and the aperture diameter and beam diameter have to be fitted (see chapter 5.6). Even if the results have no counterpart in reality, these values define a ration which is valid for your machine and should be used for measuring layers the same way. If your layers or substrates may show absorbance you should include a transmission measurement in your calculations, because this is very helpful to fit and differ absorbencies as well as layer thicknesses.

[11] B. Heinze, „Optische Konstanten von Halbleiter-Mehrschichtsystemen", Diss. Aachen 1991
[12] J.A.Woollam, Doc. of VASE spectroscopic ellipsometer

5.3 Assistant for Evaluation of Errors and Stability Issues

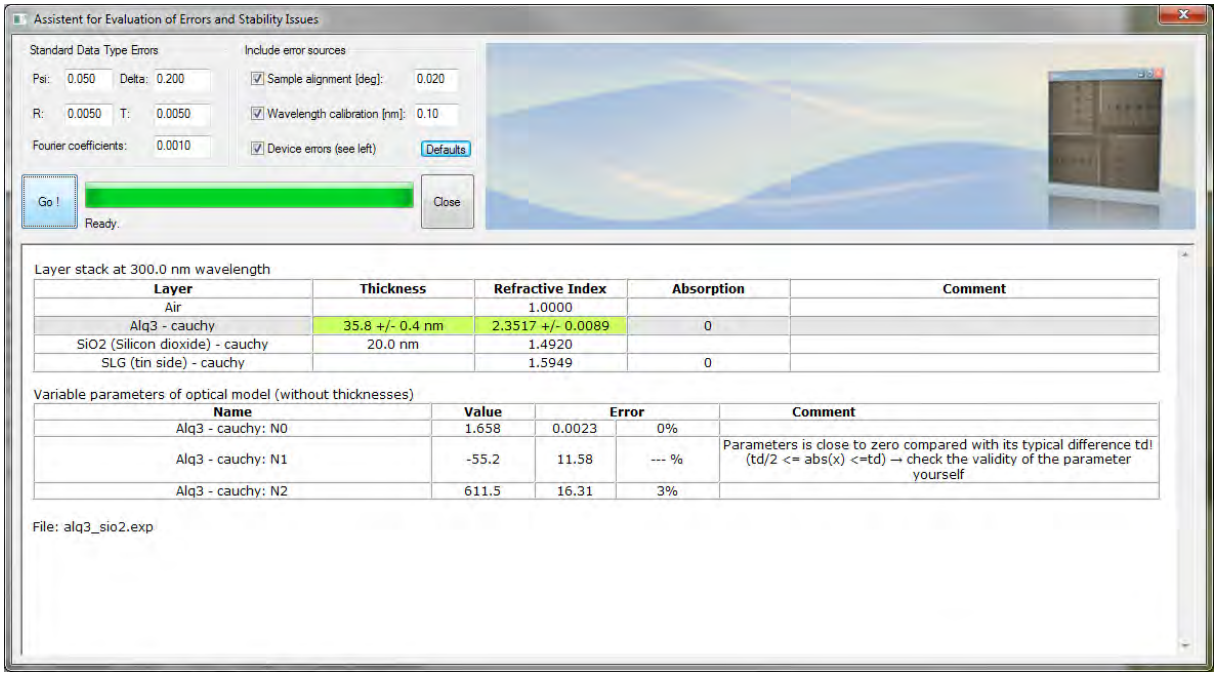


Fig. 5-124 Assistant for Evaluation of Errors and Stability Issues

The assistant helps to evaluate the accuracy of a measurement and gives remarks which parameter may introduce instabilities. It allows avoiding the common problem that over determined optical models result in nicely fitted spectra but give wrong or unstable data. It incorporates systematic errors, interprets the results and gives advice on problems.

5.3.1 Introduction

Spectroscopic ellipsometry is evolved to a powerful tool with general acceptance as well in science as in industry. The precision for measuring stacks of thin films is accompanied by a complexity which is a demand for users when exploring the full power of this method. In the recent years the hardware for ellipsometry has been developed to a high level which allows detecting sub-nanometer changes in the thickness of a film. This leads usually to the assumption that the results can believed as displayed.
However the high precision of the instruments reduces only the errors which are usually covered by the so called reproducibility. Such analysis runs a series of measurements which leaves the sample in place and gives a result reflecting the statistical errors and its propagation through the modeling of the sample. Such precision measurement can be done either manually by running the series of measurements or by theory which uses the correlation matrix to derive parameter errors for known statistical errors of the primary results (here the ellipsometric angles Psi and Delta).
With the advance of the method and the low precision values another source of error is becoming the dominating problem. Any analysis uses a model which incorporates several assumptions on the layer stack, on the material dispersion and on side effects as stray light. As well the sample is not ideally aligned and the wavelength calibration of the spectrometer has also a limited accuracy. All these problems are related to systematic errors, which are the reason for developing an assistant in SpectraRay which helps to discover the impact of some of these sources on the results. Another difference in the approach used here is that the analysis does not require the model to perfectly fit and gives trustworthy error bars even if the model does not fit the measurement in the whole spectral range. In contrast the usual method of using the correlation matrix gives only error bars which follow the practical experience if the model fits perfect and the statistical errors are exactly. However this is difficult to setup, since such simple things as the averaging of intensity readings easily changes from recipe to recipe and affects the device precision. For this reason a simpler approach needed to be developed.

5.3.2 Systematic error sources and method

There are several sources of systematic errors which can be taken into account. Here we cover some effects of the aging of instruments and the systematic errors which arise from sample positioning.
The typical measurement sequence is started by putting the sample onto the ellipsometers sample stage. In the next step the sample needs to be aligned in height and tilt to the optical system of the ellipsometer. If this is done manually by the user he has to use an optical tool as the auto collimating telescope which gives an accuracy of typically 1 arc minute. From uses to user – some of them wearing glasses – the real accuracy depends. If the alignment is done by an automatic tool, the user is no influence. However the recipe settings (scan range, averaging) and the samples (dust, bow) introduce a limit in the accuracy of alignment. Hence we have a systematic error which needs to be taken into account.
Another source of error is the wavelength calibration of an instrument. Spectrometers for the visible and UV range are usually calibrated by using special calibration lamps (for HG or Ar gas) which produce a series of very narrow spectral lines. The standard spectrometers usually have limited spectral resolution (of about 1 nm) to have good sensitivity per channel. With this resolution the spectral channel position is derived from finding the top intensity position. It is typical that the accuracy of the calibration is at 10% of the spectral resolution and we have a typical error in spectral positions of 1 A.
Device errors do not only arise from statistical sources as the noise of intensities. After a device is calibrated during its installation at the user site, it may be moved to another location or operating the mechanics may decrease the tightness of mechanics slightly. If light sources are exchanged they need to be repositioned with limited accuracy and change the local intensity distribution of the beam used for measurement. Another effect is the temperature change in the ellipsometers environment. If the machine incorporates a waveplate (i.e. a biaxial element with a thickness of more than 100 µm), the retardance depends on the temperature and 0.1 degree difference cause a change the ellipsometric angles which is above the detection limit of the device. Even with thermal stabilization such elements cause a drift which is not zero. A third device error source is the limited accuracy in aligning the optical elements as polarizer prisms to the plane of incidence. These errors come from component imperfections, limited tilting accuracy and measurement noise during calibration. If the samples show local in homogeneities (as it is the case for rough solar cells) the device error should be set to the local deviation of Psi and Delta in the measurement spot area. All these effects together are depicted here as device errors.
The following values reflect the results obtained from measurements on many samples:

- $\delta\psi$=0.05° (combination of sample tilt and absolute offset calibration accuracy)
- $\delta\Delta$= 0.1° (combines the drift caused by light source changes and temperature changes)
- δR = 0.003 (caused by positioning accuracy between reference and sample as well as noise)
- δT = 0.003 (same as R)
- δs = 0.001 (Fourier coefficients, typical noise value plus several minor sources)
- $\delta\phi$ = 0.02° (Angle of incidence: sample alignment accuracy)
- $\delta\lambda$ = 1 A (Spectrometer calibration accuracy of spectrometer, see above)

Please note that all these errors are given as an estimate reflecting practical results while different ellipsometers (low cost to high precision) require adapted sets of error values. A reflectometer usually has no good tilt alignment (the angle of incidence error is higher in this case) and a NIR spectrometer based on an FTIR is far better in its wavelength scale since it counts the fringes of a HeNe laser. So update these values for a specific device.
The method for taking these error sources into account is a simple approach. For measured values, the effect of an error is primarily a shift in the values. A measured value of ψ, Δ, s, R or T within a certain spectral range is considered as a set of 5 spectra for each value:

- x[0] … x[N] – the original spectrum
- x[0]+δx … x[N]+δx – the original spectrum plus an offset
- x[0]-δx … x[N]-δx – the original spectrum minus an offset
- x[0]-δx … x[N]+δx – the original spectrum with a diagonal offset in plus direction
- x[0]+δx … x[N]-δx – the original spectrum with a diagonal offset in minus direction

Each of these 5 spectra gives a parameter set $p_k[i]$ after fitting. The original spectrum gives $p_0[i]$ and the shifted spectra give $p_k[i]$. The estimated error of a parameter is given as

$\Delta p[i] = \max (p_k[i]-p_0[i])$ for k=1..4 (offsets) and i=1..N (fitting parameters)

The same approach can be used to determine the refractive index and thickness of each material with variable parameters after each fit. These values for refractive indices and thickness (n,k,th) are $n_k[j]$m, $k_k[j]$ an $th_k[j]$ (j is

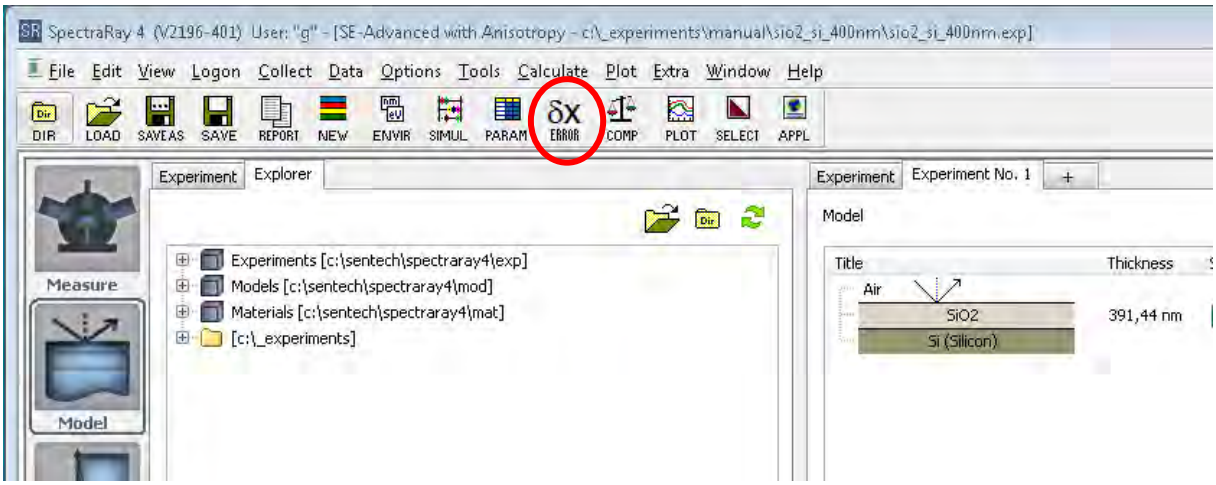
the layer number, k is the offset index). Hence we have the same formula as above to derive the stability of the refractive index at a selected observation wavelength for each material. The thickness is a parameter which is already a fitting parameter but in contrast to other parameters it is directly a stack parameter – others are elements of a dispersion relation and do not directly allow to understand the influence on the refractive index. An example of this may be the oscillator strength of the Drude-Lorentz dispersion, which influence the refractive index after complex calculation only. So it makes sense to apply the same error rule to the refractive index stack for easier understanding. In practice you can have the situation where the (n,th) is stable while the involved dispersion functions may show higher correlations. In such case the material properties are measured trustworthy despite the instabilities of the model. This is the reason to analyze not only the parameter set and to retrieve the errors of the refractive index stack as well.
While the approach given above only takes systematic errors of the instrument into account, it is easy to extend this to other sources of error. Here we take into account the tilting error (influences angle of incidence and mainly Psi) and the wavelength accuracy (important for thick layers). The process does the above calculations (4 with shifted values plus 1 with the original values) for the angle of incidence (ϕ-$\delta\phi$, ϕ, ϕ+$\delta\phi$) and wavelength (λ-$\delta\lambda$, λ, λ+$\delta\lambda$) as offset to the current values (i.e. an angle offset ($-\delta\phi$,0,+$\delta\phi$) and a wavelength offset (-$\delta\lambda$, 0,+$\delta\lambda$)).
The number of fits is then 1+4 3 3 = 1+36 = 37 (if all sources of error are taken into account.
After applying this approach there is a set of parameter errors $\delta p[i]$ and a set of refractive index errors $\delta n[i]$ and $\delta k[i]$. With these values additional tests may be applied:

- is the accuracy of a refractive index as expected by ellipsometry ($\delta n[i] < 0.01$)
- check if the thickness as accurate as expected ($\delta th_k[j]/ th_k[j]<0.01$ – i.e. 1 %)
- check if a parameter is correlated (error>20%)
- check if a parameter is too correlated an should not be fitted at all (error>50%)
- check if a parameter is after a fit at its maximum allowed range
- check whether the fitting process took too much iterations (i.e. the fit itself does not converge with the given number of maximum iterations)

All these considerations are taken into account and are used to derive helpful hints on whether the current modeling gives reliable results or not and which setting may cause instabilities. With this functionality it is recommended that any result of modeling should be approved by the approach given here. There are more useful and in detail more accurate models available to describe the influence of systematic errors, but in practice this approach depicts the real world precise enough. Since the approach is simple enough to be applied by any user it is considered a new helpful tool which adds a treatment of systematic errors to the method of correlation matrix handling statistical errors.

5.3.3 Description of the assistant tool

The assistant requires to load a combination of sample stack with some fit parameters and at least an associated measurement (ellipsometric or RT spectrum). Before entering the assistant verify that the fit will converge within the analysis window. If this test is successfully you may open the assistant by clicking in the “δx” icon in the toolbar (since SpectraRay is highly configurable the icon may be found at other positions in the toolbar). If there is no such icon, please update SpectraRay.



After opening the assistant will start the calculation automatically. If the settings are not correct, you may stop at any time (update and press "Go!" to restart the calculation). When the calculation is finished, you get an output like this (**100 nm oxide on silicon**):

Layer stack at 632.8 nm wavelength

Layer	Thickness	Refractive Index	Absorption	Comment
Air		1.0000		
SiO2 (Silicon dioxide) - therm.	105.3 +/- 0.1 nm	1.4645 +/- 0.0010	0	
Si (Silicon)		3.8717	0.0158	

Variable parameters of optical model (without thicknesses)

Name	Value	Error		Comment
SiO2 (Silicon dioxide) - therm.: N0	1.458	0.0012	0%	
SiO2 (Silicon dioxide) - therm.: N1	26.0	1.56	6%	

File: 02 - SiO2 100 nm on Silicon.recipe.xml

This shows a stable model with the typical output structure:

1. Layer stack showing values and errors of thickness, refractive index and absorption
2. Parameter list with value, absolute error and error in percent
3. Remarks section (in this case this is empty)

In the sample above the measurement is precise enough (green values in the model, no color in the parameter list, no comments and no remark section). This is typical for a 100 nm oxide on silicon.

Another **example shows a 20 nm oxide** with thickness and refractive index (Cauchy N0+N1) both fitted:

Layer stack at 632.8 nm wavelength

Layer	Thickness	Refractive Index	Absorption	Comment
Air		1.0000		
SiO2 (Silicon dioxide) - therm.	23.4 +/- 1.0 nm	1.4456 +/- 0.0413	0	lowered accuracy: δn>0.01
Si (Silicon)		3.8717	0.0158	

Variable parameters of optical model (without thicknesses)

Name	Value	Error		Comment
SiO2 (Silicon dioxide) - therm.: N0	1.431	0.0453	3%	
SiO2 (Silicon dioxide) - therm.: N1	59.8	16.30	27%	error > 20%

Remarks:

- SiO2 (Silicon dioxide) - therm.: N1 has 27% error
- SiO2 (Silicon dioxide) - therm. has lowered accuracy: δn>0.01

File: 09 - SIO2 20 NM ON SILICON.RECIPE.XML

Here we see that the accuracies are worse than expected by ellipsometry (yellow fields), but the results still make sense. Here we used a spectral range of 320 … 800 nm. However the situation changes, when the UV part is not used. The same sample within 600 … 800 nm spectral range gives:

Layer stack at 632.8 nm wavelength

Layer	Thickness	Refractive Index	Absorption	Comment
Air		1.0000		
SiO2 (Silicon dioxide) - therm.	22.7 +/- 1.4 nm	1.4726 +/- 0.0582	0	lowered accuracy: δn>0.01
Si (Silicon)		3.8717	0.0158	

Variable parameters of optical model (without thicknesses)

Name	Value	Error		Comment
SiO2 (Silicon dioxide) - therm.: N0	1.456	0.0756	5%	
SiO2 (Silicon dioxide) - therm.: N1	65.0	87.28	134%	error > 20% → it is recommended to uncheck this fit parameter

Remarks:

- SiO2 (Silicon dioxide) - therm.: N1 has 134% error → it is recommended to uncheck this fit parameter
- SiO2 (Silicon dioxide) - therm. has lowered accuracy: δn>0.01

File: 09 - SIO2 20 NM ON SILICON.RECIPE.XML

In this model we see an instability which is marked with red background and with a comment recommending a change. In the bottom the “Remarks” section summarizes problems and “ToDo” items.
A third example shows the output for a three layer model (Poly Si on oxide with surface roughness):

Layer stack at 798.0 nm wavelength

Layer	Thickness	Refractive Index	Absorption	Comment
Air		1.0000		
SiO2 (native) - cauchy	3.42 +/- 0.10 nm	1.4577	0	
P-Si (Polysilicon) - Leng-Lorentz	94.7 +/- 0.4 nm	3.7280 +/- 0.0124	0.0108 +/- 0.0015	lowered accuracy: δn>0.01
SiO2 (Silicon dioxide) - cauchy	100.0 nm	1.4577		
Silicon (100) (Jellison)		3.6826	0.0069	

Variable parameters of optical model (without thicknesses)

Name	Value	Error		Comment
P-Si (Polysilicon) - Leng-Lorentz: E1(inf)	0.0840	0.08120	97%	error > 20% → it is recommended to uncheck this fit parameter
P-Si (Polysilicon) - Leng-Lorentz: M0	-0.099267	0.0766171	77%	error > 20% → it is recommended to uncheck this fit parameter
P-Si (Polysilicon) - Leng-Lorentz: X0	2.334762	0.0278516	1%	
P-Si (Polysilicon) - Leng-Lorentz: K0	0.3159	0.04828	15%	
P-Si (Polysilicon) - Leng-Lorentz: C0(0)	309.252	4.3818	1%	
P-Si (Polysilicon) - Leng-Lorentz: Beta(0)	-0.61142	0.025484	4%	
P-Si (Polysilicon) - Leng-Lorentz: Eg(0)	3.6081	0.04653	1%	
P-Si (Polysilicon) - Leng-Lorentz: Gamma(0)	0.49388	0.020556	4%	
P-Si (Polysilicon) - Leng-Lorentz: My(0)	-0.793147	0.0604468	8%	

Remarks:

- P-Si (Polysilicon) - Leng-Lorentz: E1(inf) has 97% error → it is recommended to uncheck this fit parameter
- P-Si (Polysilicon) - Leng-Lorentz: M0 has 77% error → it is recommended to uncheck this fit parameter
- P-Si (Polysilicon) - Leng-Lorentz has lowered accuracy: δn>0.01

File: polysi_sio2_si.exp

A last example given here analyses a **reflectivity measurement on a 100 nm oxide** in silicon. The first step uses an accuracy of R of ±0.5%. This gives:

Layer	Thickness	Refractive Index
Air		1.0000
SiO2 (Silicon dioxide) - therm.	104.3 +/- 0.9 nm	1.4532
Si (Silicon)		3.8717

If we set the error of R to 0 and check only angle of incidence (0.5°) we get a thickness error of 0.002 nm (i.e. this sample is rather insensitive against the angle of incidence). If we do the same for 0.1 nm wavelength error we get a thickness error of 0.03 nm. This allows us to conclude that the main source of error is the absolute accuracy of the reflectivity reading. If all sources of error are combined we get the same 0.9 nm error for the thickness.
In the next step we will try to measure the refractive index as well. The refractive index is modeled by a Cauchy dispersion with nonzero N0 and N1 parameters. For determination of refractive index we use only N0. This results in the following:

Layer	Thickness	Refractive Index
Air		1.0000
SiO2 (Silicon dioxide) - therm.	104.3 +/- 1.2 nm	1.4532 +/- 0.0163
Si (Silicon)		3.8717

We see that the thickness accuracy is slightly lower. The refractive index is accurate enough to tell that we have an oxide (instead of nitride), but not sufficient to qualify the oxide itself. The result shows the well-known fact, that refractive indices are an order of magnitude less accurate compared to ellipsometry readings.

5.3.4 Sensitivity analysis

The above samples show the analysis of measurements. Another benefit is received in combination with the simulation. If a specific model is used, the simulation can theoretically calculate spectra for different spectral ranges (do we need DUV or NIR?) or multiple angles of incidence (which gives optimum sensitivity, is the multiple angle measurement required?). In combination with the simulation this tool can be used for sensitivity analysis (i.e. the error bars depending on varying experimental settings).

5.4 Simulation

5.4.1 Basics: Data types, Curves, Multicurves and Networks

The outputs of a measurement are data sets. Simulations are per definition theoretical experiments. Grouping the creation of data into measurements and simulations is the basic of any software dealing with spectrometry or especially with spectroscopic ellipsometry.
The following section describes the simulation part, necessary steps and types of output. A theoretical experiment starts with the setup of a sample. A sample is the theoretical description of a series of layers stacked onto a substrate. This setup is performed within the model editor, see chapter 0 “Modeling a sample” on information on this. After you set up the sample you have to set the environment. Any parameter which is not modified during the run of the simulation has to be set to desired values (for example angle of incidence). A detailed description on these settings is contained in chapter 5.2.6 “Environment”.
After sample (“model”) and environment are set up, you may want to perform a simulation. A calculation needs the following information:

Which physical quantity should be calculated (R, T,...)?
What parameters should be varied?
What type of curve is required (Curve, Multicurve or Network)?

Ellipsometry differs from spectroscopy a bit, because it measures two data at each angle or wavelength. All physical quantities used for calculation can be either pairs or single data. Classical pairs are (Ψ, Δ) and a typical single data is the reflectance R. If a single parameter p is calculated with the wavelength λ you have pairs of (λ, p). A (Ψ, Δ) pair calculated is stored as a triple (λ,Ψ , Δ). The results available in the simulation are listed in the table Tab. 5-14.

All parameters available in the model definition and within the environment can be varied. Typical parameters are the wavelength and a thickness. The current set of fit-parameters is visible if you open the summary on fit parameters (see

Appendix B: Icon reference).

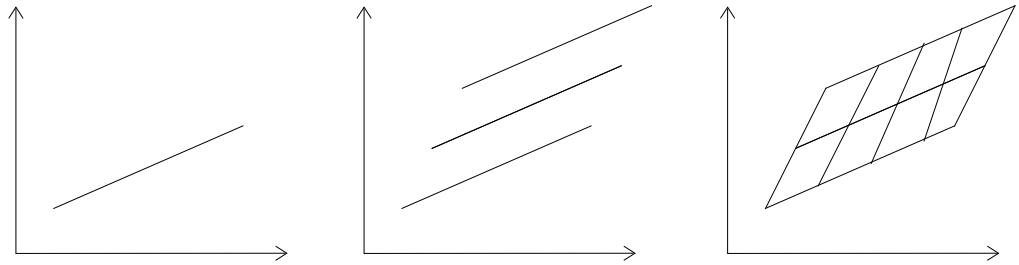


Fig. 5-125 Curve types: Curve (left), Multicurve (center), Network (right)

The third question defines the amount of data calculated. There are three types available:
Curves are a set of data created by varying one parameter from a start to an end value step by step. If you additionally vary a second parameter and go through the first each time you get a set of curves the **multicurve**. The third type creates a multicurve and changes the roles of curve and trace parameter to create a second multicurve. Combining both results a **network** is calculated.

Type	Name	Description
beam properties	Delta(Psi)	ellipsometric angles for 2D-plots Δ(Ψ), as for measurements with retarder
	Delta180(Psi)	ellipsometric angles for 2D-plots Δ(Ψ), but Δ<180° as for measurements without retarder
	CosDe(TanPs)	trig. functions of ellipsometric angles for 2D-plots cosΔ(tanΨ), the same with and without retarder
	Psi	ellipsometric angle Ψ
	tanPsi	trig. function of ellipsometric angle Ψ
	Delta	ellipsometric angle Δ, as for measurements with retarder
	Delta180	ellipsometric angle Δ, but Δ<180° as for measurements without retarder
	cos(De)	trig. function of ellipsometric angle Δ
	R	reflectance
	Rp	reflectance in p-direction (parallel to the plane of incidence)
	Rs	reflectance in s-direction (perpendicular to the plane of incidence)
	T	transmission
	Absorption	absorbance (A=1-R-T)
layer information	n(k) layer	n(k) 2D-plot, useful for EMA theory considerations
	n layer	refractive index of a layer
	K layer	absorption of a layer
	e1(e2) layer	$\varepsilon_1(\varepsilon_2)$ 2D-plot, useful for EMA theory considerations
	e1 layer	ε_1 of a layer
	e2 layer	ε_2 of a layer
scanner for fits	MSE-Diff.	calculates the least square difference between measured and calculated curves, see below

Tab. 5-14 Output values for simulations

All calculated data are stored within files or added to the actual data list:

1. The standard output is to a *.dat file for immediate display by the PLOT program.
2. Additionally the data can be stored in the same format as measurements *.dob.
3. If the calculated data should be used for fits or comparison you should add them to the data list.

5.4.2 Setting up and running a simulation

This chapter explains the settings and functions of the simulation dialog. On the top are two boxes containing parameters for curves and traces. On the bottom six checkboxes are used to setup the output of data. A “display” button directly views the last dataset contained (the corresponding file name is contained in the edit field labeled “Name of transfer file”). The functions of the checkboxes are explained in the table below.

Item	Function
Add simulated data to experiment	save the result of the calculation to the actual data listbox (in memory!)
Add line colors	additional commands for colors are added to the data output (ASCII, PLOT program format) to create different colors for the first curves in a multicurve or network
Mark first data	additional commands for colors are added to the data output (ASCII, PLOT program format) to add a marker to the first point of all curves
Overwrite transfer file	the output overwrites the current file, otherwise data are appended
Display data in plot module	runs the PLOT program with the current data file immediately after each simulation
Create *.dob-file	saves the next simulation to a file *.dob with the name taken from the output file (change of the extension only); if a network is calculated two typed data files *1.dob and *2.dob are created

Tab. 5-15 Checkboxes in the simulation dialog

5.4.2.1 Creating curves

A curve is the simplest type of data and needs one parameter varied within an interval using a step while all other parameters stay fixed. Typical applications are calculation of spectra or angle dependencies.
The simulation dialog displays all data necessary to create a curve, all other elements are hidden. If you cannot calculate a curve, set TYPE to “Net” and check, whether all parameters have correct values.
The example is to calculate a curve between 250 nm and 1000 nm and using a step width of 1 nm. The element “Curve parameter” must be set to “wavelength”. The unit “[nm]” depends on the unit settings within the environment. If “µm” was chosen “0.25” and “1.0” and “0.001” have to be used, respectively.

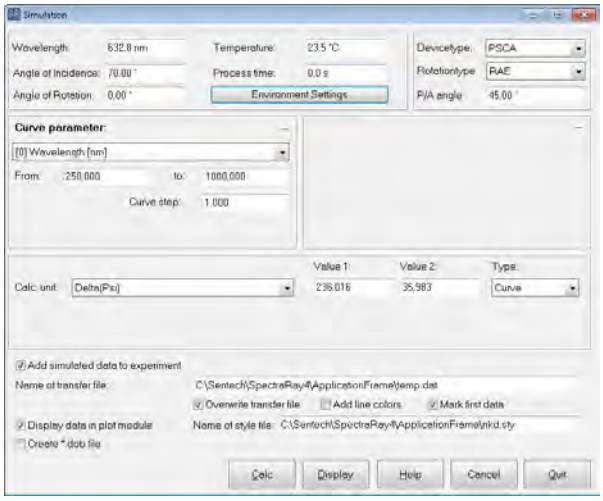


Fig. 5-126 Simulation: Curves setup

The calculation starts by pressing “Calc”. This causes the button to change to “Cancel”. Aborting a calculation is very useful if your step width would create too many data points or would take too much time. The progress is displayed during the calculation by a percentage bar allowing detecting long term calculations. After a simulation was successful the following things happen, depending on the flags listed in Tab. 5-15:

1. The output of data to the current output file is closed.
2. The data set in memory is added to the data list displayed in the main screen.
3. The same data are stored as a data object (*.dob) to load the calculated dataset later.
4. The PLOT program is run to display the ASCII output file.

These actions allow you quick views on spectra, using them as data input and comparing them with your measured data.

5.4.2.2 Retrieving layer information

If you defined a material by dispersion functions or by tables you may want to study the dielectric constant versus wavelength or other parameters. The curve/multicurve/network calculations allow you to study the influence of parameters to the dielectric constant.
The first example of using this feature is to compare two materials in its dielectric functions. It requires the calculation of n(λ) for two materials (k,ε_1,ε_2 is the same). Set up the simulation mask as visible in Fig. 5-127. This adds two elements to the dialog:

1. a listbox to select the material
2. an “edit” button to quickly edit the selected material

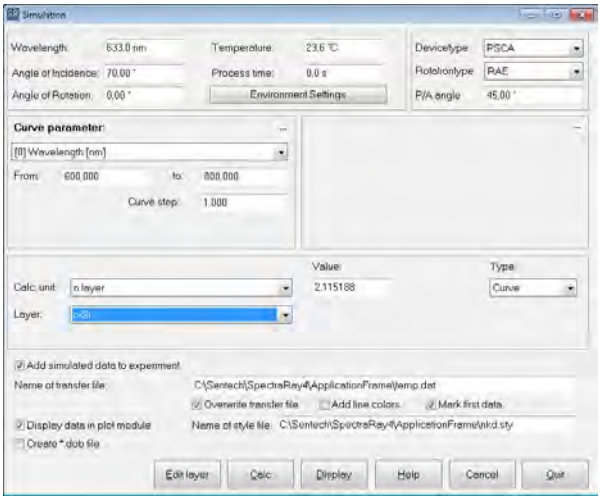


Fig. 5-127 Simulation: Retrieving layer information

You create a comparison between two materials as follows. First check the “Overwrite transfer file” box and select the first material. If you have an empty data list (1) check “Add simulated data to experiment”. Now select the curve parameters (example is shown in Fig. 5-127). Uncheck “Display data in plot module”, because the view of data is needed only after calculating the second data set. Press “Calc” to run the calculation. After this was successful you have the first data set and you have to append the second. Uncheck “Overwrite transfer file” and check “Display data in plot module”. This appends the following data and since the second data set is the last to be calculated the automatic data display is useful (the same function is achieved by pressing the button “Display” after the calculation has finished). Select the second material and rerun the simulation by pressing the button “Calc”. This creates the second data set and automatically runs the PLOT program with the ASCII file containing both data sets. This should display the two desired curves.

5.4.2.3 Multicurves

Many applications require calculating more than one curve. You can study how the thickness of a layer changes a spectrum or the angle dependency for different refractive indices (the angle dependency has the same importance for a single wavelength ellipsometer as the wavelength scale for a spectroscopic ellipsometer).
The following example for using a multicurve calculates the dependency of the ellipsometric angle Ψ from wavelength and angle. The results should be saved untyped to the output file for quick display and print-out. Additionally the created multicurve should be added to the data list.
Multicurves consist of several curves. The parameter varied within each curve is the "Curve parameter". The second parameter fixed during the calculation of each curve and changed from curve to curve is the "Trace parameter". The step width of the curve parameter makes the number of points in each curve and the step width of the trace parameter is responsible for the number of curves. The example in Fig. 5-128 creates 5 curves each of 201 data points.

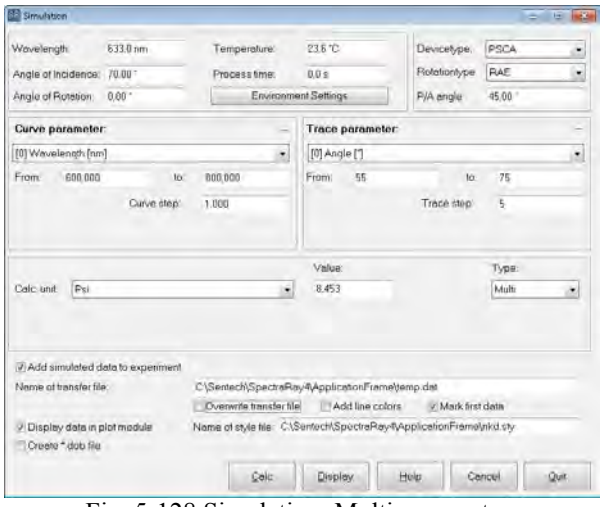


Fig. 5-128 Simulation: Multicurve setup

The flag "Add simulated data to experiment" is checked to save the results to the data list displayed in the main screen. "Add line colors" should be checked if you want to see the first curve (55°) in a different color. "Mark first data" is used to mark the first point of a curve (600 nm). "Overwrite transfer file" is important to avoid a display mixed with old data. "Display data in plot module" starts the PLOT program immediately after the calculation has finished successfully. Since the data are saved in memory ("Add simulated data to experiment"), no data object file is needed ("*.dob"). After pressing the button "Calc" the calculation is started and the multifile is displayed within the plot program.
If you want to see the colors in the PLOT program uncheck "Black and White" in its "Option" dialog. For output to black and white printers the flag easily converts colors to a black and white scheme.

5.4.2.4 Networks

The calculation of networks is a task mainly used for single wavelength ellipsometers, where single measured points compared with plots in the (Ψ,Δ)-plane give more information on accuracy and separation of parameters than numbers calculated.
The support for networks is still needed since this software package covers all ellipsometric devices from the SE400adv series (discrete wavelength) to the SENresearch family.
A network is the superposition of two multicurves, where the roles of the curve and trace parameter change. The dialog display needs therefore two additional steps width. The curve parameter acts during the calculation of the second multicurve as the trace parameter and needs a "Trace step", greater than the "Curve step". Just the opposite is for the trace parameter, it acts as the curve parameter for the second multicurve and needs an additional "Curve step", smaller than the "Trace step".
The output to the file changes for networks: A network is the parametric plot in the result plane. If (Ψ, Δ) pairs are calculated, the x-axis is ψ and the y-axis is Δ. For (ε_1, ε_2) the x-axis is ε_1 and the y-axis is ε_2. When only a single value is calculated a network is senseless.

The output “Add simulated data to experiment” saves in all cases the two multifiles calculated and the same applies for the data object output (see Tab. 5-15) “*.dob”.

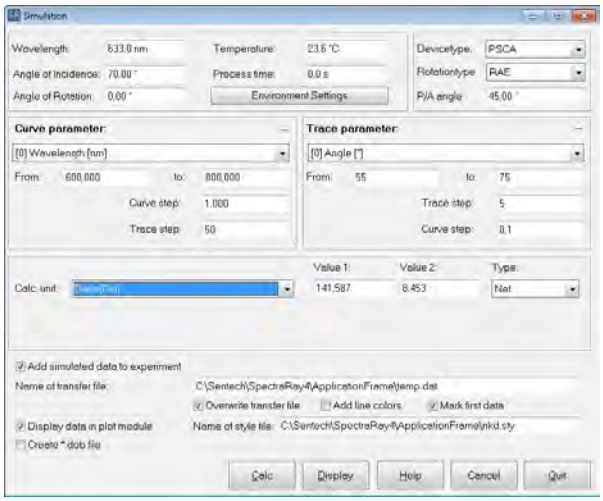


Fig. 5-129 Simulation: Network setup

In Fig. 5-129 the settings for steps are demonstrated. An application should set the output file to an appropriate name (if the path used does not exist or the file name is invalid, no calculation is performed).

5.4.2.5 Scanner for start values

The simulation contains a built-in scanner for fit assistance. In many situations you have an unknown sample and have no guess which thicknesses (or other parameters) belong to these samples. In this case you would manually test a set of hypothetical parameters by changing the model and comparing theory and measurement. This is needed for example for the SIMOX problem, where the dependency of the spectrum is very sharp for different thicknesses and even a difference of a few nanometers could cause large deviations between theory and fit. So the manual search for good start values is required but deadly boring and much time consuming.
The idea of the scanner is to automatically check a series of parameters, always calculate the theoretical data sets and the resulting figure of merit and to save these data the same way as for other parameters. Doing the automated scan is still time consuming, but enables the operator to do other things meanwhile.
The scanner function of the simulation requires a valid model and valid data. This means the ranges of the data must be in the ranges allowed within the environment, must have valid unit types and much more. If any of the conditions fails you will get an error message “Cannot create fit ...” during the start of the simulation dialog.
The handling of the scanner is the same as for a calculation of (Ψ, Δ)-pairs. You have to select “MSE Diff.” from the “Calc unit” list. MSE is the abbreviation for Mean Square Error.

The least squares are the basis of the figure of merit. In the case of a set of (Ψ, Δ)-pairs it becomes:

(31) $$MSE = \sqrt{\frac{1}{2N}\sum_{i=1}^{N}\left\{\left(\frac{{\Psi_i}^m - {\Psi_i}^{th}}{\delta\Psi}\right)^2 + \left(\frac{{\Delta_i}^m - {\Delta_i}^{th}}{\delta\Delta}\right)^2\right\}}$$ figure of merit for a single data set consisting of a number of N Ψ values and the same number of Δ values.

The values δΨ and δΔ are the errors of your measurement as given within the environment settings. Similar expressions are used for other measured data types as s1 and s2. If you have an experiment with multiple data sets the formula is extended by a weighing factor for each data set (see data editor page “title”).
For a more general discussion of the MSE value see chapter 5.6.1.

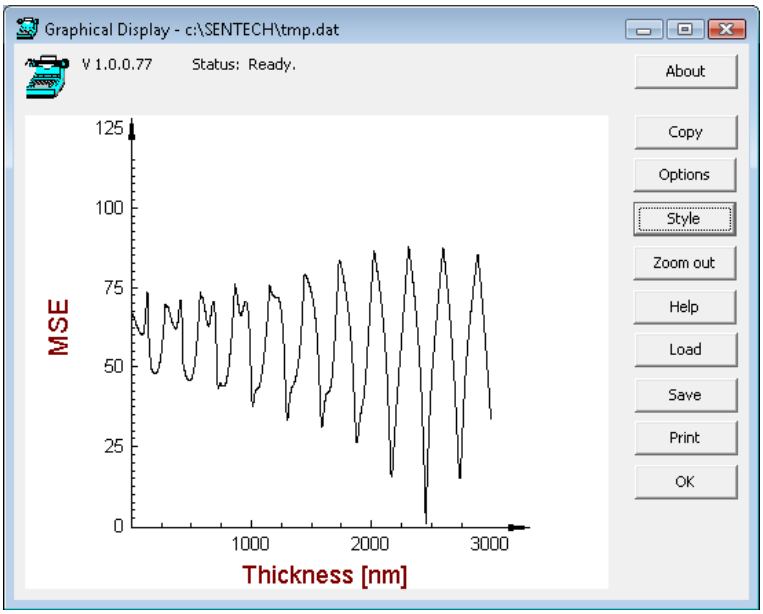


Fig. 5-130 Scanner example: 2.45 µm silicon dioxide on silicon

The example illustrated in Fig. 5-130 bases on a multiple angle measurement made on a SE400adv single wavelength ellipsometer. The sample was a thick thermal oxide on silicon. For maximum accuracy 100 angles were measured (40°...90°, step 0.5°). The refractive index was fixed to 1.46 because this would be a good guess for a thermal oxide. The calculation of the FOM was carried out in the range 0...3000 nm by using the scanner. A sharp minimum was found at 2450 nm, no other local minima have sufficient small MSE's. This indicates 2450 nm is a good guess for the thickness.

5.5 Data sets

5.5.1 Basics

Data sets play an important role within SpectraRay. Measurements and simulations are stored as data sets. A broad support of the import of data from other sources is included to convert other data to SpectraRay data sets. What is a data set in SpectraRay? Each time you measure a spectrum you generate a series of measured values y_1, y_2,... at a series of x-values x_1, x_2,... where the y-values belong to the z-axis z_1, z_2,... Typical examples of the x-, y-, and z-axis are the wavelength, the ellipsometric angles and the angle of incidence. The z-axis of a dataset makes up a table of data where the x-values are the rows and the z-axis creates columns filled with y-values. Each column has a set of header information (unit type, z-value etc.). This allows combining all types of measurement in one data set if the x-axis fits each other.

Many ellipsometers create evenly spaced data sets. SpectraRay supports both evenly spaced and none evenly spaced x-axis types. For example if you convert an evenly spaced spectrum in nanometers to electron volts, the x-axis can no longer be evenly spaced. This would generate additional points on the right and fewer data points on the left if interpolation would be used. For avoiding such problems an x-axis is introduced anyway.

SpectraRay is designed for supporting the full spectral range from ultraviolet to the far infrared. For measurements in the infrared the x-axis needs special enhancements. Since all polarizers available in the far infrared show absorption bands, each measurement contains intervals, where the information is invalid because of polarizer absorption. These intervals have to be excluded from the fitting routine to avoid bad fitting behavior. SpectraRay supports x-axis inclusion and exclusion intervals for support of such absorption bands.

Each measurement was done under certain conditions as there are wavelength, angle of incidence, time and temperature. These values overwrite at fitting sessions the environment values. This set of parameters, the internal "environment", may interfere with the x- and/or z-axis. In these cases the x-axis overwrites the internal "environment":

Fig. 5-131 Overwrite sequence for environment settings

If the x- and z-axis have the type "none" (see below) the internal environment is used, otherwise it is temporarily overwritten (from single columns).
The file representation of all this information is the *.dob (data object) format. The same format is used to store combinations of models and data to experiments (*.exp). The automatic import "*.spc" files interprets the type information contained in the "*.spc" files and creates the relating header information. Since the SPC files cannot contain all header information, some information are lost if you save a data set to the SPC format: z-axis type, columns selection, x-axis intervals. Most measurements are stored within the SPC format because the above limitations do not apply for measured data sets. Only if they are fitted you may want to change the default settings and you should save your desktop to experiment files then.

Limitations: A dataset can contain a maximum of 4 million data. The number of columns is limited to a maximum of 200.

5.5.1.1 Header information

Each data set consists of one or more columns containing the same type of data in each column. The description of each column is contained in the column header. The header consists of six elements:

Element	Type	Description
Color		displays the color used for plots
y-axis	selection	type of data stored in the column
z-axis	selection	type of z-axis
z-value	value	value of the z-axis
Use	flag	use this measurement for display and fit
View	flag	display this column during fits (if selected)
Mod	flag	reserved (currently fits the modulation instead of absolute values)
Minimum	value	minimum value of y-axis
Maximum	value	maximum value of y-axis

Tab. 5-16 Header of data sets

The “y-axis” describes the type of data stored in the column. A (Ψ, Δ)-spectrum has two columns, “Psi” and “Delta”. The z-axis is per default the angle of incidence (SPC-import, otherwise “none”). The z-value is needed if the z-axis is not “None”. For example if the z-axis is the angle of incidence the value of the angle is stored in this element.
Very important is the “Use” flag. It allows to use/not to use single columns during fitting sessions. If you have complicated samples it will be difficult to understand a full spectrum on the first try. It is much simpler to find parameters fitting a Ψ-spectrum only than the full (Ψ, Δ) combination. The “Use” flag allows you to disable columns during displays and fits of data without changing your data set. A consequence of this feature is a drastically reduced number of “working” files and increased speed.
The last flag “Mod” is reserved for future support of fitting derivations of spectra.

5.5.1.2 Unit types for x-, y- and z-axis

Now the header elements are explained. The x- and z-axis base on the same set of types listed in the following table:

Label	Description
“Wavelength”	wavelength in nm
“eV”	photon energy in eV
“Wavenumber”	Wavenumber in cm^{-1}
“Phi”	angle of incidence
“Theta”	sample rotation around the normal to the surface
“TimeSec”	process
“Temperature”	temperature
“None”	no selection
“Simulation”	calculated by simulation, but no basic type
“PolaPos”	position of polarizer

Tab. 5-17 Types of x- and z-axis

Label	Description
“Reflectivity”	reflectivity
“Transmission”	transmission
“Psi”	ellipsometric angle Ψ
“Delta”	ellipsometric angle Δ
“TanPsi”	ellipsometric angle ψ as tan Ψ
“CosDelta”	ellipsometric angle Δ as cosΔ
“Delta180”	ellipsometric angle Δ in the range 0..180°, as measured without retarder
“Psidelta”	
“Psidelta180”	
“Tanpsi_cosdelta”	
“Mat._refractive_index”	refractive index
“Mat_absorption”	Absorption coefficient
“TimeSec”	process time
“None”	untyped
“Epsilon1”	e1 of a material
“Epsilon2”	e2 of a material
“Temperature”	process temperature
“Absorption”	absorption
“Nk”	
“E1,e2”	
“Reflec_p”	p-reflectivity (parallel to the plane of incidence)
“Reflec_s”	s-reflectivity (perpendicular to the plane of incidence)
“Simulation“	calculated by simulation, but no basic type
“S1”	Fourier coefficient S1
“S2”	Fourier coefficient S2
“S1c”	Fourier coefficient S1 (with compensator)
“S2c”	Fourier coefficient S2 (with compensator)
“S1, s2”	
“S1p, s2p, s1c, s2c”	
“Polgr”	degree of polarization
“R, t”	
“Intensity”	Intensity of light
“Transmission_p”	p-transmission (parallel to the plane of incidence)
“Transmission_s”	s-transmission (perpendicular to the plane of incidence)
“M11” … “M44”	16 Mueller matrix elements
“Retphase”	Phase of the retarder
“Retaxis”	Axis of the retarder

Tab. 5-18 Basic data types (y-axis)

The selection of the types can be made on the header page of the editor, see chapter 5.5.2.4 for more information.

5.5.2 Editing the data

The data editor is available by double clicking a data set or using the menu. It allows changing any of the elements contained within a data set. It consists of several pages each for editing a certain subset of information.

5.5.2.1 Graphical View

The graphical view allows a quick overview on all data actually used for fitting sessions. It displays only the columns selected on the header page. It allows interactive operations on single curves: Smoothing, erasing spikes, deriving data and managing x-regions.

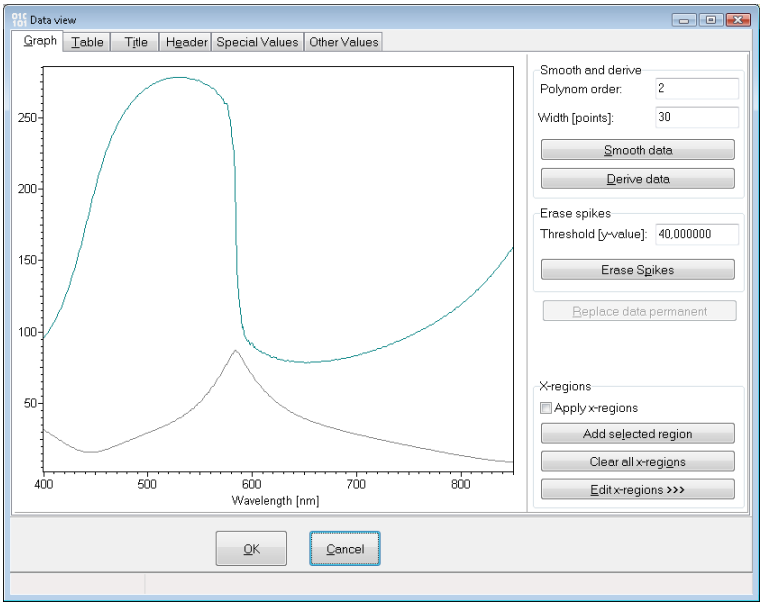


Fig. 5-132 Data editor view page

A useful function is the zooming. You can use your mouse to zoom into your data by clicking into the plot area and dragging the rectangle you want to zoom in. After releasing the left mouse button the picture is redrawn in the new (zoomed) range. You return back to the original floating point window by clicking and releasing the left mouse button without dragging a float rectangle.
The viewer is capable to draw any number of data available to load into the memory of your computer; progress info is displayed when redrawing larger data sets. The colors used are listed on the header page of this editor. You can change these colors as explained in Appendix E: Color setup.

Note: Smoothing, deriving and erasing spikes works with up to 4095 data points, otherwise the trim function should be used to reduce the amount of data.

5.5.2.1.1 Smoothing

A typical problem with measurements is the noise. This can be caused by bad measurement conditions or wrong settings used. Often the measurement cannot be repeated because the device is busy by other operators or there is not enough time.
In all these cases a smoothing operation is very helpful. The smoothing routine of SpectraRay bases on polynomials smoothing pieces of a spectrum. Polynomials are very powerful when applied to sufficiently small intervals. This is the same as expanding the analytical function by a Taylor series to a N-th order and reducing the residual by selecting appropriate intervals around the development point.
For applying this method a polynomial and the interval must be defined. The polynomial requires only the input of the polynomial order N (the coefficients are calculated). Since the dataset consists of points a number of points W (Width) is used to define the x-interval used. The method starts on the left of the spectrum and calculates the least square fitted polynomial for the first W points. Calculating the polynomial for the first W/2 points gives the first W/2 smoothed points. Then the interval is shifted 1 point right and the procedure is run again. The

polynomial is calculated at the middle of the interval and gives the W/2+1 smoothed point. The procedure repeats until the interval reaches the most right data point and the last polynomial gives the last W/2 smoothed points. This procedure has the advantage, that no W/2 data remain unsmoothed at the left and right. The smoothing power is contained in the ratio of N to W. For the SER 800 typical values are N=3 and W=30.

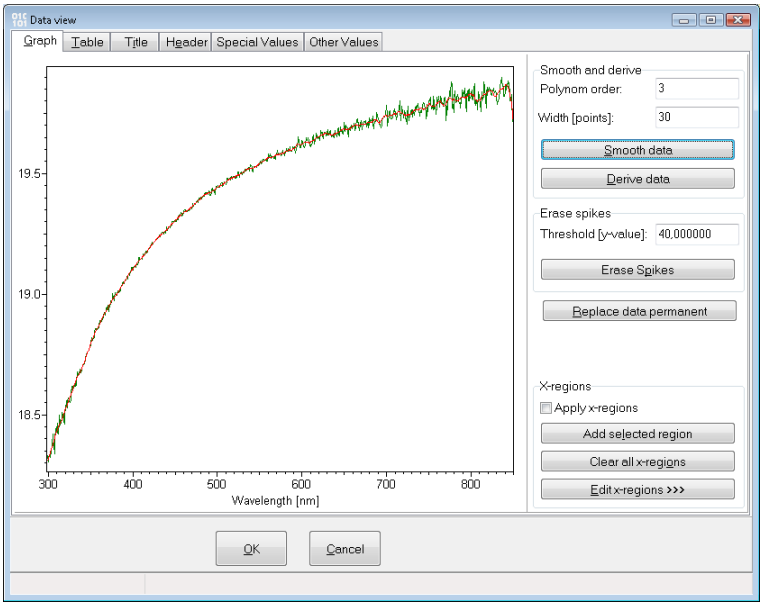


Fig. 5-133 Smoothing data

A smoothing session is done by selecting the order of the smoothing polynomial, the number of data points the polynomial uses and pressing “Smooth data”. The result is displayed as red curve in the plot. If this theoretical curve is good, you can press “Replace data permanent” to copy this smoothed curve to your data set. Otherwise you can change order and width and rerun the smoothing to improve the results.
If you have a smooth curve with single peaks in it, a single smoothing session may not give good results. You can use the x-regions to exclude the peak-area and run the smoothing with settings valid for the plain part of the curve and replace these data. When you change the exclusion interval to the peak area only you can smooth this part of the curve individually.

A special function is contained, when the number of points used for the smoothing is larger than half the number of points of the data set. In this case the whole curve is fitted by a single polynomial (you can read the number of points from the “Title” page of the editor) and the coefficients are displayed in a message box. The formula of the smoothing polynomial is:

$$p(x) = \sum_{i=0}^{N} C_i x^i \qquad (32)$$

C0 is the constant, C1 the linear and C2 is the parabolic coefficient. This allows you to “abuse” the smoothing for your own regression purposes.

It is recommended to avoid larger orders (N>10) because a polynomial regression calculates powers of 2N of each number ($x^{2N}<10^{4192}$!).

The spike reduction and smoothing always process only a single curve. If you selected more than one curve (header page: “Use” flags), the last selected column is used for smoothing and spike reduction.

5.5.2.1.2 Erasing spikes

Sometimes a spectrum contains so called spikes. This occurs when the signal noise creates virtual degrees of polarizations larger than 1. Ψ and Δ are not defined in this case and set to default values. The same occurs when a set of data is taken under weak intensity conditions.
A spike is in this understanding a drastically increased noise of measured data in a limited area. Spikes are treated as illegal data and the replacement of these illegal data is the linear average of the last W points extrapolated to the invalid point. Since the spike is defined by the increase in the noise, a threshold is required to separate good and bad points. A threshold aware method looks for points which differ from their neighbors more than allowed. If this is the case the above extrapolation method replaces the "wrong" data point.
Starting this method is critical because the left and right portions of a spectrum contain the most signal noise and the most spikes. This would lead to fail the extrapolation and a totally senseless result would appear. For this reason a noise analysis is executed prior to spike elimination to determine an appropriate starting point and working directions.
The spike reduction and smoothing always process only a single curve. If you selected more than one curve (header page: "Use" flags), the last selected column is used for smoothing and spike reduction.
For removing spikes you should set the threshold value to the difference between spike values and spectrum. Press "Erase spikes" to run the calculation. After this is finished, a red curve displays the result. If it is ok, press "Replace data permanent" to copy the result to the data set. Otherwise you have to change the settings and retry again.
It should be mentioned that the original data are unchanged until you press the "Replace data permanent" button. Don't forget to save the changed data set if needed!

5.5.2.1.3 Deriving curves

Derivations of spectra are used for example for critical point analysis of semiconductors. SpectraRay does not support this analysis in the current version but allows calculating derivations of data sets.
This problem is very close to the smoothing of data. Any measured spectrum contains a certain amount of noise, so that the classical discrete derivation

$$y'(x_i) = \frac{y(x_{i+1}) - y(x_i)}{x_{i+1} - x_i} \tag{33}$$

produces large amount of noise in the derivation and is no longer of use. This comes from the fact that the measured data are no analytical functions. The solution of the problem is very close to the smoothing. Because at each data point the result of the smoothing is a polynomial of the order N its derivation can be calculated easily:

$$y'(x_i) = \sum_{i=1}^{N} iC_i x^{i-1} \tag{34}$$

The procedure and parameters are the same as for smoothing. You should keep in mind that you have to change the data type to "None" if you replace the original data column with the derived curve. Otherwise the fitting procedures could show unpredictable behavior.

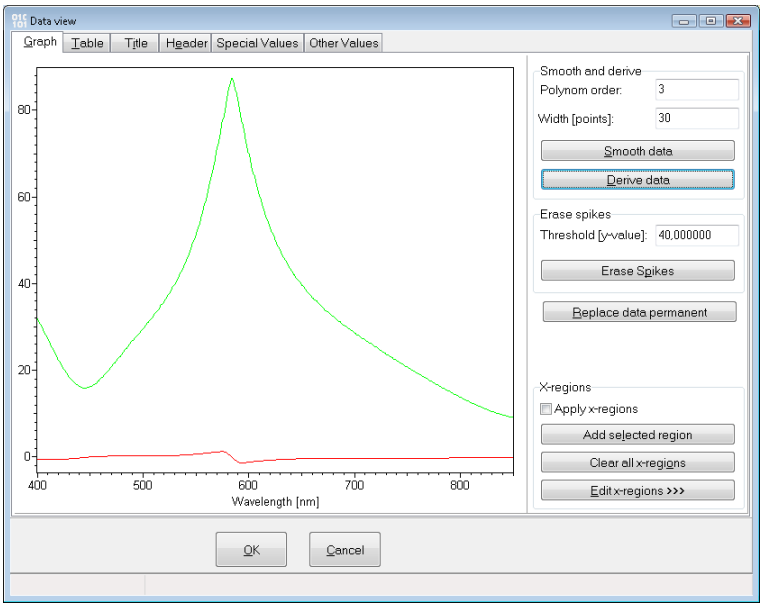


Fig. 5-134 Deriving spectra: example data set and derived spectrum (red)

5.5.2.1.4 Applying x-regions

An x-region is an interval definition with include or exclude functionality. The reason to include this feature into SpectraRay is the support for the infrared. Ellipsometers in the infrared have the same basic configuration as within the UV/VIS but use other components. One of the most critical components is the polarizer, often a metallic wire grid created from an evaporated metal on a polymer film, the grooves created mechanically. The substrate material polymer always contains certain absorption bands. The ellipsometric spectra cannot be measured at these bands, because absorption causes weak (or no) intensity. This causes spikes or illegal values for the ellipsometric angles in the data sets. Since the polarizers are the same for each measurement these bands should be removed automatically. The basis for removing bands is the definition of intervals. All these intervals make up the list of absorption bands (in the application for IR-ellipsometers).

SpectraRay data sets store a list of such interval definitions. Moreover a flag is used to indicate the usage of the interval definitions (i.e. the x-regions). The editor for these x-regions is contained in the graphical viewer. There are two ways to create a list of intervals:

1. Zooming the desired interval
2. Manually editing the list or loading it from a file.

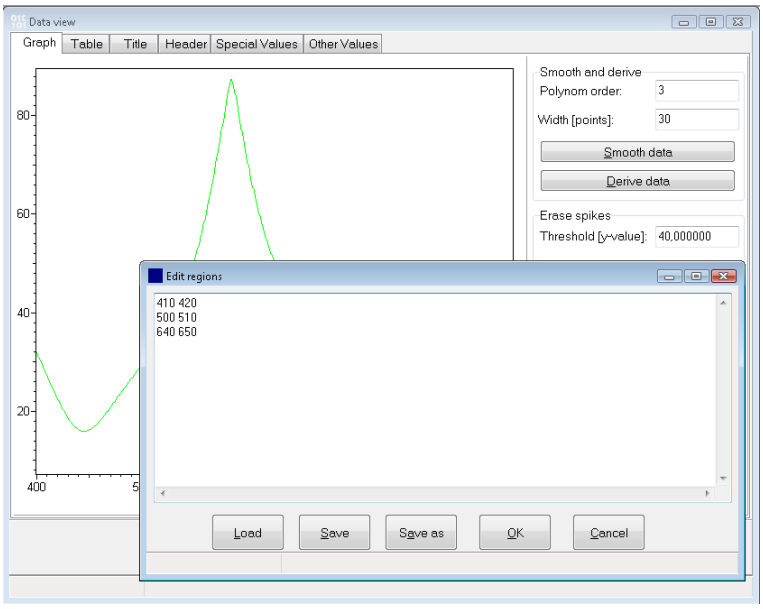


Fig. 5-135 Editing the interval list by using the ASCII editor

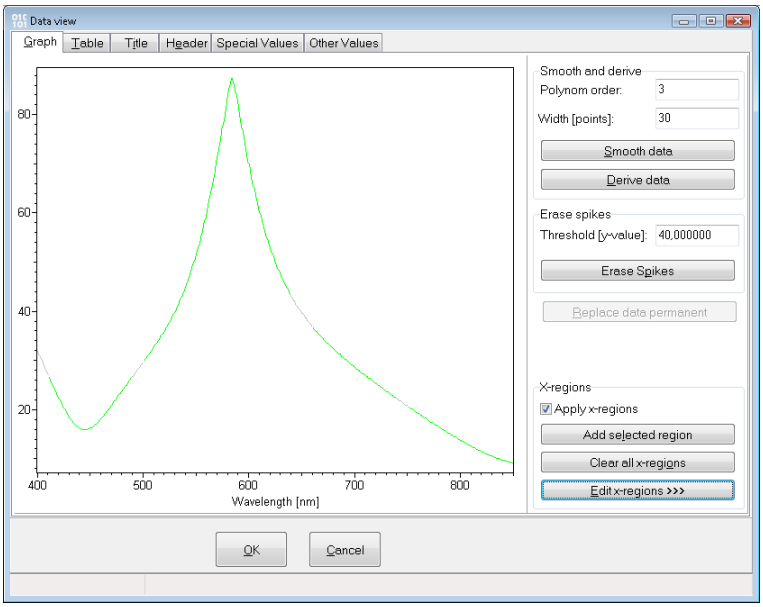


Fig. 5-136 Data points within x-regions are displayed grayed

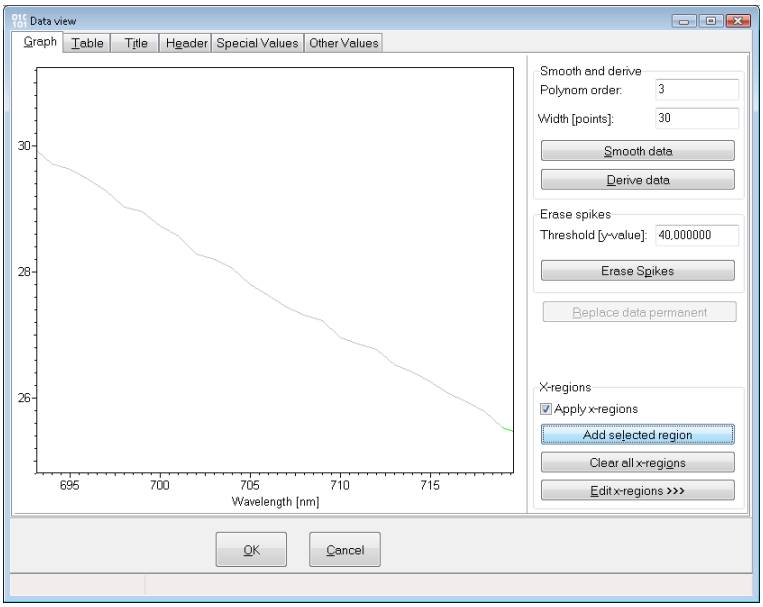


Fig. 5-137 A zoomed interval can be added to the x-region list by “Add selected region”

The first method uses the zooming of the plot window. You use your mouse to zoom into your data by clicking into the plot area and dragging the rectangle you want to zoom in. After releasing the left mouse button the picture is redrawn in the new (zoomed) range. If you press “Add selected region” the current x-interval is added as an exclusion region to the list. After you added the interval (or if it was wrong and you did not add it) you return back to the original floating point window by clicking and releasing the left mouse button without dragging a float rectangle. This sequence is repeated until you set up all intervals.
The second method could be used if you have predefined intervals. As you see from Fig. 5-135 the editor contains “Load” and “Save” buttons. This allows saving or loading predefined intervals.
A second application of x-regions is smoothing, erasing spikes and calculating derivations. The replace button copies only (!!!) the values not excluded to the original data. This allows individually processing each part of a curve.

The x-region definition written in files for predefined intervals can contain inclusion or exclusion regions. Each region is defined in a single text line following this syntax:

[“[+]” | “[-]”] <start> <end>

The “[+]” or “[-]” prefixes are optional and define the interval to include or exclude data. If you want to use only a small interval you should combine an exclusion interval of the whole data range followed by an inclusion region of the interval you want.

The definitions of the x-regions apply to the following things:

- display in the graphical editor
- calculation of the figure of merit

If an interval influences the fit depends on:

1. the interval defined in the environment reduces the set of data first
2. if a column is not used, it does not influence the fit
3. if the remaining data points still are valid the x-regions are checked

5.5.2.2 Editing the data table

The second page of the data editor views and edits the data. The first column is the x-axis and the following contain the y-data. If you edit the data changes are stored immediately after leaving a cell.
If a large number of data is displayed (many columns) an hourglass indicates the activity.

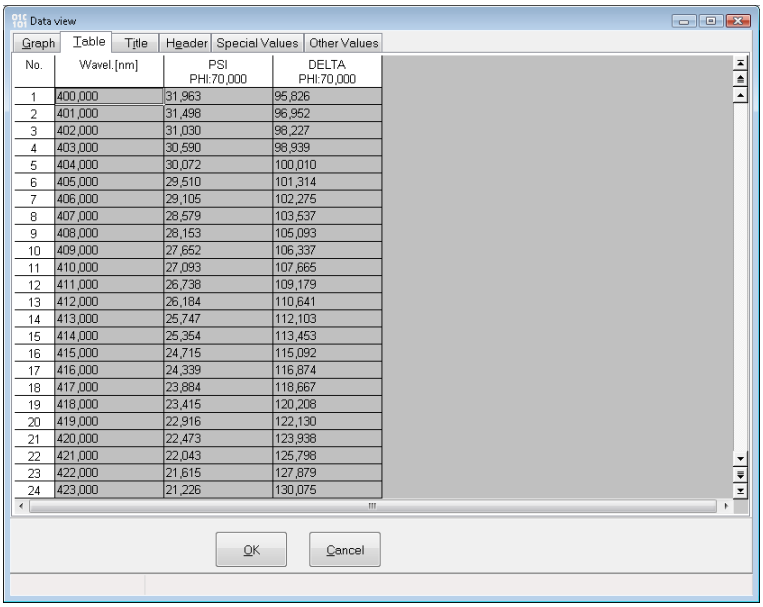


Fig. 5-138 Data editor table page

If you want to change the x-axis for evenly spaced data sets see the “Title” page of the data editor. The x-axis of a non-evenly spaced data set cannot be changed (except by exporting it to ASCII, changing and re-importing).

5.5.2.3 Title

A data set contains additional information on the measurement. This covers the name of the measurement (displayed in the data set list, the default for non-"*.dob" files is their filename), user name, date, time as strings (255 characters). A multiline comment can contain up 10000 characters.

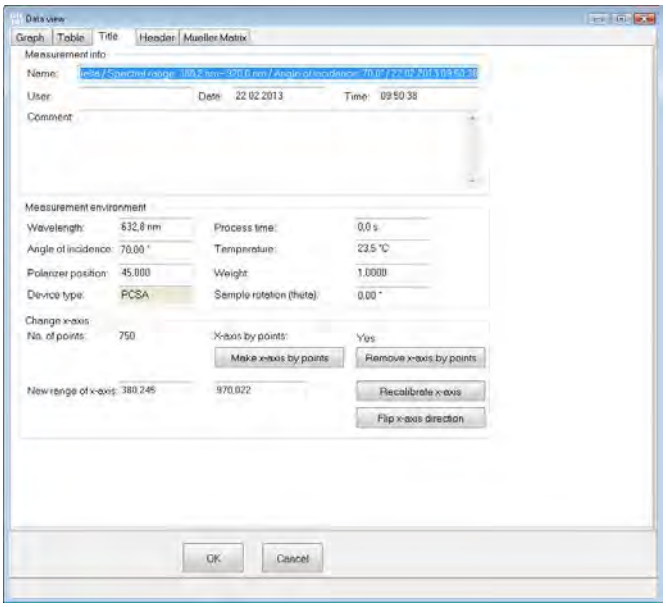


Fig. 5-139 Data editor title page

This page additionally contains the measurement environment. The four values for wavelength, angle of incidence, temperature and process time are needed to fix the parameters NOT defined in the x- and z-axis.

Some of the measurement settings like polarizer position, sample rotation and device type are saved here too. These values may be useful for later analysis.

The information on the number of data points (i.e. rows) is useful for the smoothing section where a maximum of 4095 data points is required. If you have more you can read it here. If the data set is evenly spaced the flag "x-axis by points" shows "no" otherwise "yes".
The x-range of evenly spaced files can be changed if you edit the two fields at "Range of x-axis". A special function is the button "Flip x-axis direction" which exchanges the minimum and maximum values for the x-axis.
If the x-axis is non-evenly spaced the x-axis cannot be edited.

5.5.2.4 Header

This page edits the column headers mentioned in chapter 5.5.1 and the x-axis type and contains an extensive trim function.

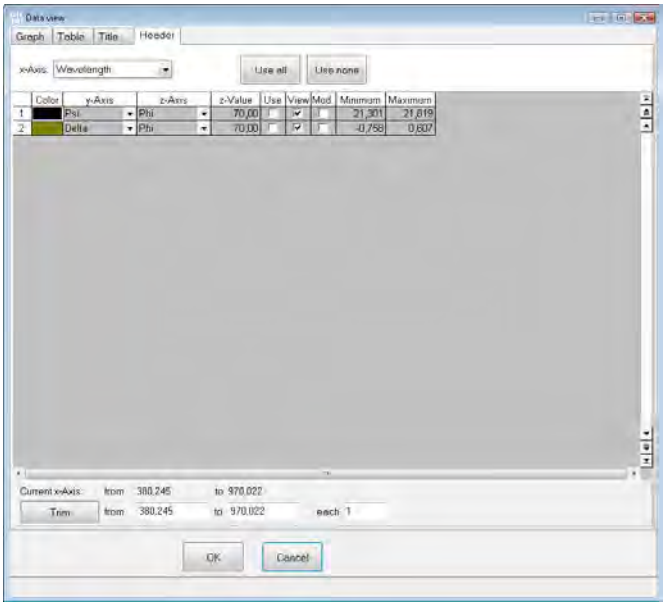


Fig. 5-140 Data editor header page

The x-axis type is selected by the first combobox. If you change this type two possible functions are executed. If the types are similar, only the label is changed. Otherwise a calculation is executed. For example for converting "eV" to "wavenumber" a multiplication is needed. If "eV" is changed to "nm" the density of points on the x-axis changes. Such calculations need additionally a non-evenly spaced x-axis inserted. If only a label change is necessary, you are prompted to confirm the label change.

	Phi	eV	none	Theta	Sim	T	t	nm	cm^{-1}
Angle of incidence (Phi)	--	l	l	l	l	l	l	l	l
Energy [eV]	l	--	l	l	l	l	l	cx	c
none	l	l	--	l	l	l	l	l	l
Sample Rotation (Theta)	l	l	l	--	l	l	l	l	l
Simulation (Sim)	l	l	l	l	--	l	l	l	l
Temperature (T)	l	l	l	l	l	--	l	l	l
Time (t)	l	l	l	l	l	l	--	l	l
Wavelength [nm]	l	cx	l	l	l	l	l	--	cx
Wavenumbers (cm-1)	l	c	l	l	l	l	l	cx	--

Tab. 5-19 Conversion rules between x-units: l - only label change, c - additional calculation, x - force creation of a non-evenly spaced x-axis

The central element of this dialog is the column header table. It contains the header elements as columns and the data set columns as rows. Important are the two comboboxes for y- and z-types. The usage flag is very important for fits and displays (see chapter 0 for selecting data).

The y-types and their explanation were already listed in Tab. 5-18. Changing the y-types again has double functionality: The type label is changed and - if possible - appropriate calculations are executed. Calculations are possible for the ellipsometric angles as listed below.

From	To
Psi	tan(Psi)
Delta	cos(Delta)
Delta180	cos(Delta)
Delta	Delta180
tan(Psi)	Psi
cos(Delta)	Delta180

Tab. 5-20 y-type conversions with calculations

If the change in the y-type does not follow Tab. 5-20 you are prompted to confirm the conversion:

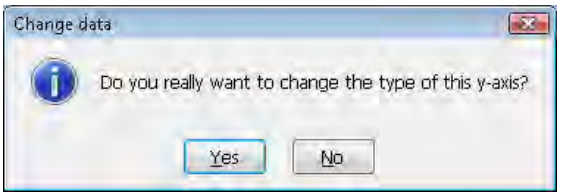


Fig. 5-141 Prompt before changing an axis type

The other fields of the table do not require more explanations (see Tab. 5-16 Header of data sets). The z-Value is displayed only, if the type of the z-axis differs from “none”.

The two buttons “Use all” and “Use none” are useful for selecting columns: “Use all” checks all “Use” flags and “Use none” resets them. These buttons are very convenient for multiple angle spectroscopic measurements.

The remaining fields on the bottom are used by the trim function. See chapter 5.5.2.5 for more information.

5.5.2.5 Trimming of data

The trimming of data is a very important function for any application. It is the tool for the following purposes:

1. clipping noise from borders of the measured interval
2. selecting only special columns from a large data set
3. decreasing the number of data points

This list of functionality requires several settings, which are located on the data editor's header page (see Fig. 5-140). The first item "clipping" requires the intervals of the clipped data set. Default values are the whole x-axis range as displayed in the two edit fields on the bottom of Fig. 5-140.
The second influence on the clipping is the column selection in the header table. If the "Use" flag of a specific column is checked the column is copied to the clipped (new) data set, otherwise the column is not copied. When you use the data select dialog (see chapter 0) you can trim for example all "Psi" columns from a multiple angle measurement for 3D-display.
Decreasing the number of points is achieved by not copying every data point but each N-th point.

5.5.2.6 Mueller matrix page

In Fig. 5-142 the Mueller matrix page of the data editor is shown. This tab is only visible in data sets containing Mueller matrix elements.

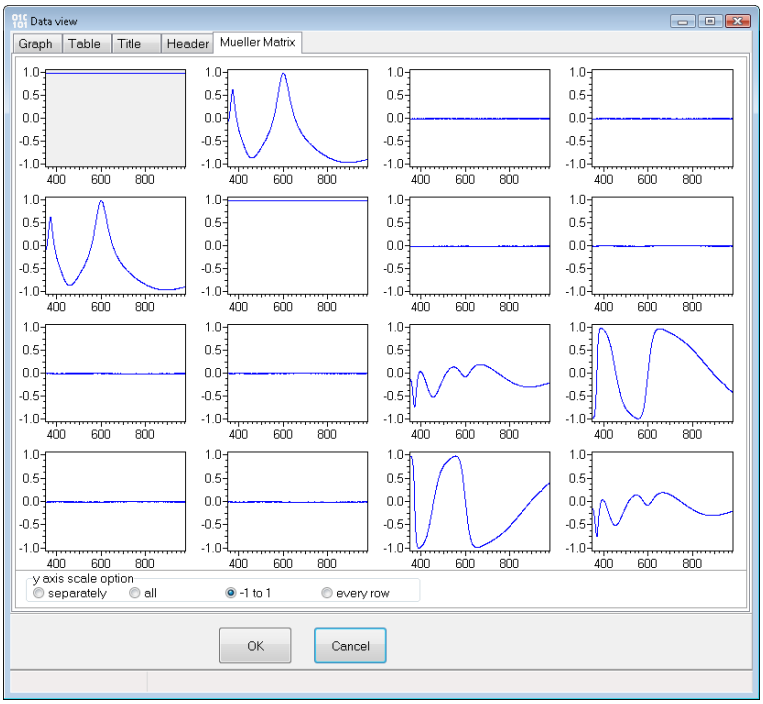


Fig. 5-142 Data editor Mueller matrix page

The 16 graphs in this tab show the 16 Mueller matrix elements in dependence of the wavelength. Depending on the measurement device (see Fig. 5-139) 12 (PCSA[13] or PSCA) or 16 (PCSCA) elements can be measured. A PCSA-device can measure the first three rows of the Mueller matrix, a PSCA-device the first three columns and a PCSCA-device can measure the complete matrix (see Fig. 5-143). The first element M11 of the Mueller matrix is used for scaling and is fixed to 1 (-> grey background).
The scale options below the graphs allow changing the scaling of y-axis of all plots. "all" set identical y-axes for all elements, "separately" scales each plot individually, "-1 to 1" sets the limits of all plots to -1 to +1 and "every row" sets identical y-axes for each row.

[13] Setup principle of the ellipsometer with component list from source to detector (P-polarizer, C-retarder, S-sample, A-Analyzer).

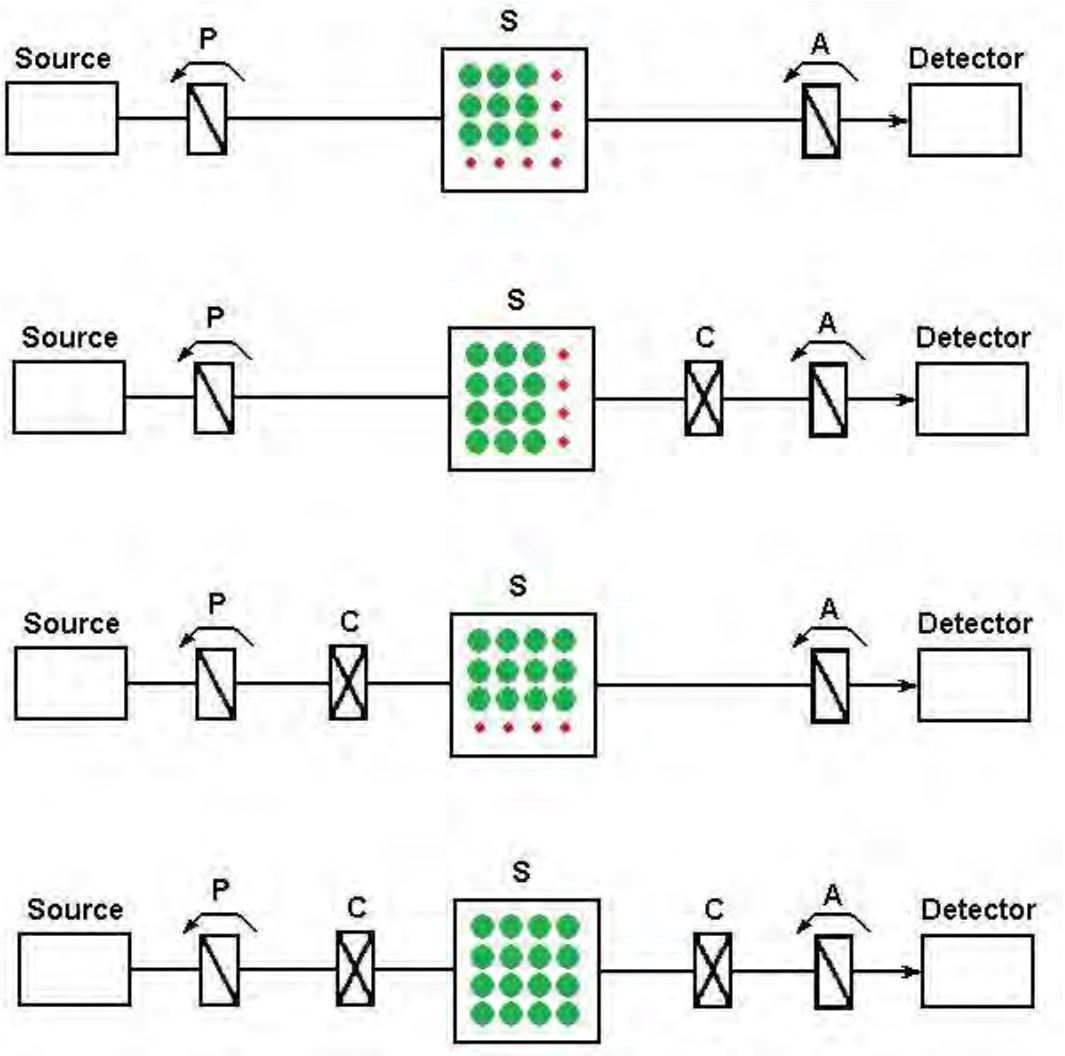


Fig. 5-143 Setups for measuring the Mueller matrix elements

5.5.3 Selecting data

Some samples need a lot measured data to get reasonable results: Multiple angle measurements of Ψ, Δ, Rp, Rs and transmission data. If you want to detect biaxial anisotropy you additionally have to rotate the sample. All these measurements belong to a single sample and should be fitted. Since this amount of data takes much time to fit, the first steps in a fitting session should use a subset of data.
The creation of subsets of data would create mountains of working files: TempR50.spc, TempR55.spc, TempPD70.spc and so on. The idea of column selection can be used for multiple data sets and avoids the extensive file handling and is therefore quicker in usage.
Each data set contains the list of "Use" flags on the header page. If you check these flags each data set can be checked partially. This state is displayed in the data set listbox by icons preceding the data set names:

Icon	Description
	all columns are selected
	some columns are selected, but not all
	none of the columns is selected

Tab. 5-21 Icons in the data set listbox

The use of these icons gives an excellent overview on the current selection of columns. There are two more ways to select data columns: the first uses the select mask application from a dialog and the second uses the mouse cursor.

The columns have y-types each of the types described in Tab. 5-18. A selection mask makes it possible to select or deselect a certain group of y-types through all data sets. You open the dialog displayed in Fig. 5-144 by pressing the icon bar button  or selecting the menu "Data/Select data types…". This opens the data selection dialog.
It consists of a series of checkboxes each for a basic y-type. The actions "Select" and "Deselect" affect the checked y-types. The checking of y-types is supported by two buttons "All" and "None". This does not perform a selection, but sets default states.
If you press "Select" or "Deselect" you immediately see the changes in the selection state icons of the data set listbox in the main screen.

Examples:

1. Select all measurements:
   "All", "Select"

2. Select only reflectivity:
   "All", "Deselect", "None", "R", "Select"

3. Select all Psi-delta pairs
   "All", "Deselect", "None", "Psi", "Delta", "Select"

If you close the dialog the current selection mask is kept for the second selection method using the cursor. When the cursor is moved through the data set listbox and is located on a selection icon it changes from the arrow to  . If this is the case and you click with the left mouse button, the selection mask is applied to toggle the selection state of the data set under the mouse cursor. Toggling means all columns affected by the mask are selected if they were not and deselected if they were selected.

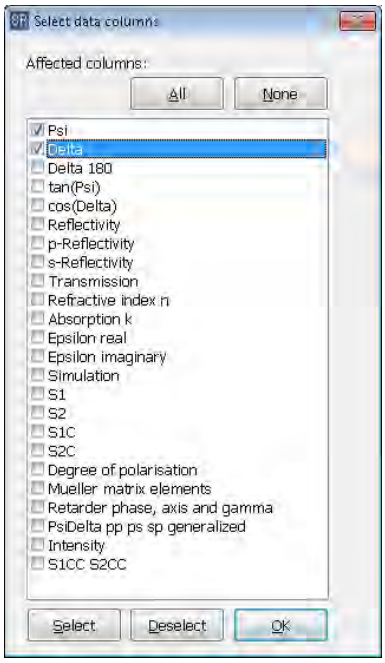


Fig. 5-144 Data selection dialog

The usage of the cursor allows a more detailed quick selection scheme. The following examples show the flow:

A. The second data set should be selected.

Press the icon bar  to open the selection dialog. Press “All”, “Deselect”. Close the dialog by “Ok”. Click on the icon of the second data set until you see a  .

B. Choose all Psi’s of the second and third data set.

Press the icon bar  to open the selection dialog. Press “All”, “Deselect”, “None”, “Psi”. Close the dialog by “Ok”. Click on the icon of the second and third data set until you see a  there.

5.5.4 Comparing data

You can compare data quickly by pressing the icon bar button 

. This function opens a quick data viewer. The display shows all columns selected and uses the colors shown on the header page of each data sets editor.

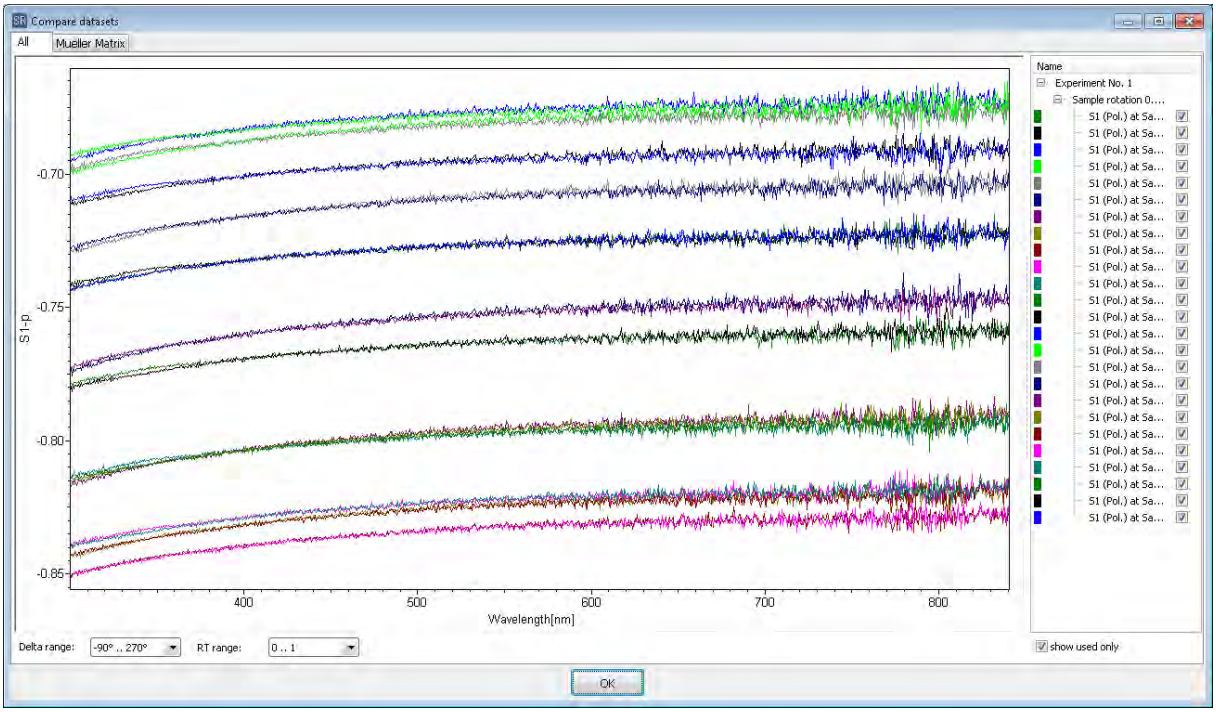


Fig. 5-145-5-146 Compare data columns viewer

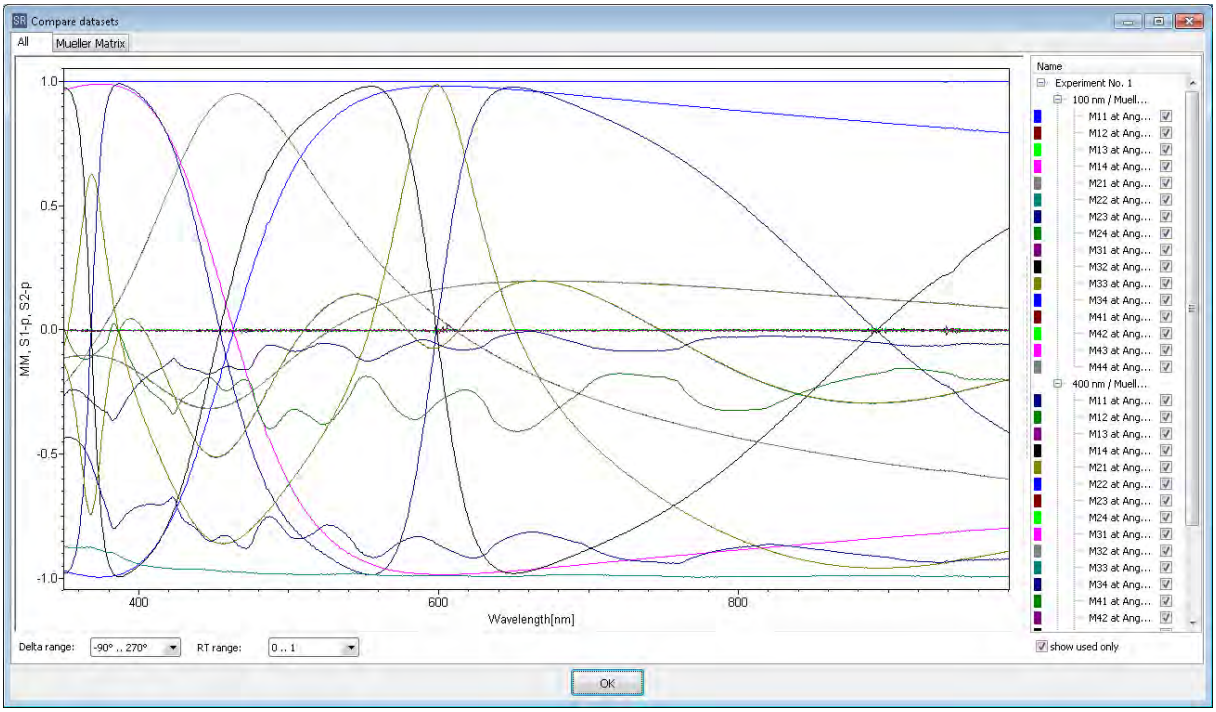


Fig. 5-147 Compare data sets containing Mueller matrices

If one of your selected data sets contains Mueller matrix data the “Compare” dialog looks like shown in Fig. 5-147. The additional tab allows comparing the Mueller matrix elements of two measurements.

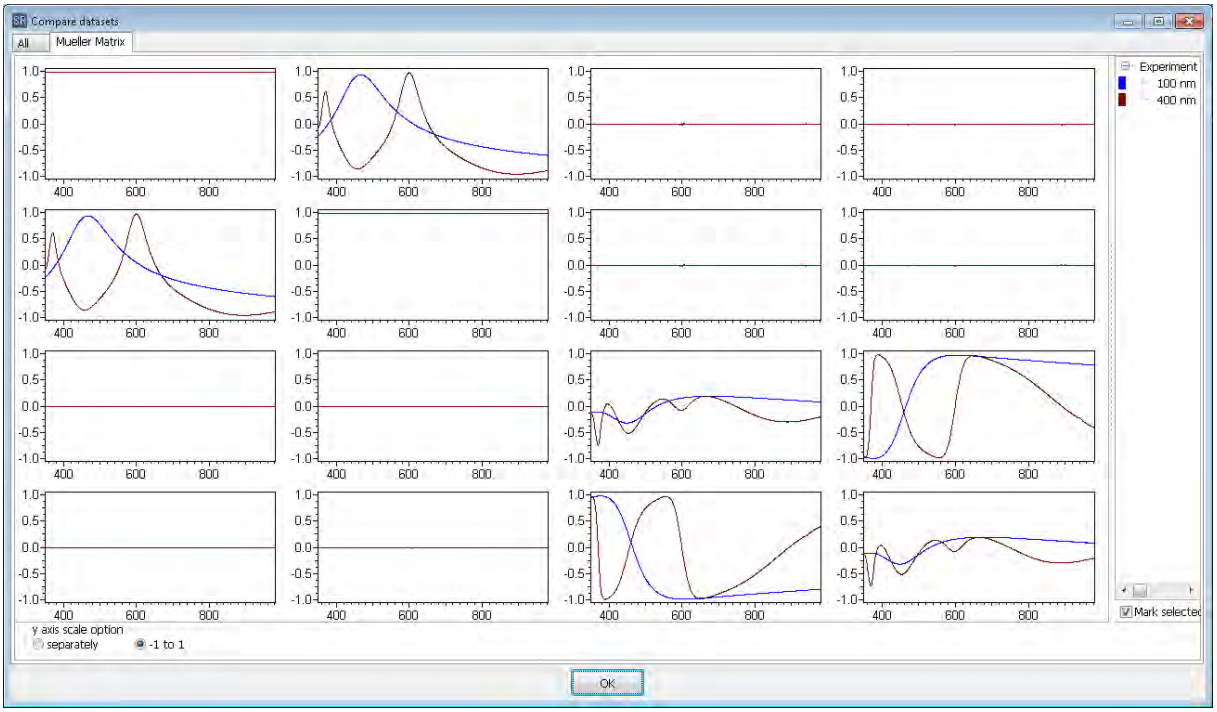


Fig. 5-148 Comparing two Mueller matrices

This viewer is designed for quick display, not for high quality prints. For these purposes the SpectraRay Grams portion could be used (predefined plots are possible by loading appropriate views) or running the Plot utility.

5.5.5 Swapping x- and z-axis

The swapping of x-and z-axis is useful for

- extracting the angle dependency at one wavelength from a multiple angle spectroscopic measurement
- extracting the theta dependency at one wavelength from a multiple theta angle spectroscopic measurement

The swapping function is started by using the menu “Data/Swap x- and z-axis”. Swapping of data is more complicated than changing the axis only, because ellipsometry data consist of column pairs (Ψ, Δ) and these pairs must stay.

The swapping moves data like in these two examples:

1. example: reflectivity measurement

	z_1	z_2	z_3	z_4
x_1	R_{11}	R_{12}	R_{13}	R_{14}
x_2	R_{21}	R_{22}	R_{23}	R_{24}

is swapped to

	x_1	x_2
z_1	R_{11}	R_{21}
z_2	R_{12}	R_{22}
z_3	R_{13}	R_{23}
z_4	R_{14}	R_{24}

2. example: (Ψ, Δ)-measurement

	z_1	z_1	z_2	z_2
x_1	ψ_{11}	Δ_{11}	ψ_{21}	Δ_{21}
x_2	ψ_{12}	Δ_{12}	ψ_{22}	Δ_{22}

is swapped to

	x_1	x_1	x_2	x_2
z_1	ψ_{11}	Δ_{11}	ψ_{12}	Δ_{12}
z_2	ψ_{21}	Δ_{21}	ψ_{22}	Δ_{22}

Since the maximum of columns is limited to 200, the data points must be reduced. The maximum number of columns created is contained in PModell.Ini entry “maxSwapColumns”. Change this entry if needed.

Note: Swapping clears any x-region used!

5.5.6 Combining data

If you measure a complicated sample a lot of data sets are generated. On a mechanical goniometer additionally multiple angle measurements appear as single data sets. All these data have the same x-axis (i.e. spectrum with wavelength limits and resolution) in common. For avoiding large numbers of files belonging to the same samples the combination of data and the storage within experiments is possible. The first method reduces the amount of data sets within an experiment. Opening the editor of combined data sets offers more columns directly than editing each column directly. The second method is to load all measurements of a sample into the data set list and to save all data together into an experiment. The role of experiments is therefore twice: Storing the actual work space on fitting a sample and storing all data in one file. This avoids trouble in file naming and speeds up reloading old work spaces. This section describes how the first method is applied. You first load all data you want to combine into your data set list or make your measurements by using the measurement dialog. As a result several data sets are contained in the list.
The combination simply proceeds by choosing “Data/Combine data” from the menu. The combination procedure tries to find all combinations possible. If no combination is found to be valid, you get informed by a message box. The preconditions for combinations are (except agreeing x-axis) the same environment values. The name, time and user entries may differ. The comments are appended.

5.6 Fitting of data

5.6.1 Mean square error (MSE)

The basic function of fitting data is to take a set of measurements and a set of parameters from a model and trying to find the best agreement between the theoretical and measured data points. The term “agreement” is defined by the figure of merit, based on Gaussian least squares:

$$F(\vec{p}) = \frac{\sum_{j=1}^{M} \frac{\sum_{k=1}^{C_j} \frac{\sum_{i=1}^{N_j} \left(\frac{\left(m_{ik}^j - t_{ik}^j(\vec{p})\right)}{w_k^j} \right)^2}{N_j}}{C_j} \cdot v^j}{\sum_{j=1}^{M} v^j}$$

$$MSE(\vec{p}) = \sqrt{F(\vec{p})}$$

with

M = number of used data sets (measurements)
N_j = number of used rows of the k-th column in the j-th data set
C_j = number of used columns in the j-th data set
m_{ik}^j = **m**easured data point in row i of the k-th column of the j-th data set
$t_{ik}^j(\vec{p})$ = **t**heoretical value of the data point in row i of the k-th column of the j-th data set calculated from the parameter vector $\vec{p}$
w_k^j = relative precision of a data point of the k-th column of the j-th data set (one column k has a certain data type and therefore a certain weight for all rows i)
v^j = weight of j-th data set
MSE = mean square error of the whole experiment

The above formula takes into account multiple columns and multiple datasets. The parameter vector p represents the list of fit parameters. The task of a fit is to find the global minimum of F. Since no algorithm exists for finding global extrema of any function, all methods search for local minima.
The method used by SpectraRay is the “Simplex” algorithm. It is very stable if your initial values differ from the minimum. A method to find a valid starting point is to use the scanner, see chapter 5.4.2.5.

The formula for F has a very general appearance. The general approach of the fomula makes it possible to combine ellipsometric data with reflection or transmission measurements and other data types. The values of these different data types usually have different ranges. For example the ellipsometric Ψ has values between 0° and 90°, the ellipsometric Δ has values between 0° and 360°, Stokes parameters have values between -1 and 1, and reflection and transmission coefficients have values between 0 and 1. In order to compensate for these ranges the relative weights shown in Fig. 5-149 are used. Usually the values should be set to the default values, but is also possible to introduce relative precision weights according to the quality of the measured data in these coefficients.
In addition it is possible to set a relative weight for a whole data set as shown in Fig. 5-150.

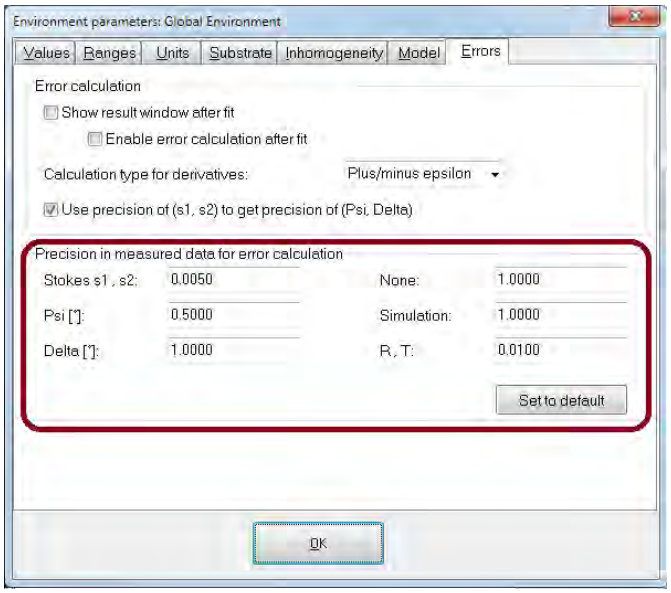


Fig. 5-149 Relative precision values for data types

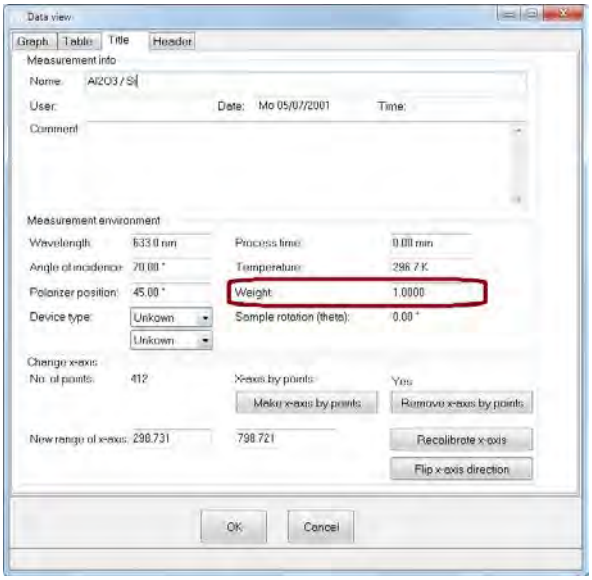


Fig. 5-150 Weight for data set

5.6.2 Fit parameter list

The preconditions of a fitting session are

1. the model contains at least two layers
2. at least one column of data is selected
3. the spectral ranges of all layers agree with the environment
4. the range of selected data contains points within the ranges allowed by the environment
5. the model contains at least one parameter to be fitted

Conditions 1 to 5 are automatically checked and would cause error messages if one of these conditions fails. Since all parameters are situated in the layers or environment pages a quick overview is useful to view and edit all parameters together.

The list of fit parameters is opened by pressing the icon bar button 

or using the menu “Calculate/View parameter list…”. This opens the editor shown in Fig. 5-151. The list of parameters is influenced by a series of settings:

1. The environment contains the flags “Display environment parameters in list of fit parameters” and “Display RAE parameters in list of fit parameters”: if these flags are not set, only layer parameters are visible
2. The environment contains some non-ideal effects; the number of parameters varies with the use of these effects
3. Splined table layers have a flag “Report spectral points as fit parameters”: If this is not set, only thicknesses are displayed. Otherwise only those points are displayed which lay in the spectral range allowed by the environment.
4. Duplicate materials are displayed only once
5. Thicknesses are not reported for top and bottom layers
6. The environment settings

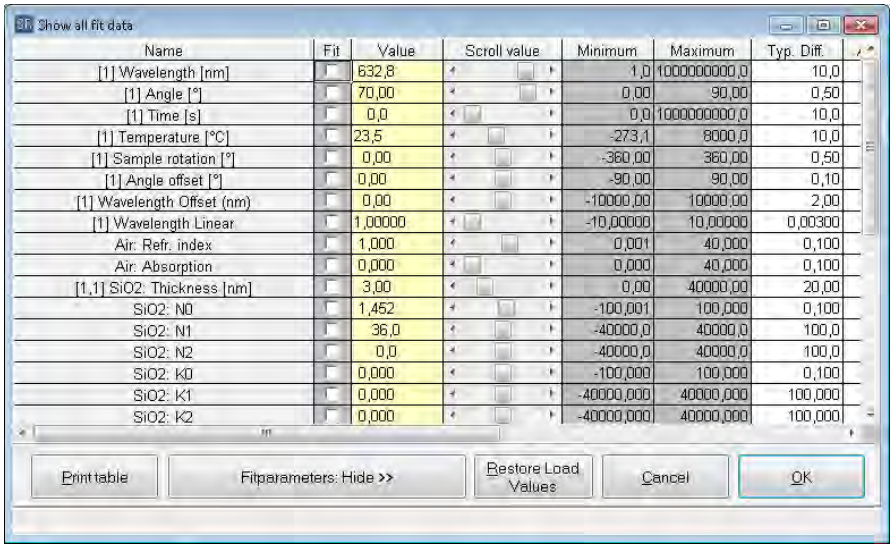


Fig. 5-151 Fit parameter list

The changes made in this editor immediately apply.

5.6.3 Fit of multiple datasets

A fitting session is started by pressing the toolbar button  or selecting “Calculate/Fit…” from the menu. This opens the dialog for fitting sessions. If you get an error message, check the error conditions 1…5 listed in the chapter above.
After the dialog appeared you will see one or two 2D-plots. If your data contain values of Ψ or tan Ψ the upper plot is used. All other types are drawn in the bottom plot. A single plot window appears if one of the two plots would appear empty (no data). This enlarges the display in a user friendly way. All theoretical curves are displayed in the same color (see Appendix E).

The fit is driven by a series of buttons and settings.

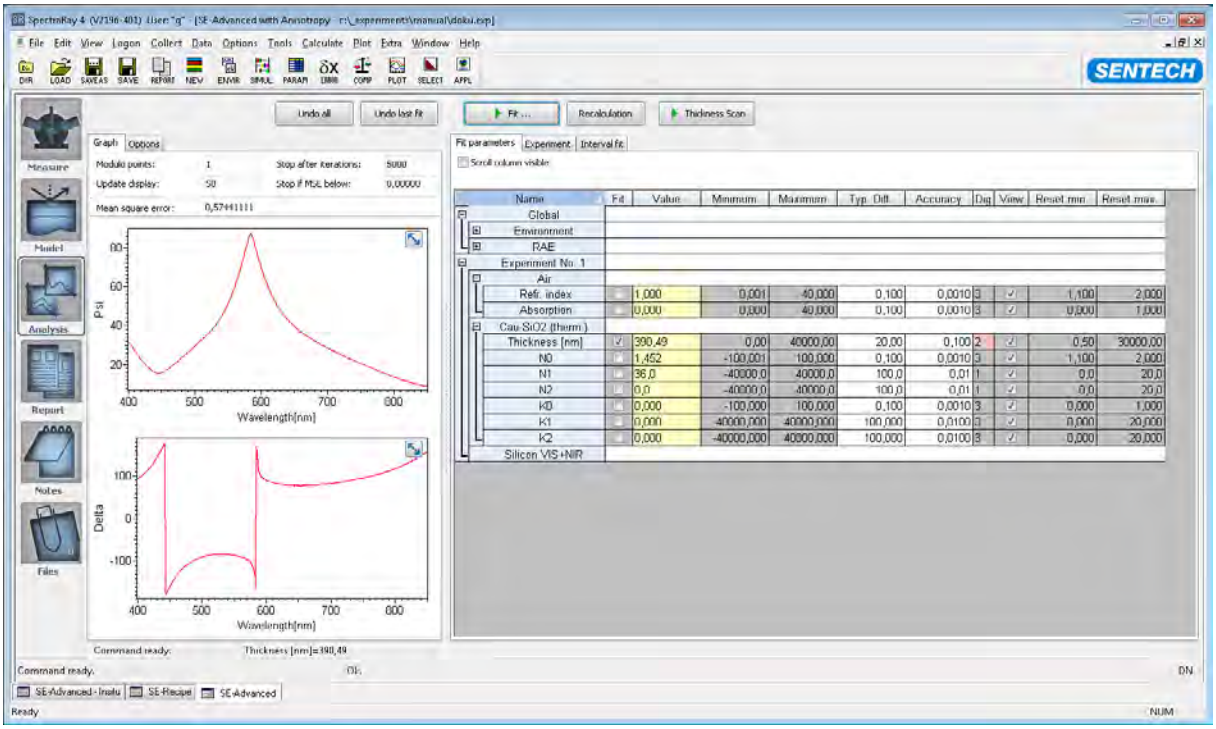


Fig. 5-152 Fitting session

Running a fit

A fit is started by pressing the “Fit…” button. This changes the text and function to “Abort fit…” and initiates the fitting procedure. The Simplex algorithm requires the calculation of a starting point (several calculations of the figure of merit at different settings of the parameter vector). The status line displays “Initializing fit in the meantime”. After this has been successful, the iteration proceeds step by step.
Each step the status line is refreshed. It displays the number of iterations made, the figure of merit and in the second line the actual fit parameters. Since the calculations take time, you may want to speed up the operation. This can be done in two ways. The first method is to reduce the number of data points. For first tries to fit a spectrum this should be the choice, because large differences between theory and measurement do not require many data points. If the agreement of the spectra is better more data points should be used. The function is driven by the integer value “Modulo points”. For example 1000 data points would be reduced to 100 by a value of 10. A second method to speed up is to reduce the overhead introduced by refreshing the display. For reducing the number of refresh’s set the integer “Update display” to a value larger than 1.
If you want to abort the fitting procedure press the “Abort fit…” button. After the next data column has been calculated the button text is changed to “Acknowledged” indicating that the procedure is being aborted. After the fit was stopped the whole data are calculated with a “Modulo points” of 1 and the display is refreshed. This may take a bit of time, don’t worry.
The same takes place if the fit was successfully and the button “Abort fit…” returns to “Fit…”. The results of the fitting procedure are displayed in a dialog window which is the same as for the fit parameter list (see Fig. 5-153). Changes are made to prevent the user from editing the data and only the fitted parameters are displayed. This

allows to print the results easily (“Print table” button) and to copy them to the clipboard. Select the cells you want to copy and press the CTRL and INS keys simultaneously.

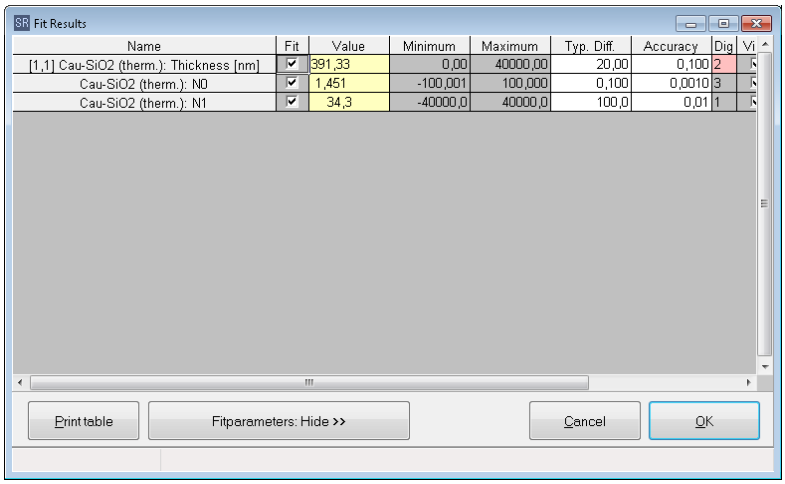


Fig. 5-153 Fit result display

Other settings

“Undo all”	undoes all actions
“Undo last fit”	undoes the last fit
“Recalculation”	initiates a new calculation of theoretical values and a refresh of the display
“Thickness scan”	initiates a thickness scan by searching the best agreement for thicknesses between minimum and maximum
“Stop after iterations”	number of maximum iterations used for fitting
“Stop if MSE below”	stopping condition for the fitting

5.6.4 Shifted interval and point by point fits

A special method of fitting spectra is available in the frame „Interval fit“ in the fitting session dialog (see Fig. 5-152). This frame contains a special tool for fits which work in certain intervals or point by point. A single fit is a sequence of selecting some parameters to fit and setting up the environment ranges and data. The output is a single vector of parameters, the results.

The idea of the interval or shifted fit is to run multiple fits each on its own interval. This is very helpful to understand difficult dispersion relations as for example polymers with absorption bands or edges. The output of this procedure is either a set of resulting parameters or the desired dispersion as a curve.

The interval fit works as follows: A small interval is selected within the environment where the selected curves are fitted well (if not, do not start the interval fit and put your attention to fitting the small interval). A fit is run, the results are stored and the interval is shifted to the left or right. The next fit is run, again the results are stored and the interval is shifted. This is repeated, until the interval has finally moved through the whole spectrum.

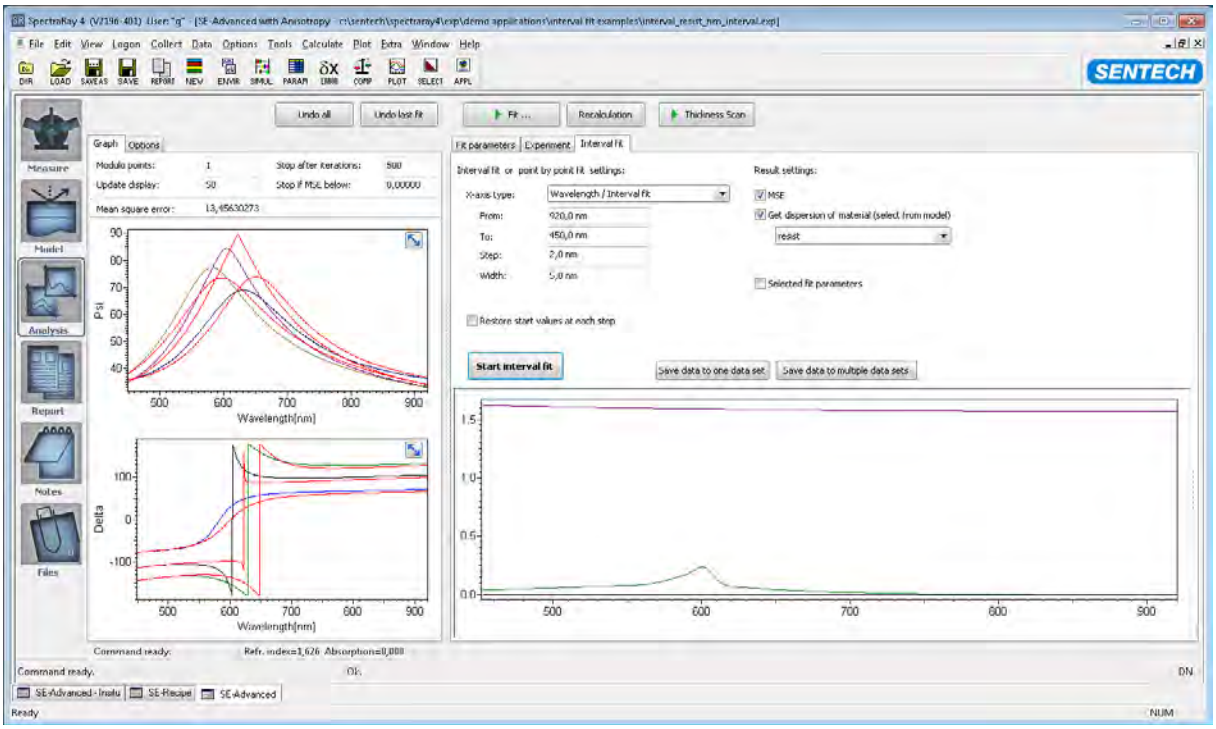


Fig. 5-154 Shifted interval fits

The settings needed to set up this interval fit are:

X-axis	type of X-axis, select from Wavelength / Interval fit Data set - rows / Point by point fit Time / Interval fit Angle of incidence (phi) / Interval fit Angle of rotation (theta) / Interval fit Temperature / Interval fit Data set columns / Point by point fit
From	center of the interval at start
To	center of the interval at the end
Step	shift of the interval from fit step to fit step
Width	width of the interval
Restore start values at each step	restores the start values before fitting each interval
MSE	save MSE values for the fit
Get dispersion of material	If this flag is checked, the output is the dispersion of the material selected by the combobox below the checkbox. Be sure that the

	fit influences the dispersion of the selected layer.
Selected fit parameters	saves the values of all selected fit parameters and shows the results in the graph
Start interval fit	starts the interval fit
Save data to one data set	save the results to one data set
Save data to multiple data sets	save the results to multiple data sets

In the following chapters examples are given for interval fits on different data types.

5.6.4.1 Example 1a: Interval fit versus spectral axis (nm)

As an example a resist layer on a silicon substrate is chosen.
In a first step the data can be very well described by a Cauchy model in the visible part of the spectrum.
In a second step the data is analyzed by an interval fit to demonstrate its functions. (An extended example of similar type is given in the advanced tutorial in chapter 8.7.3).

5.6.4.1.1 Example 1: Step 1: Cauchy model

The film thickness of the photoresist film is analyzed first in the transparent part of the resist (spectral range: 450…920 nm). Multiple angle measurements are necessary. Here (Ψ, Δ)-measurements of 50, 60 and 70 deg are used.

A simple Cauchy model is applied to model the measurement.

Title	Thickness	State	Layer Type	Info [633,0 nm]
Air			NK layer	n=1,0000
Resist	112,84 nm		Cauchy layer	n=1,5882
Si DUV-UV-VIS-NIR			File layer	n=3,8736 k=0,01455

Set the used spectral range to 450 nm to 920 nm.

The fit parameters of the resist film are the film thickness and the Cauchy coefficients N0, N1, N2.

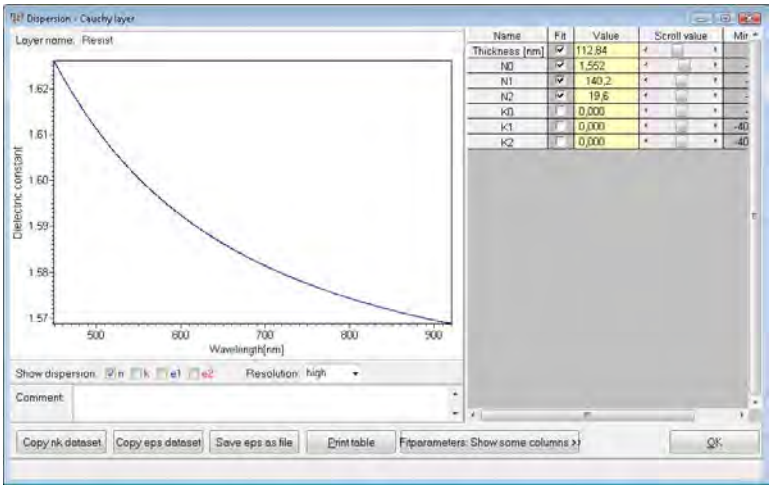


Fig. 5-155 Cauchy model of the resist film

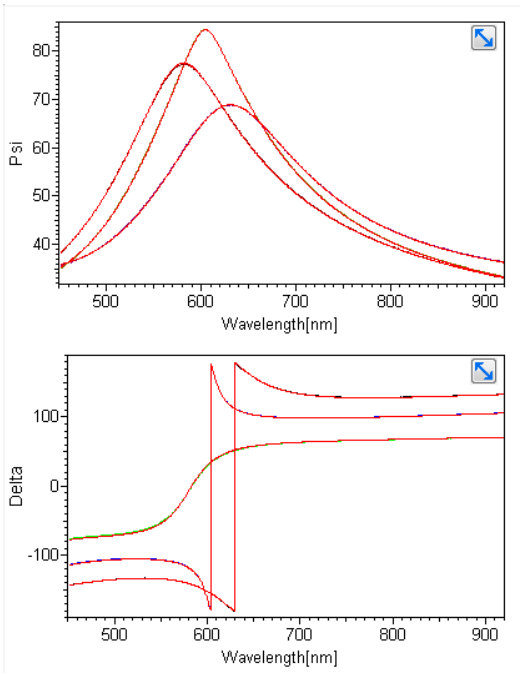


Fig. 5-156 Measured and calculated data after fit with Cauchy model

The model shows an very good fit to the measurement. A film thickness of 112.8 nm is obtained.

5.6.4.1.2 Example 1: Step 2: Set up the interval fit

It is necessary to know the film thickness of the photoresist accurately from the previous step, because the film thickness is not a fit parameter during the “interval fit”. This becomes important because in the absorbing spectral range (in this case in the UV) the interval fit is less sensitive or even insensitive against the film thickness.

The Cauchy layer is removed. At its position a “Fixed refractive index and absorption”, also called “N,K layer” layer is inserted. Press the “New” icon from the icon bar. The “Create new material” window is opened.

Select the “NK layer” type and Press “ok”.

Fig. 5-157 “Create new material” window

Double click the “NK layer” layer to open the dialog. Enter the film thickness obtained from the former modeling (Here: th = 112.84 nm). Select n and k as fit parameter. Set a starting value for n of n=1.6.

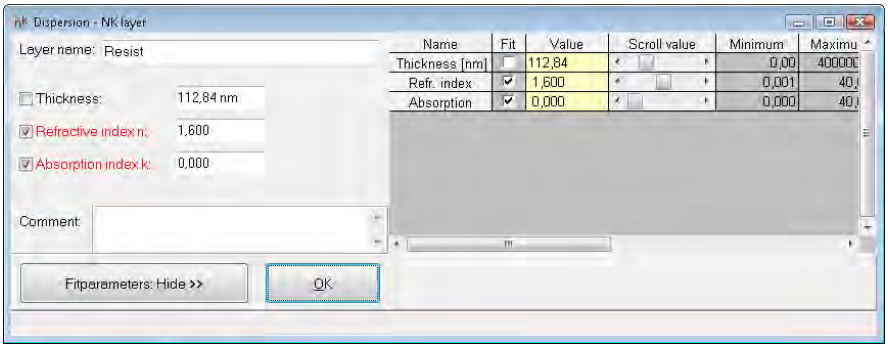
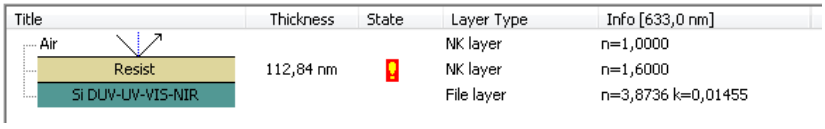


Fig. 5-158 “NK layer” window

Press “Ok”. The layer is inserted into the model. Move it to the correct position. The model appears now as follows:



5.6.4.1.3 Example 1: Step 3 Perform the interval fit

Open the fit screen and check the measured and modeled data. Because the constant refractive index is used now the calculated data do not fit exactly to the measured data.

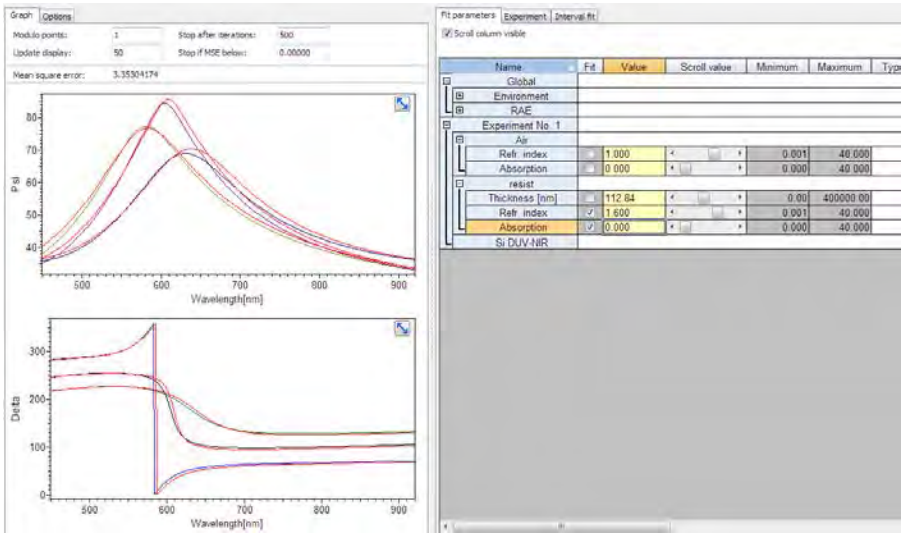


Fig. 5-159 Measurement and model with new model with “N,K layer”. The model fits not exactly as a constant refractive index is used now.

Now select the “Interval Fit …” frame on the right side. The “Shifted Interval Fit” window is shown. Select the following settings:

x-axis: Wavelength (nm) / Interval fit

from: 920 nm (the scan is done from the highest wavelength, because the starting values of the model are correct here, because they are known from the former modeling. In the UV they are less well known, so starting at 240 might lead to a wrong solution)

to: 450 nm

step: 2.0 nm (the step size for the intervals. It should be sufficiently narrow in order not to skip any structures in the spectrum)

width: 5 nm (width of the fitted interval. It should be sufficiently narrow in order not to average the structures in the spectrum)

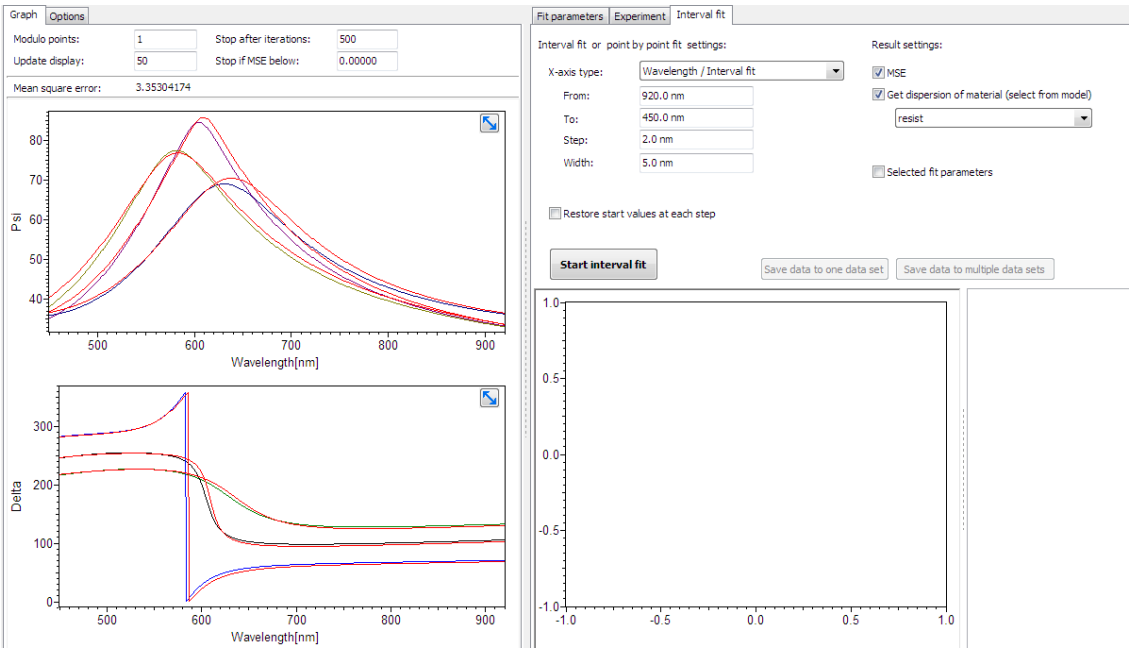


Fig. 5-160 “Shifted interval fit” window

The “Start interval fit” button is pressed to initiate the fitting procedure. The fit is now done step by step. The fitting window shows the progress for each interval. The results are stored in the results window. When the shifted interval fitting procedure is finished the results are shown in the graph. The dispersion of n and k as well as the MSE value are displayed.

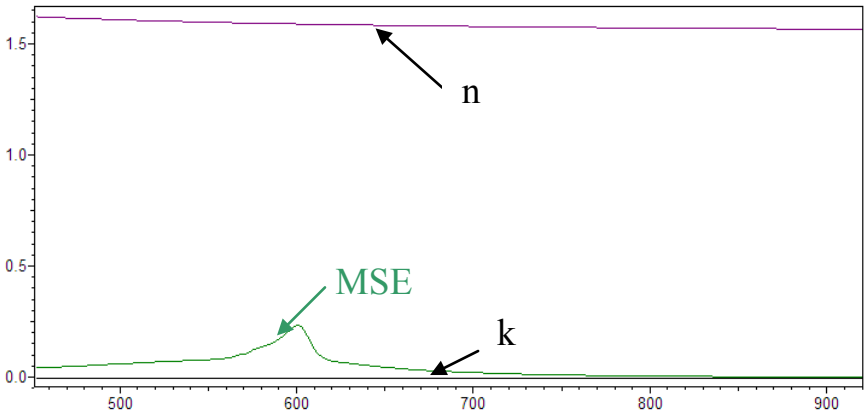


Fig. 5-161 “Shifted Interval Fit” results

The results of the fitting procedure can be saved by pressing the “Save data to one data set” or “Save data to multiple data sets” icon. In case you click on “Save data to one data set” all fitting results are saved into one data set as shown in Fig. 5-162:

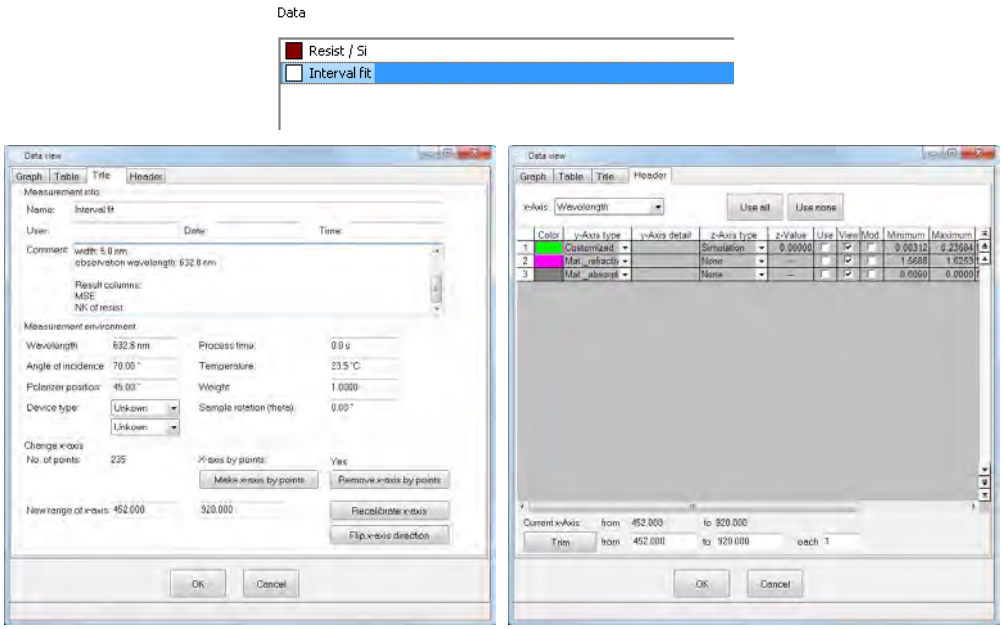


Fig. 5-162 Results of interval fit in one file

In case you click on “Save data to multiple data sets ” each fitting result is saved into one separate data sets shown in Fig. 5-163.

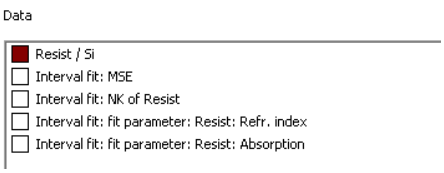


Fig. 5-163 Results of interval fit in multiple files

5.6.4.2 Example 1b: Interval fit versus spectral axis (eV)

Very similar to the example given in 5.6.4.1 where a spectral axis in nm is used it is also possible to perform the fit with a spectral axis in eV.
Different units for the x-axis (such as nm, eV, 1/cm etc.) may be set in

a) in the data set
b) in the environment
c) in the edit fields in the interval fit dialog

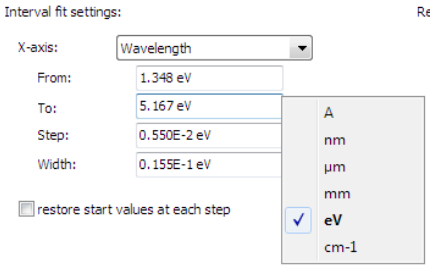


Fig. 5-164 Unit settings in edit fields

It is possible to enter values in the edit fields in different units by just entering the desired unit. In addition a right mouse click in the edit fields opens the menu which allows to select the desired unit as shown in Fig. 5-164. All values in the fields will be converted. The 'Step' and 'Width' parameter are differences and they are converted according to the derivative (for example from nm to eV) at a nominal wavelength of 633nm.

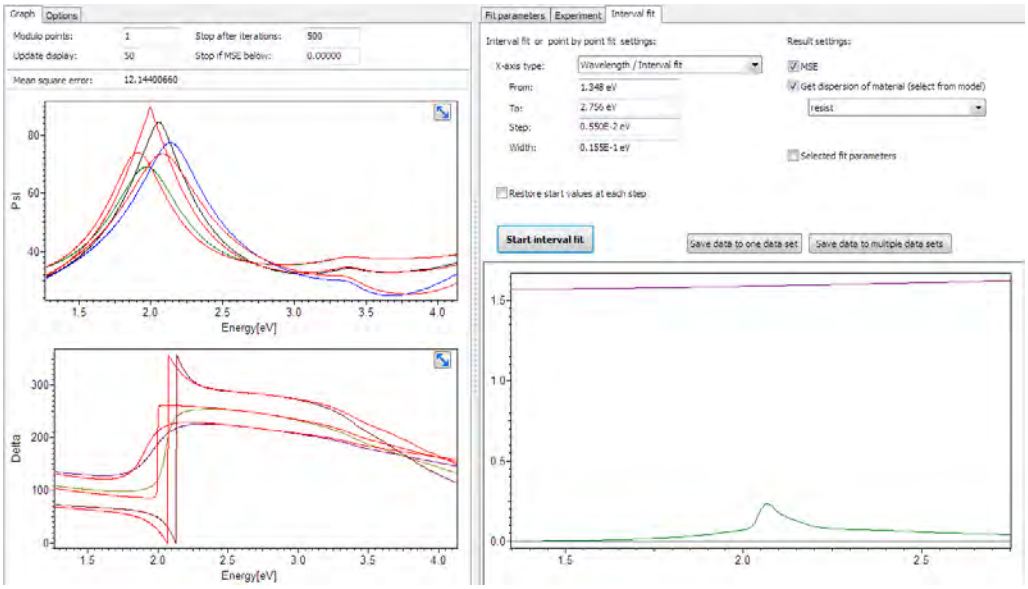


Fig. 5-165 Interval fit with data versus spectral scale in eV

Fig. 5-165 shows the results of the interval fit with the spectral scale in eV. The data are the same as in the example in chapter 5.6.4.1.

5.6.4.3 Example 1c: Interval fit versus spectral axis (1/cm)

Very similar to the example given in 5.6.4.1 where a spectral axis in nm is used it is also possible to perform the fit with a spectral axis in 1/cm.

Different units for the x-axis (such as nm, eV, 1/cm etc.) may be set in

a) in the data set
b) in the environment
c) in the edit fields in the interval fit dialog

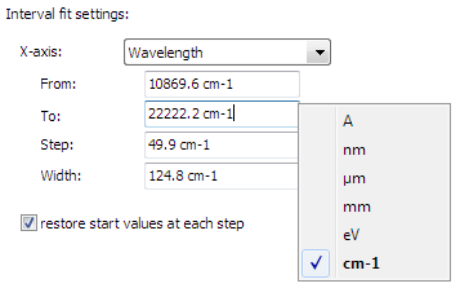


Fig. 5-166 Unit settings in edit fields

It is possible to enter values in the edit fields in different units by just entering the desired unit. In addition a right mouse click in the edit fields opens the menu which allows to select the desired unit as shown in Fig. 5-166. All values in the fields will be converted. The 'Step' and 'Width' parameter are differences and they are converted according to the derivative (for example from nm to eV) at a nominal wavelength of 633nm.

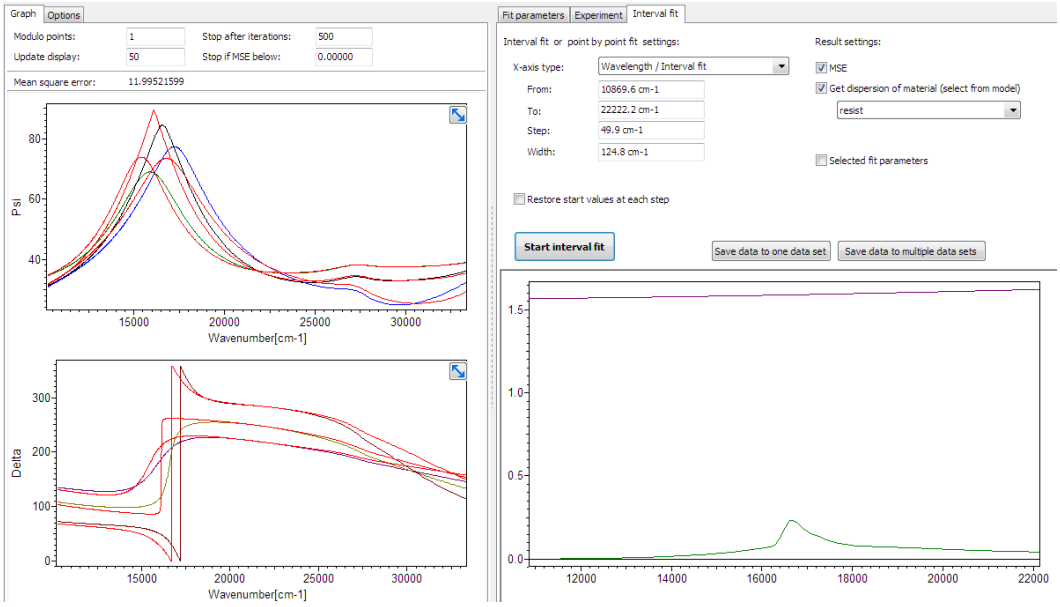


Fig. 5-167 Interval fit with data versus spectral scale in 1/cm

Fig. 5-167 shows the results of the interval fit with the spectral scale in 1/cm. The data are the same as in the example in chapter 5.6.4.1.

5.6.4.4 Example 2: Interval fit versus time

In this example the evaluation of time dependent data with the interval fit is demonstrated.
For example deposition or etch processes can be monitored with in-situ ellipsometers.

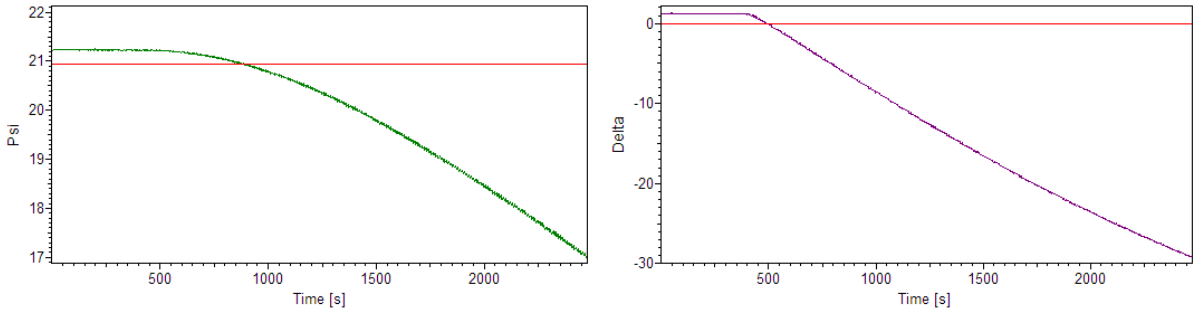


Fig. 5-168 Time dependent ellipsometric data

Time-dependent data from an atomic layer deposition process on glass are shown in Fig. 5-168.

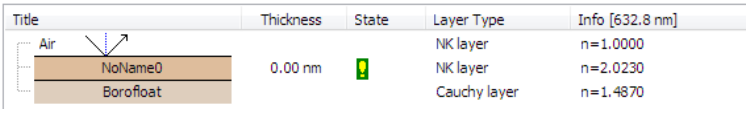


Fig. 5-169 Simple model

A simple model is set up containing an NK layer for the deposited film and the glass substrate.

Between 0 and approx. 500 s the Ψ and Δ values in Fig. 5-168 remain constant, so no deposition is going on here. The calculated values (straight red lines) do not match the measurements exactly. In in-situ applications this situation may occur due to different substrate materials, additional layers that are not precisely described in the model or systematic shifts due to the windows which the optical beam has to pass.
In order to correct for these non-ideal starting conditions offsets can be set as shown in Fig. 5-170

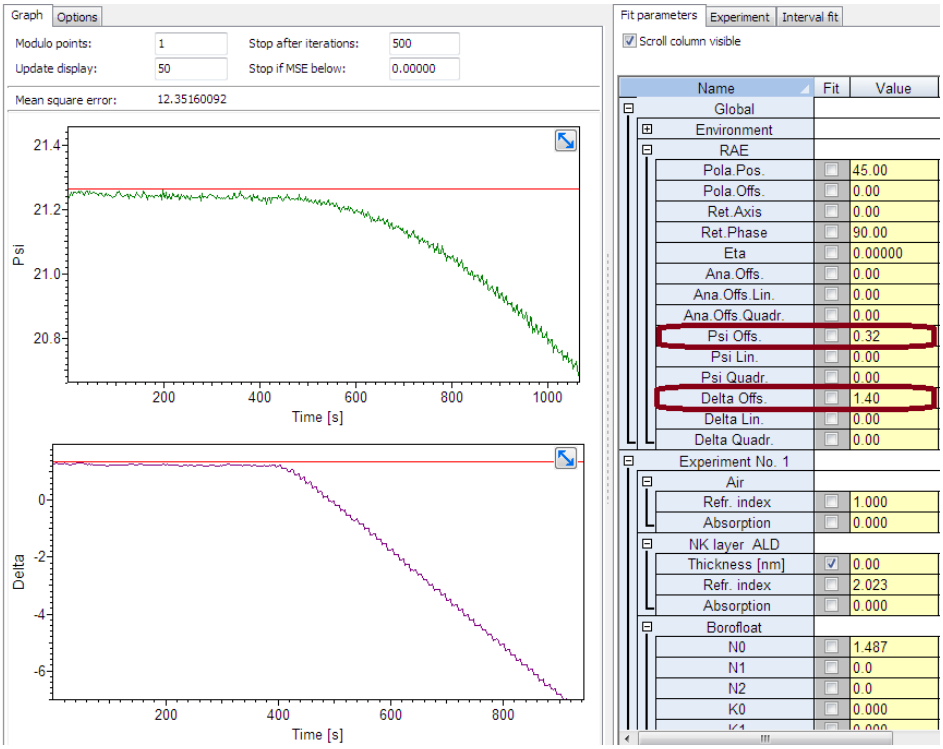


Fig. 5-170 Offsets for compensation of the starting conditions

The interval fit can now be set up for time-dependent calculations as shown in Fig. 5-171.

In this example the film thickness is fitted.

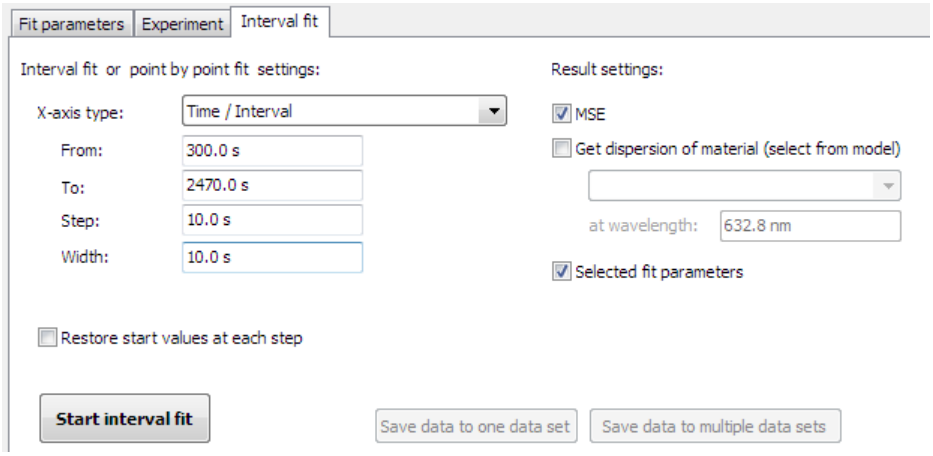


Fig. 5-171 Interval fit settings for time dependent calculations

For a reasonable fit it is advisable to check the starting value for the film thickness - in this case 0 nm as shown in Fig. 5-172. Otherwise wrong solutions may be found and MSE values may be very high to indicate bad fit results-.

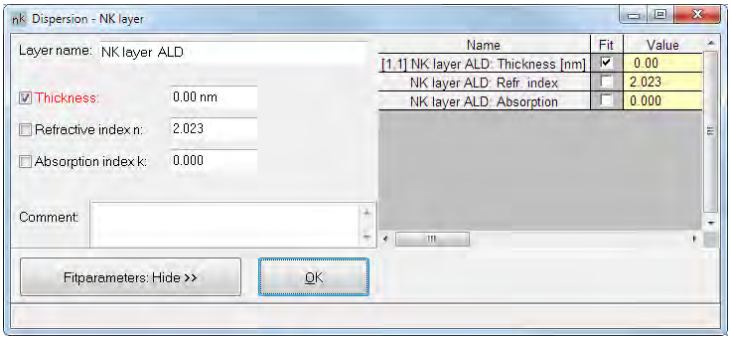


Fig. 5-172 Starting thickness and fixed refractive index for interval fit

The fit procedure can be started with the button 'Start interval fit'. The result is shown in Fig. 5-173. The film thickness grows quite linearly with time and the MSE value is small indicating a good fit quality.

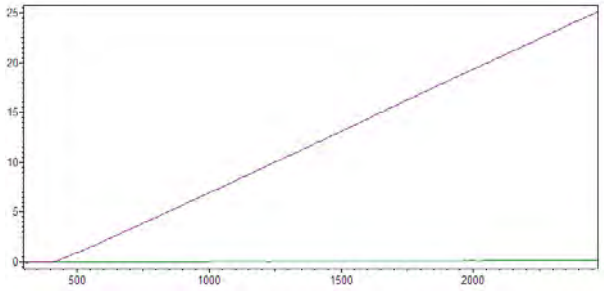


Fig. 5-173 Resulting film thickness versus time (purple) and MSE (green)

Due to the setting '10 seconds' for the 'Width' of the interval the result appears to be 'smoothed'. It is possible to choose different values in order to optimize results.
See chapter 5.6.4.5 for further treatment of the data with calculations at each point.

The results can be saved to files which appear in the main data box as datasets as shown in Fig. 5-174.

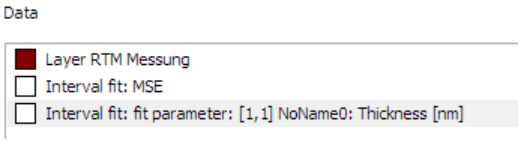


Fig. 5-174 Datasets with results

5.6.4.5 Example 3: Point by point fit versus x-axis values from a dataset

This example continues the example in chapter 5.6.4.4.

It may be desirable to use the x-axis values of a certain dataset for the calculations at every point. This is point by point mode which does not use an interval width as each point is treated individually.

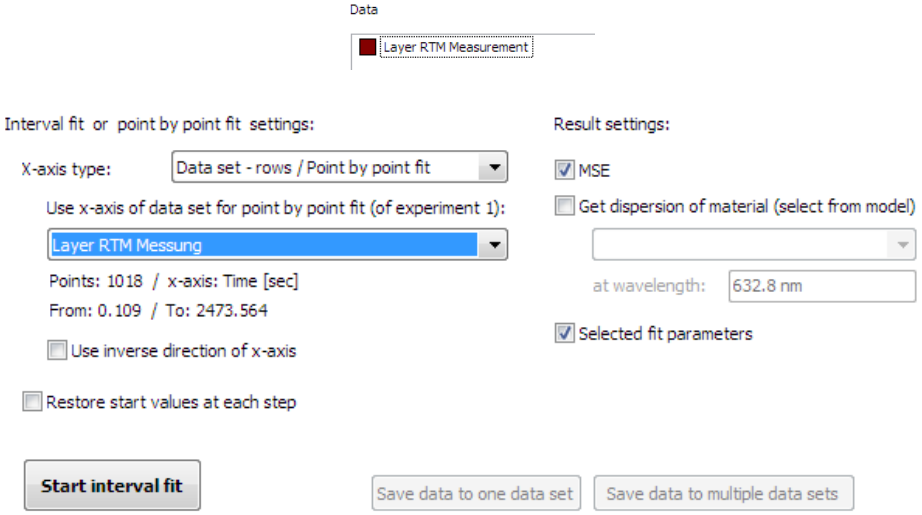


Fig. 5-175 Interval fit settings for x-axis according to the data set rows.

The option 'Data set - rows / point by point fit' has to be chosen and the data set which contains the x-axis values has to be selected from the list of data sets (in this example only one data set is present). The number of points to be calculated, the type of the x-axis and the x-axis range is shown.

The starting values are set as shown in Fig. 5-176.

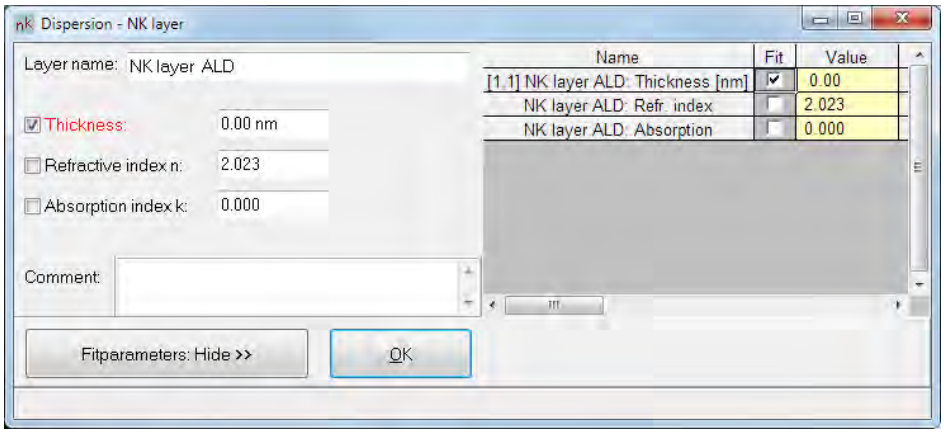


Fig. 5-176 Starting values

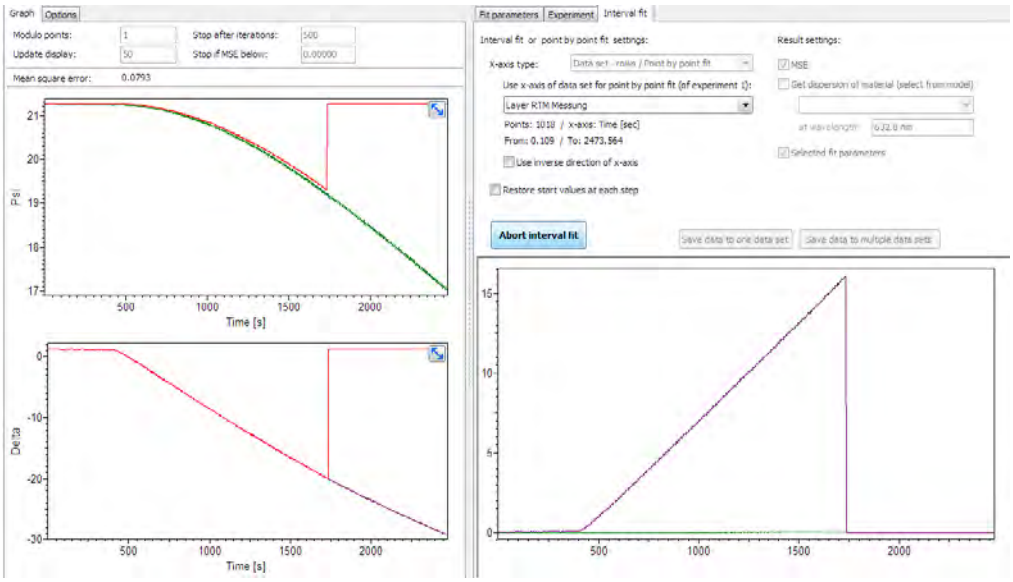


Fig. 5-177 Interval fit in progress

When the interval fit is in progress the measured and fitted data and the results are shown in Fig. 5-177.
The fit now determines results at each point. In this example it is very helpful as the small 'steps' in the measured curve are correctly evaluated as stepwise varying thickness values as shown in Fig. 5-178. This result is typical for ALD deposition processes where the thickness varies from step to step in the shown manner.

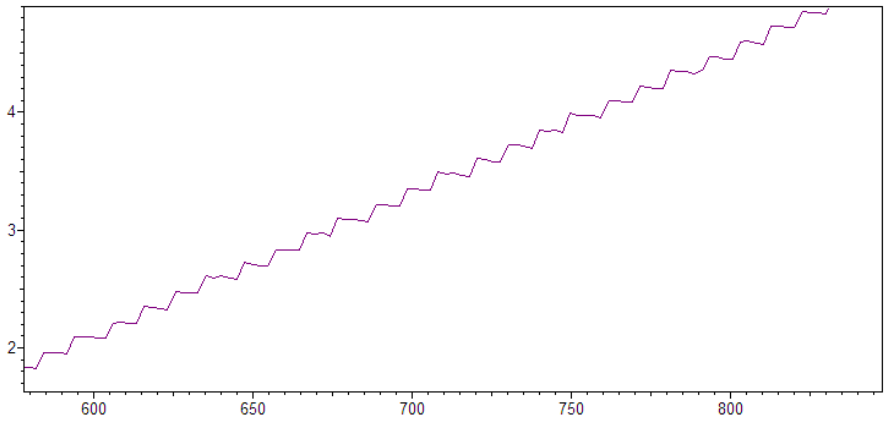


Fig. 5-178 Resulting thickness versus time showing the individual steps of an ALD deposition.

The results can be saved to files which appear in the main data box as datasets as shown in Fig. 5-179.

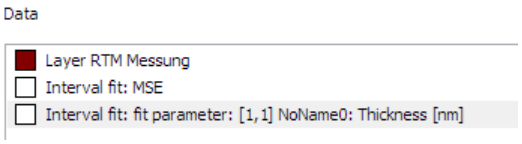


Fig. 5-179 Datasets with results

5.6.4.6 Example 4: Interval fit versus angle of incidence (phi)

In this example the treatment of a multiangle measurement data set is shown with a fit versus the angle of incidence.

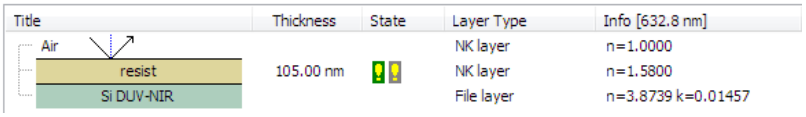


Fig. 5-180 Model for layer on silicon wafer with starting values

The data to be analyzed contains Ψ and Δ values versus angle of incidence. The model consists of an NK-layer with reasonable initial values. The initial data do not give a good description.

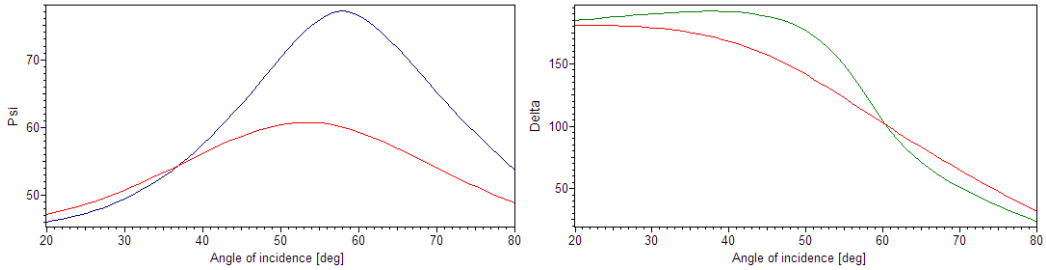


Fig. 5-181 Data to be analyzed and calculated data from initial values

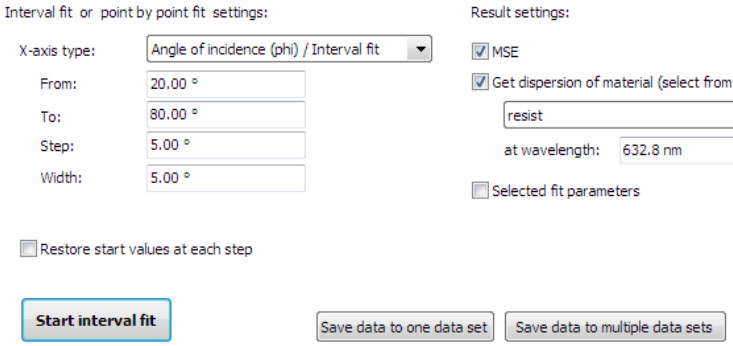


Fig. 5-182 Settings for interval fit versus angle of incidence

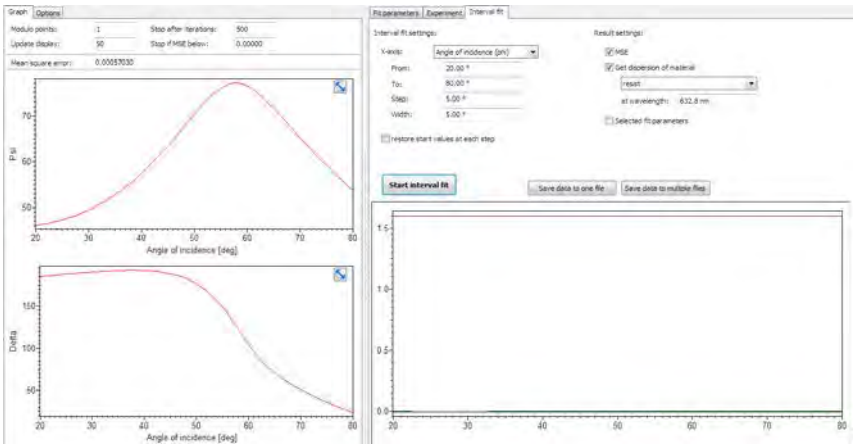


Fig. 5-183 Results of interval fit

The result of the interval fit with the settings shown in Fig. 5-182 gives the thickness and the refractive index of the film as shown in Fig. 5-183.

5.6.4.7 Example 5: Interval fit versus angle of rotation (theta)

In this example the treatment of a measurement data set from an anisotropic sample is shown with a fit versus the angle of rotation ϑ. The extraordinary axis is in the sample surface. Therefore a rotation of the sample will show a strong dependence of the ellipsometric data from the rotation angle. The mode l is shown in Fig. 5-184and Fig. 5-185.

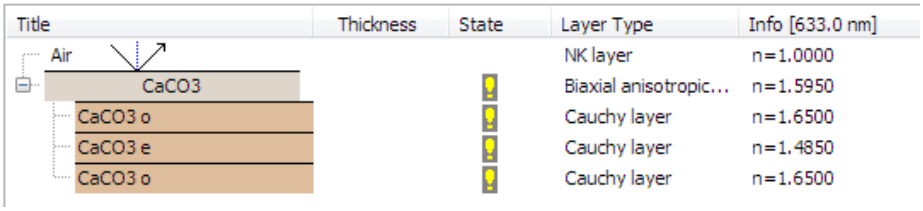


Fig. 5-184 Model for biaxial sample with extraordinary axis in the sample surface

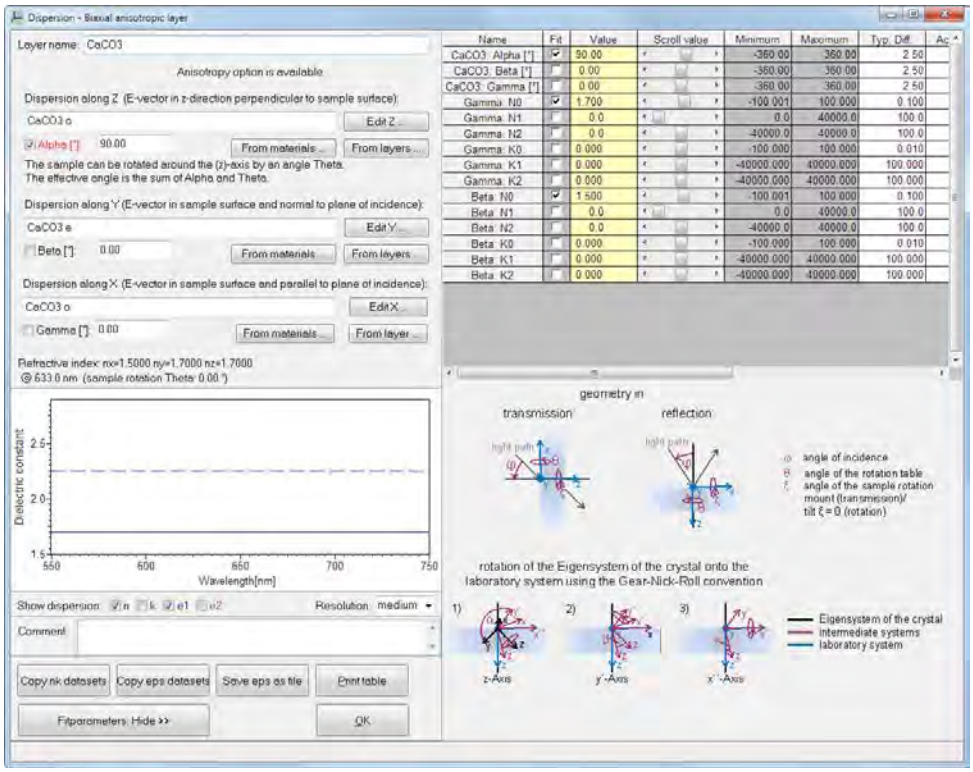


Fig. 5-185 Biaxial layer settings - initial values

The data to be analyzed contains Ψ and Δ values versus angle of incidence. The model consists of an NK-layer with reasonable initial values. The initial data do not give a good description.

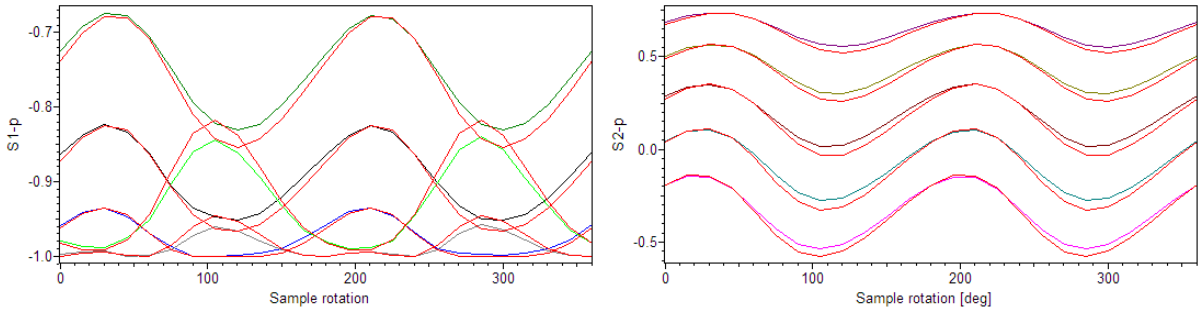


Fig. 5-186 Data to be analyzed and calculated data from initial values

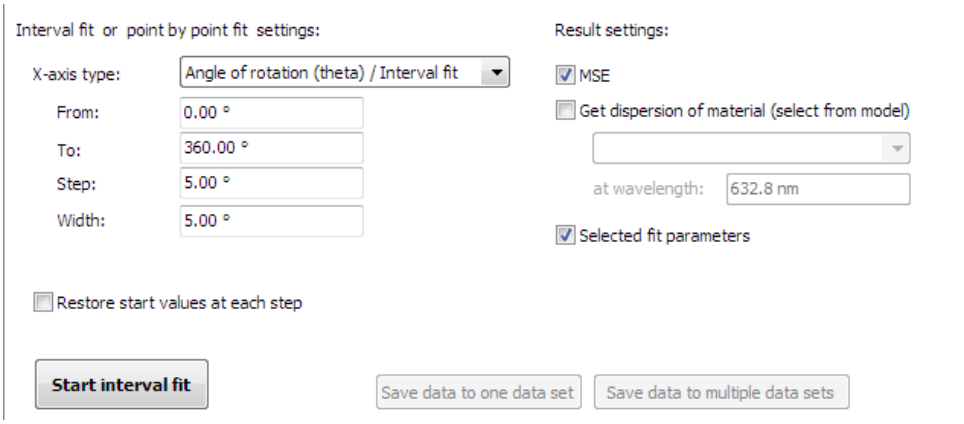


Fig. 5-187 Settings for interval fit versus angle of rotation

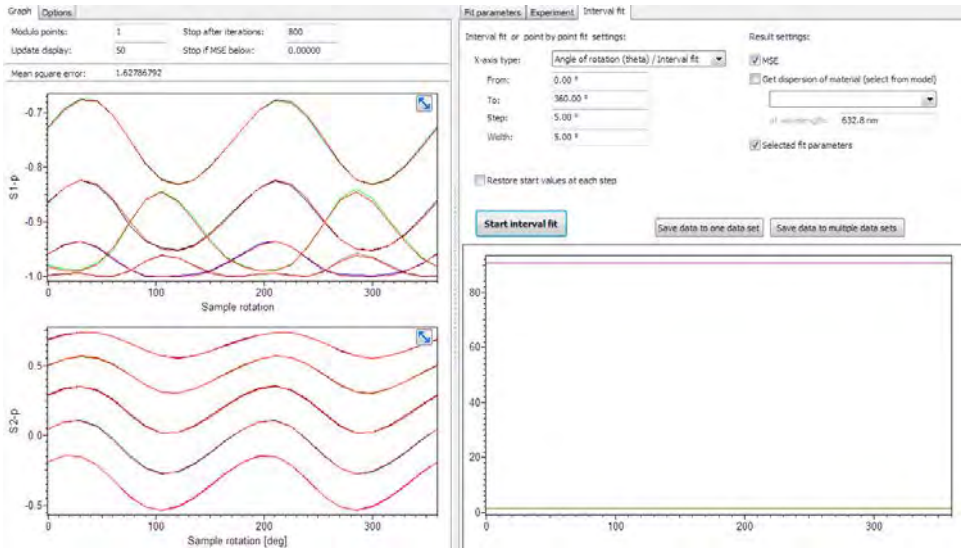


Fig. 5-188 Results of interval fit with calculated data and resulting fit parameters

The result of the interval fit with the settings shown before gives the rotation angle Alpha of the sample and the refractive indices of the sample as shown in Fig. 5-188.

5.7 Plot Utility

5.7.1 Basics

The plot program serves as SpectraRays interface to text processing or presentation programs. SpectraRay holds many data and allows filtering of data to be displayed in a very comfortable manner. The plot utility comes into play when a report is generated and xy-graphs are needed. Also when you click on the Plot utility icon within SpectraRay, the current data are exported and plotted within this small utility. Once you have images here, you may copy them into the clipboard or save as Bitmaps (*.bmp not resizable) or Metafiles (*.wmf resizable) onto the hard disc. An example is shown in Fig. 5-189.

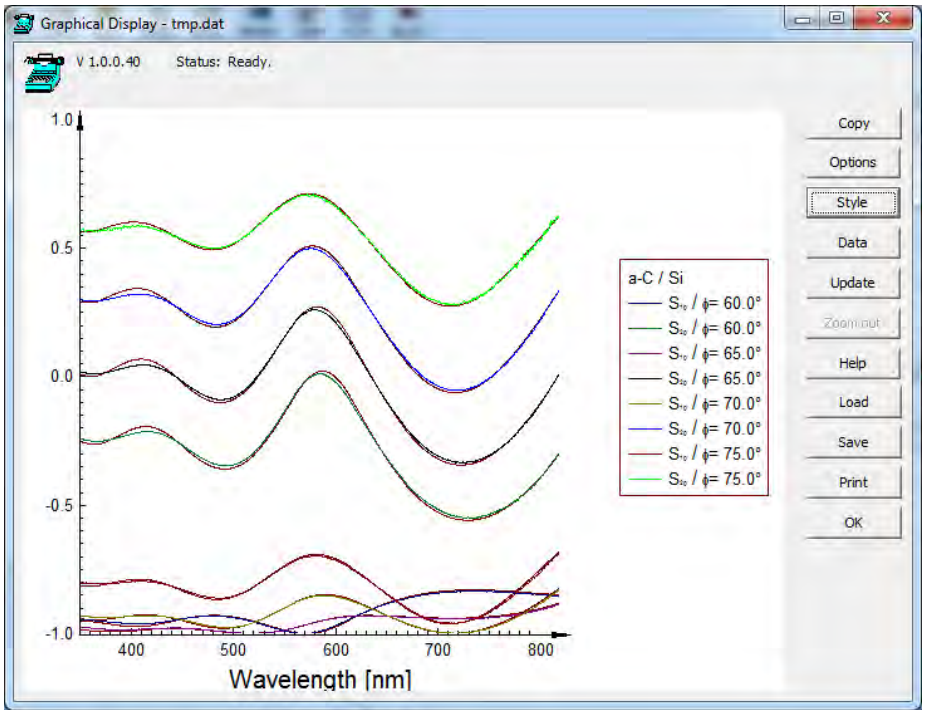


Fig. 5-189 Plot utility main screen

The function differs from typical DTP programs and is designed as an interpreter for data and style commands. This makes it favorable for applications generating data output, because it allows easy creation of ready-to-print xy-graphs. A xy-graph is always generated by combining a data file, background data and a style file. All these files are pure ASCII data and can easily be edited or changed. The program has no enhanced editor for styles, but the script format is so easy, that there is no need for the large number of windows and dialogs required for this purpose. The plot utility is very compact and designed as an add-on for other programs (here for SpectraRay). The principle of operation is interpreting ASCII files by combining data and commands. A picture is made up by combining data, background and styles. For changing the generated graph, you need to edit the text input and retrigger the rendering (“Update”). A broad set of commands allows modifying the plotting in a very detailed manner. You should read the following reference before making changes. In most cases it is only needed to edit the styles.

5.7.1.1 Data files

The simple but powerful way to create a plot is to load a data file. This data file must be an ASCII format file and can contain data in each line as follows:

<y1> <y2> <y3> ... or <y1> <y2> <y3> ...

The first row (here y1) is by default the x-axis and the others the y-axis. All possible separation characters (“.” and “,”) are accepted. This allows columns as “a=5 b=6”, where “a=” and “b=” are ignored. Each line within the

file can be either a row of data (as above) or a command. A command is also is understood as a delimiter between two curves (a data file may contain more than one dataset). This allows setting up the individual curves color and style by adding some heading commands directly into the data file.

5.7.1.2 Style files

A style file is the set of commands interpreted **before** scanning a data file (like a preset). The data file is interpreted afterwards in two steps: The first scans the floating point range needed and the second draws the data. During the first run it is possible to overwrite settings in the style file by commands in the data file.
The difference of style and data files is that data contained in style files are ignored.

Example:

```
;Title=Sample DT 231/1
;SubTitle=(Thickness homogeneity)
;xAxis=Distance [mm]
;yAxis=Thickness [nm]
```

This example sets the title, subtitle and the axis descriptions. The order of the commands can be any sequence of valid instructions. Invalid commands are ignored without message boxes popping up.

5.7.1.3 Background files

A background file is a data file, read before the selected data are drawn. This function is used especially for displaying an amount of measured data drawn on a pre-calculated set of curves. Since background files are useful for serving as a plotter only, background files can be set only by the command line. The application of these files is interesting only to the developer.

5.7.1.4 Command line options

The plot program accepts the following options at start up:

/C	only create image and display as small window, auto close (for use as batch command)
/D:<file>	data file
/B:<file>	background file
/S:<file>	style file
/X:xx	sets the image width to xx mm
/Y:xx	sets the image height to yy mm

Plot accepts any combination or none of these options. The files are used only if the path is correct and the files could be read (check access rights in case of problems).

5.7.1.5 Creating plots

A plot is simply created by loading (i.e. interpreting) the data file. The style file is specified in the options dialog. After a new file name is specified the data file is scanned to retrieve the floating point range and the message “Scanning ...” appears. The second step draws the data and “Reading ...” will appear. After completion “Ok” is shown in the status line. During the drawing process you can stop by pressing the Ctrl-key. A message box asks if the process should be aborted.

If you cannot see a plot of your data check the following:

- the path to the style file is invalid (see “Options” dialog)
- there are no data in your file

- you specified a wrong range of columns to display (“row”-command)
- the x-axis you selected does not exist (“xrow”-command)
- no marker and no lines were selected (“marker...”, “lines”, “linecolor”, “pattern” commands)
- you zoomed into an empty rectangle
- the multi-plot command “nodraw=1” may be set, but the other commands are missing

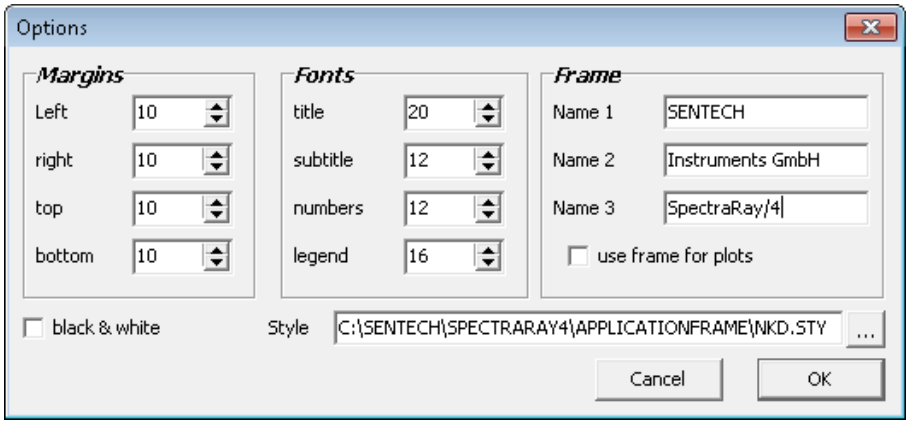


Fig. 5-190 Option screen for selecting presets and style file

5.7.1.6 Options

The options dialog (see Fig. 5-190) is a small editor for basics and settings related to printing. These settings are presets and could be overwritten by the style file. The options for printing cover the margins, some font sizes, informational presets and support for black and white printers.

The frame settings cover three text strings used to add a frame with three text items. If you don’t want the frame uncheck “use frame for plots”. The frame will not be used for saving to image files or copying to the clipboard. If you want the frame in a file, you may print to a PDF printer. A sample print with a frame is shown in Fig. 5-191-5-192.

The option “black&white” translates automatically a color scheme to black and white without changing the color definitions. You can use colors but simply switch to BW mode for print outs. The alternative would be to create a style file, with all background areas white and only lines, text and axis colored. Such styles are recommended for color printers.

A central role plays the style file defined in the edit field at the bottom. The button “…” helps to select such a file. The style file here is applied after the presets in the edit fields. For example, if you check “black&white” and the style contains a line “;BlackAndWhite=0” the checkbox has no effect.

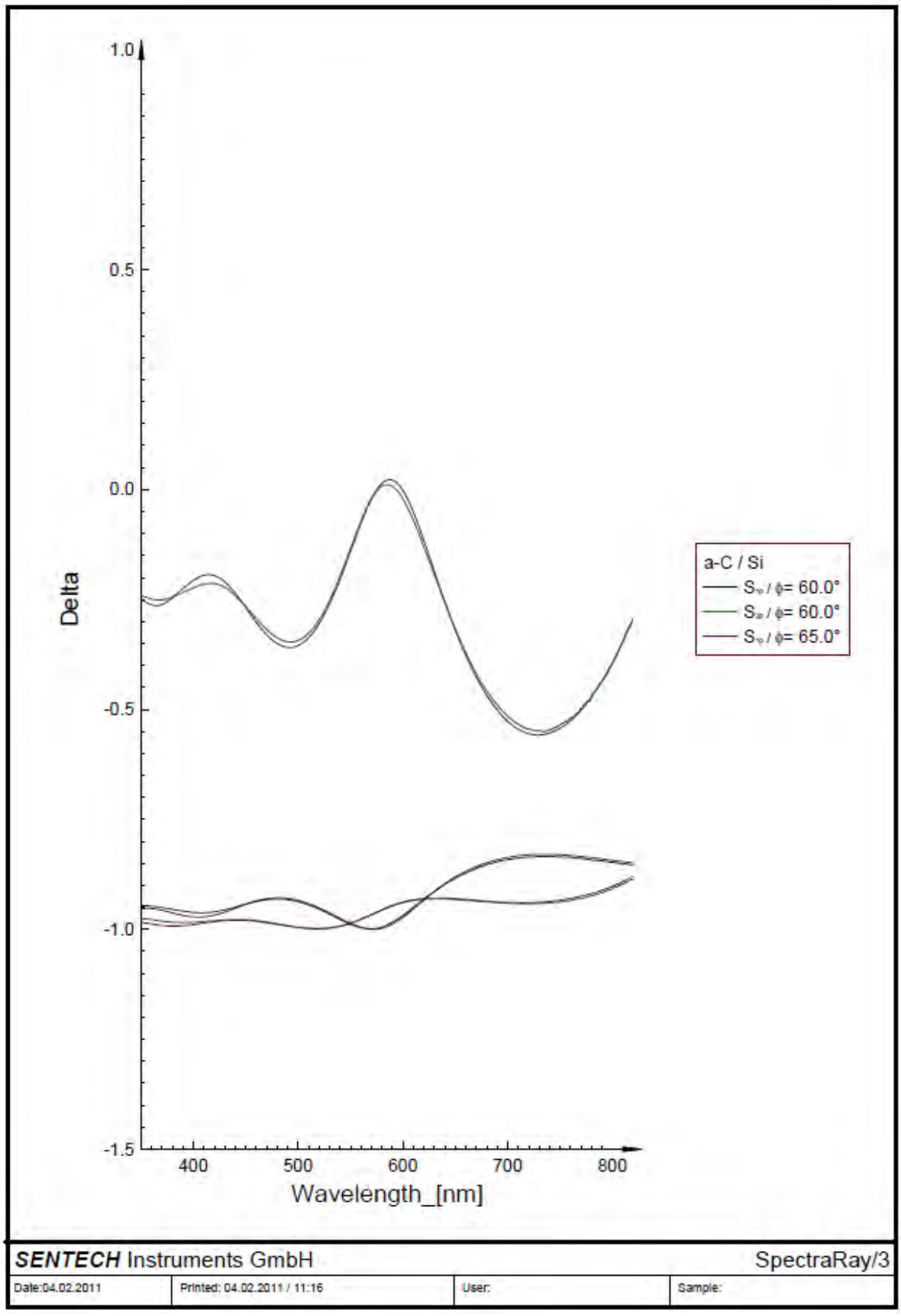


Fig. 5-191-5-192 Printout with information frame

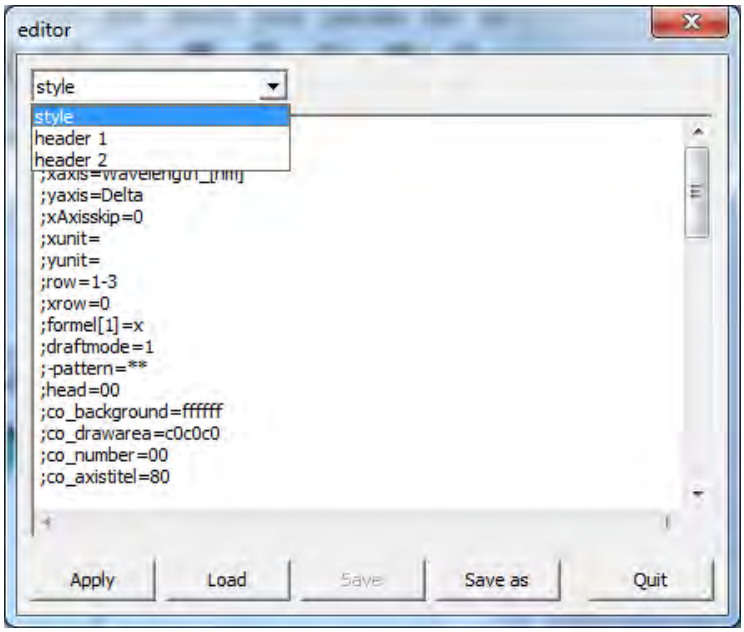


Fig. 5-193 Editing the style file

5.7.2 Editing styles

Since the style contains the layout of the picture is has to be edited very often. The “style” button on the right of the main screen opens an editor box. On the very top of the editor you may select the section to edit. The default is “style” which is exactly the style file. Since the data may also have heading commands, the editor lists the commands found preceding each data set. In the sample above we have the colors for the theory (header 1) and for the measurement data (header 2) – both in a single data file.

When you change the style, you must click on “Apply” to initiate an update. If you only click on “Quit” the changes are not used for a screen update.

You may also load an external text file into the editor box or save the box content into a new file. After you saved into a file, the save button is enabled.

Hint: You should have a style file which contains all the settings you usually need. In such case the style editor is like a property box and you don’t have to memorize the command names each time.

5.7.3 Printing

The printout opens a printer setup window. Here you may select the target printer as well as paper size and paper orientation (landscape or vertical).

The frame around the plot with fields for user and sample appears only when printing.

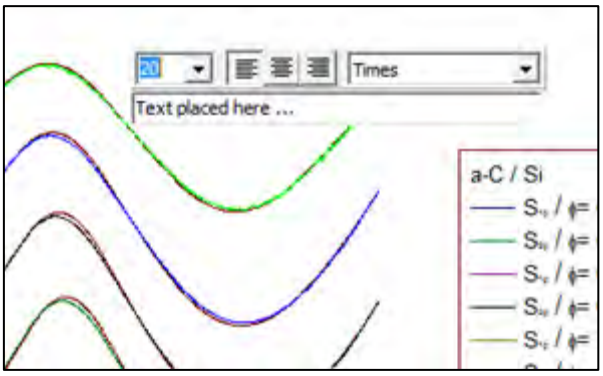


Fig. 5-194 Adding text to a plot

5.7.4 Adding text to the plot

After the plot was drawn you may want to add some text to the picture. Click the right mouse button on the position you want and the box shown in Fig. 5-194 appears. You can enter the text, font attributes and alignment. When you pressed OK the necessary instructions are *appended* to your data file. The text becomes visible after the next "Update".
If you want to edit or remove the text you should edit your data file (see the caption for the file name) and find the "MoveTo" and "Text" commands.

5.7.5 Columns, multiple files and plots, Greek symbols

Displaying columns
Even if your data have many columns you can display any subset you want by using the "row" and "xrow" command.

Multiple files in a plot
Multiple files can be plotted to a picture by using a separate command file as data file. See "Drawscale" and related commands for more information.

Multiple plots in a picture
Multiple plots in a picture require a separate command file as data file. See "Part" and related commands for more information.

Greek symbols
Any text element can consist of multiple fonts. See "Multiple font text" for more information

Zooming
This is no command but a feature of the display. You can zoom into the display by clicking the mouse button into the graphics window, holding the button, sizing the zoomed window and releasing the left mouse button. If the zoomed rectangle is larger than 5x5 pixels a zoom is performed after releasing the left mouse button. This is indicated by changing the cursor to a crosshair. If the rectangle is smaller than 5 pixels in x- or y-direction the cursor returns to an arrow, because this is no valid zoom. If you want to abort the zoom, decrease the size of the zoom rectangle until the cursor appears as an arrow.

The minimum interval you can zoom into is 0.0001.

5.7.6 Multiple font text

Most text elements can contain multiple fonts within the text. This is a normal text with commands added in "\ ... \" pairs. Such text can be used for titles, subtitles, axis descriptions and numbers (XUnit, YUnit).

Command	*Parameter*	*Description*
Arial	Size	selects the Arial font and sets the size in points if the optional parameter is used.
Times	Size	selects the Times font and sets the size in points if the optional parameter is used.
Courier	Size	selects the Courier font and sets the size in points if the optional parameter is used.
Symbol	Size	selects the Symbol font and sets the size in points if the optional parameter is used.
Arrow	Length	draws an arrow of 40 pts or the length specified (optional)
Back		move to the last character position. Multiple BACK's are not allowed
OX	Width	add an offset to the current point x-coordinate in points (for creating indices)
OY	Width	add an offset to the current point y-coordinate in points (for creating indices)

All commands can be connected by adding a ";". The standard syntax is:

\<command>[;<Command>[...]\

Remark: The "*" character is converted into a small circle (for multiplication characters).

See also:
XUnit, YUnit, XAxis, YAxis, Title, SubTitle, Text

Examples:

"This is a Greek Delta: \Symbol\D\Arial\ (as multi-font text)"
"Wavelength [nm] \arrow=12\"
"\Arial=12\H\Arial=8;OY=-4\2\Arial=12;OY=0\O is water"

5.7.7 Button Reference

Button	**Description**
Copy	Opens a window allowing copying the plot into the clipboard. The size of the generated image may be given.
Options	Opens the options window (see Fig. 5-190 on page 241)
Style	Opens the style editor (see Fig. 5-193 on page 243)
Data	Allows you to save the loaded data into an ASCII text file (export)
Update	Regenerates the window after changes
Zoom out	If zoomed, the full plot will be restored.
Help	Opens the electronic help
Load	Allows to load a file in plots internal format (*.pf) or in text format (rest of file formats)
Save	Allows to save in plots internal format (*.pf), ASCII data, sizeable images (*.wmf) and non-sizeable images (*.bmp)
Print	print to a selectable printer
OK	Quit the program

5.7.8 Command Reference

List of available commands:

AutoScale	BlackAndWhite	BorderWidth	BottomGraphSkip
Co_Axistitle	Co_Background	Co_Border	Co_DrawArea
Co_Number	Co_Line	Co_SubTitle	Co_Text
Co_Title	Date	Draftmode	DrawScale
DrawWmf	EdgeAdjust	ElliBreak	FloatWindow
Fo_Axis	Fo_Number	Fo_Title	FO_SubTitle
Formula	Frame	GridX	GridY
Head	LeftGraphSkip	LineColor	Lines
LineWidth	LockYMax	LockYMin	Marker
MarkerBorder	MarkerColor	MarkerWidth	MaxCount
MinToHour	MoveTo	NoDraw	NoLines
Numbers	OverflowDelete	Part	Pattern
Plot	RightGraphSkip	Range	Read
Row	Sample	Scale	Spectrum
StopAtMax	SubTitle	Text	Ticks
Title	TopGraphSkip	UpdateFrequency	User
Wrap360	XAxis	XAxisSkip	Xrow
XUnit	YAxis	YAxisSkip	YUnit

5.7.8.1 AutoScale and AutoScaleEx

```
;AutoScale=0|1
;AutoScaleEx=<x> <y>
```

Automatic scaling is the default mode of operation. The covered floating point range is |x|<1e7. This mode can be enabled/disabled by use of this command. If you want to use manual scaling refer to Scale and FloatWindow.

The “AutoScaleEx” allows to enable automatic scaling for x and y axis separately. For example “AutoScaleEx 0 1” sets automatic scaling off for the y-axis while it is used for the x-Axis. This is helpful if you need plots for reflectivity files which are scaled 0 ... 1 for the y-axis while the x-Axis depends on the current data. If you are using a fixed scale for one axis only, you still need to have a valid setting for both axes using the “scale” and “FloatWindow” commands.

See also:

Scale, FloatWindow

Examples:

1. Enable automatic scaling:
;autoscale=1

2. Disable automatic scaling:
;autoscale=0

3. Setup a fixed scale for y (0 ... 1) and use a dynamic x-scale

```
;Scale=200 50 1 0 0.2 0.05 1 1
;FloatWindow=0 0 1000 1
;AutoScaleEx 1 0
```

5.7.8.2 BlackAndWhite

```
;BlackAndWhite=0|1
```

The colored style is useful for screen display or color printers. If you have a black and white printer you may wish an easy conversion to your printer. You can use a special style file for these purposes. This may be useful for color printers when only the curves should be colored.
This powerful command automatically translates all colors to an economic back and white scale. This command has the same function as the checkbox in the option screen. If you use this command in your style file it overwrites the function of the button in the option screen.

Examples:

1. Set all to black and white:
```
;BlackAndWhite=1
```

2. Enable colours:
```
;BlackAndWhite=0
```

5.7.8.3 BorderWidth

```
;Borderwidth=<Size>
```

The with of frame around the plot (or the width of the scalings) is set in Pica points.

Example:

1. Smallest available line:
```
;borderwidth=0
```

2. Lines 1 pt. thick:
```
;borderWidth=1
```

5.7.8.4 BottomGraphSkip

```
;BottomGraphSkip=<Value>
```

The distance between the bottom of the plot window and the numbers at the bottom is set by this command in pica points. The value can be either positive or negative. The default layout has the value 0.

See also:
TopGraphSkip, LeftGraphSkip, RightGraphSkip, XAxisSkip, YAxisSkip

Example:

```
;BottomGraphSkip=1
```

5.7.8.5 Co_Background

;co_background=<color>

This command sets the color of background of the plot. <Color> can be a hexadecimal RGB code. See colors for additonal information.

Examples:

1. Use a blue background for plots:
```
;co_background=800000
```

2. Use a white background
```
;co_background=FFFFFF
```

5.7.8.6 Co_DrawArea

```
;co_drawarea=<color>
```

This command sets the color of the rectangle between the x- and y-axis. <Color> can be a hexadecimal RGB code. See colors for additional information.

Examples:

1. Use a blue background for curves:
```
;co_drawarea=800000
```

2. Use a white background for curves (on needle printers)
```
;co_drawarea=FFFFFF
```

5.7.8.7 Co_xxx

```
;co_<xxx>=<color>
```

This class of command sets colors of the various elements of the plot. The command relating to curves or markers are array command. Their format is:

```
;co_<xxx>[<rows>]=<color>
```

<Rows> is a set of columns for which the color should be set. If no array indicator [] is used, the color is set for all columns. See ROW for additional explanation on selecting columns.

co_number
The color of the numbers printed on the scaled axis and the color of the axis border and ticks is set.

co_axistitle
Color of the axis description (set by XAXIS or YAXIS).

co_line
The color of a line between two data points. This color can be different for any

co_border
Color of the frame, ticks and grid of the scaling axis.

co_title
Color of the main title on the top of the plot.

co_subtitle
Color of the subtitle on the top of the plot.

co_text
Color of the text plotted with the following TEXT command.

markerborder

Color of the border of the marker. This is an array command and can be used to address selected columns (“;MarkerBorder[2..4]=ffff” or “MarkerBorder=ffff” for all columns).

markercolor
Filling color of the marker. This is an array command and can be used to address selected columns (“;MarkerColor[2..4]=ffff” or “MarkerColor=ffff” for all columns).

5.7.8.8 Colors

The following list gives the R(ed)G(reen)B(lue) code of standard colors (lower cases are allowed):

```
Black             000000
White             FFFFFF
Blue              800000
Light blue        FF0000
Green             008000
Light green       00FF00
Red               000080
Light red         0000FF
Yellow            008080
Light yellow      00FFFF
Magenta           800080
Light magenta     FF00FF
Cyan              808000
Light cyan        FFFF00
Transparent      1000000
```

5.7.8.9 Draftmode

`;draftmode=1|0`

The draft mode is used to speed up drawing for large data sets. If this command uses “0” the line styles set by the pattern-command are disabled and drawn as solid lines. If the command uses “1” the pattern drawing is enabled.

Example:

1: Disable any pattern set for lines:
`;draftmode=0`

2. Enable extended line styles:
`;draftmode=1`

5.7.8.10 Date

`;Date=<String>`

If you check “Use frame for plots” a standard frame is drawn around the plot area containing several elements of text. One of these elements is the date string set by this command.

See also:
User, Sample

Examples:

```
;Date=12.1.95
;Date=01/12/95
;Date=none
```

5.7.8.11 DrawScale

```
;DrawScale
```

This command is used together with RANGE and READ to retrieve the floating point range of a file. After the floating point range is retrieved by one or more RANGE commands, the DrawScale command plots the scales. After this command one or more READ commands should plot the data.
This command requires the multiple file mode (";NoDraw=1").

See also:
Plot, Read, Part, DrawScale

Example:

The following examples requires a line ";NoDraw=1" in the style file!

This sequence combines the use of several multiple file commands. There are four files d1.dat, d2.dat, d3.dat, d4.dat to display in two plots. The two plots should be vertically stacked. The following comments should not be included in the commands:

`;Part= 2 1 2 1`	Two cells above each other and select the top cell
`;range=1,d1.dat`	Get the floating point range for plot no. 1 from d1.dat
`;range=0,d2.dat`	Expand this range with d1.dat
`;drawscale`	Draw the scales
`;read=d1.dat`	Draw the data of d1.dat
`;read=d2.dat`	Draw the data of d2.dat
`;Part= 2 1 2 2`	Two cells above each other and select the lower cell
`;range=1,d3.dat`	Get the floating point range for plot no. 2 from d3.dat
`;range=0,d4.dat`	Expand this range with d4.dat
`;drawscale`	Draw the scales
`;read=d3.dat`	Draw the data of d3.dat
`;read=d4.dat`	Draw the data of d4.dat

5.7.8.12 DrawWmf

```
;DrawWMF=<filename>
```

A Metafile can be drawn in the background if this command is used to set a valid filename. The metafiles accepted **must** be Windows metafiles without a placement header. The filling colors for the drawing area and background should be set to transparent (color code "1000000").

Example:

```
;DrawWmf=c:\temp\picture1.wmf
```

5.7.8.13 ElliBreak

```
;ElliBreak=<Value>
```

In many cases curves show sharp changes. If you use lines you might want to connect data points with small changes and not to connect those with sharp changes. This command sets the level for connecting data points. If the distance in the xy-plane is larger this value no lines are drawn. If the level is 0 all lines are drawn.
The distance in the xy-plane is calculated by d=sqrt((x1-x2)^2+(y1-y2)^2).

Example:

```
;ellibreak=100
```

5.7.8.14 FloatWindow

```
;FloatWindow=<XMin> <Ymin> <Xmax> <YMax>
```

This command is used for manual scaling. Manual scaling requires a floating point range and to define the positions for numbers and ticks. The latter definition is set be the Scale command. The parameters define the floating point range to display. The data may be outside this range, necessary clipping in floating point coordinates is performed.

See also:
Autoscale, Scale

Example:

Display only data within 0..15 for x and 7 to 9 for y.

```
;floatwindow=0 7 15 9
```

5.7.8.15 Frame

```
;Frame=<SizeX> <SizeY>
```

The plot area of a single data plot can be reduced by additional borders defined by SizeX and SizeY in Pica points. This command is useful for multiple plots in one picture (see PLOT, PART). It allows to increase the separation of each plot individually.

See also:
Plot, Range, Read, Part, Drawscale

Examples:

```
;Frame=1 1
;Frame=2 -4
```

5.7.8.16 Fo_Axis

```
;Fo_Axis=<Size>
```

The size of the axis description on the scales could be set in Pica points.

See also:
Fo_Number, Fo_Title, Fo_Subtitle

Example:

```
;Fo_Axis=12
```

5.7.8.17 Fo_Number

```
;Fo_Number=<Size>
```

The size of the numbers on the scales could be set in Pica points.

See also:
Fo_Axis, Fo_Title, Fo_Subtitle

Example:

```
;Fo_number=12
```

5.7.8.18 Fo_SubTitle

```
;Fo_SubTitle=<Size>
```

The size of the subtitle on the top of the plot is set in Pica points.

See also:
Fo_Number, Fo_Axis, Fo_title

Example:

```
;Fo_SubTitle=12
```

5.7.8.19 Fo_Title

```
;Fo_Title=<Size>
```

The size of the title on the top of the plot is set in Pica points.

See also:
Fo_Number, Fo_Axis, Fo_Subtitle

Example:

```
;Fo_Title=16
```

5.7.8.20 Formula

```
;Formula=<expression>
```

This array command allows data manipulation individual for each column (including active x-axis). The expression can contain any basic mathematical operation. It consists of a token series **delimited by one or more spaces** (this increases operational speed). Each token consists of an operator and operand. The calculation is executed from left to right.
The supported operators are “+”, “-“, “*” and “/”. An operand can be either a floating point constant or the abscissa “x”. This abzissa are the data values for the selected columns.
As many other commands the formula can be set within the style file and within the data file. This allows to switch between formula and design within data files with multiple data sets.

If x is 2 the following expressions give the results listed below:

x	2
1	1
1+x	3
1/x	0.5
x/2	1
1 +x/4	1.5
2 *x *x	8

Examples:

1. The x-axis has data in seconds, but the output should be scaled in minutes (the x-axis is the first column):

```
;xrow=0
;formula[0]=x/60
```

2. The second column is 1000 times larger than the first. A display should divide the second by 1000:

```
;formula[2]=x/1000
```

5.7.8.21 GridX, GridY

```
;GridX=0|1
```

These commands enable the drawing of horizontal and/or vertical dotted grid lines. A “0” disables the grid line while “1” enables the grid line. GRIDX is used to select horizontal grid lines and GRIDY drives vertical grid lines.

Examples:

The following example disables the vertical grid lines and enables the horizontal lines:

```
;gridx=1
;gridy=0
```

5.7.8.22 Head

```
;Head=<no>
```

The head command does literally the same as the Unix command head. Its purpose is to use only the first n lines of a large data file for display. If you have a large data set of 10000 data points and you want to design your colors, line styles, axis descriptions and titles the drawing of all data would be poorly slow. The use of head speeds up your work.
If the <no> is 0, the full file is used. Any other number gives the number of lines to read for display.

Examples:

1. Read the full file:

```
;head=0
```

2. Read only the first 100 data lines:

```
;head=100
```

5.7.8.23 EdgeAdjust

```
;EdgeAdjust=0|1
```

The first and last numbers are positioned on the beginning and end of the y-axis. If these numbers are centered the beginning of the y-axis they may overwrite the first and last x-number in some cases. The bottom adjustment is for the first y-value and the top alignment for the last y-value or centered alignment for both numbers is set by this command.
This default is adjustment enabled (the first and last are *not* centered).

Examples:

1. The first and last y-numbers should be centered:
```
;edgeadjust=0
```

2. The first and last y-numbers should not overwrite in all cases:
```
;edgeadjust=1
```

5.7.8.24 LeftGraphSkip

```
;LeftGraphSkip=<Value>
```

The distance between the left of the plot window and the numbers at the left is set by this command in pica points. The value can be either positive or negative. The default layout has the value 0.

See also:
TopGraphSkip, BottomGraphSkip, RightGraphSkip, XAxisSkip, YAxisSkip

Example:

```
;LeftGraphSkip=1
```

5.7.8.25 Lines

```
;Lines
```

This command enables lines between data points. It is an array command which allows enabling lines for selected columns.

See also:
NoLines, LineColor, LineWidth, Pattern, Draftmode

Example:

```
;lines
;lines[1..4]
```

5.7.8.26 LineColor

```
;LineColor=<Color>
```

This sets the color of lines between data points from a hexadecimal longint. It is an array command which allows setting the line color for selected columns. See colors for explanation of the color data format.

See also:
Lines, NoLines, LineWidth, Pattern, Draftmode, Colors
Example:

Set yellow lines for all columns:
```
;linecolor=ffff
```

5.7.8.27 LineWidth

```
;LineWidth=<Value>
```

This sets the width of lines between data points in pica points. It is an array command which allows setting the width of lines for selected columns.

See also:
Lines, NoLines, LineColor, Pattern, Draftmode

Example:

```
;linewidth=1
;linewidth=5
```

5.7.8.28 LockYMax

```
;LockYMax=0|1
```

The automatic scaling normally extends the y-axis to higher values to find a suitable end value for the y-axis, so that the last number is at the end of the axis. This automatic extension can be disabled by the LockYMax command. If this is used the floating point range retrieved from the data file is not expanded to higher values.

See also:
LockYMin, Spectrum

Examples:

1. Disable automatic extension to higher y-values:
```
;LockYMax=0
```

2. Enable automatic extension to higher y-values:
```
;LockyMax=1
```

5.7.8.29 LockYMin

```
;LockYMin=0|1
```

The automatic scaling normally extends the y-axis to lower values to find a suitable starting value for the y-axis, so that the first number is at the beginning of the axis. This automatic extension can be disabled by the LockYMin command. If this is used the floating point range retrieved from the data file is not expanded to lower values.

See also:
LockYMax, Spectrum

Examples:

1. Disable automatic extension to lower y-values:
```
;LockYMin=0
```
2. Enable automatic extension to lower y-values:
```
;LockyMin=1
```

5.7.8.30 Marker

```
;marker=<number>
```

A marker is the drawing of a single data point. Each marker has a layout defined by the marker number, a width, a color for the border and a filling color. Connecting of data points is set by the LINES command.

Number	Layout
0	no marker
1	rectangle
2	circle
3	triangle (baseline at bottom)
4	triangle (baseline at top)
5	rectangle with diagonal crosshair
6	rectangle with horizontal crosshair
7	hexagon
8 or higher	point

See also:
markerborder, markercolor, markerwidth, Lines

Examples:

The marker type of the second column should be “circle”, the 4th to 6th should be hexagons while all other should be only points.

```
;marker=8
;marker[2]=2
;marker[4..6]=7
```

5.7.8.31 MarkerBorder

```
;markerborder=<color>
```

This sets the color of the border of the marker. This is an array command and can be used to address selected columns (“;MarkerBorder[2..4]=ffff” or “MarkerBorder=ffff” for all columns).

See also:
Co_xxx, Colors

Examples:

Set the second marker to a yellow border with black filling color:

```
;markerborder[2]=ffff
;markercolor[2]=0
```

5.7.8.32 MarkerColor

```
;MarkerColor=<color>
```

This sets the filling color of the marker. This is an array command and can be used to address selected columns (“;MarkerColor[2..4]=ffff” or “MarkerColor=ffff” for all columns).

See also:
Co_xxx, Colors

Examples:

Set the second marker to a yellow border with black filling color:

```
;markerborder[2]=ffff
;markercolor[2]=0
```

5.7.8.33 MarkerWidth

```
;MarkerWidth=<size>
```

The size of the marker is set in Pica points.

See also:

MarkerColor, MarkerBorder, Marker

Examples:

```
;MarkerWidth=2
;MarkerWidth=5
```

5.7.8.34 MaxCount

```
;MaxCount=<Number>
```

This command is used in style files for the SE 401 insitu ellipsometer to drive the queuing of data. For the plot program itself this command has no influence.
For the SE 401 this is the maximum number of data displayed during data collection. If your computer is slower a value of 200 may be a good choice. Fast computers may work with 1000 data points. The parameter of this command can be an integer number from 100 to 2000. If the number of data exceeds the MaxCount value, the first N data are deleted (and saved to hard disk) where N is a value set by the OVERFLOWDELETE command.

Example:

```
;MaxCount=500
```

5.7.8.35 MinToHour

```
;MinToHour=0|1
```

This old command is supported only for compatibility. It has the same effect as “;formula=x /60”. It divides all x-data by 60 and emulates a conversion of minutes to hours.

Examples:

1. Enable conversion:
```
;MinToHour=1
```

2. Disable conversion:
```
;MinToHour=0
```

5.7.8.36 MoveTo

```
;Moveto=<XFloat> <YFloat>
```

This command is used for adding text to a plot. It sets the position of the next text output in floating point coordinates. This command precedes the TEXT command.
It is designed for use by programs creating data sets. If you want to add text after the data set was created use the plot dialog window for this purpose.

See also:
Text

Examples:

```
;moveto=2.3 4.5
;moveto=-3.14159 0
```

5.7.8.37 NoDraw

```
;NoDraw=0|1
```

This command is used to enable multiple file / multiple plot operations. If you want to use the Read, Plot, Part or Range command, the command NoDraw **must** be used with parameter "1". If you want to return to single file operations (standard) you must use the command with parameter "0".
If you use multiple file plotting the data file contains only the commands for reading and processing files.

See also
Read, Plot, Range, Part

Examples:

Enter multi file operations:
```
;nodraw=1
```

Return to single file operations:
```
;nodraw=0
```

5.7.8.38 NoLines

```
;NoLines
```

This command disables lines between data points. It is an array command which allows disabling lines for selected columns.

See also:
Lines, LineColor, LineWidth, Pattern, Draftmode

Example:

```
;noLines
;noLines[1..4]
```

5.7.8.39 Numbers

```
;Number=<Left> <Top> <Right> <Left>
```

This command selects the axis with plotted numbers. You can select any of the four axes available for numbers. Each of the above parameters can be “0” (select the axis) or “1” (do not draw numbers there).

Examples:

1. Numbers left and at the bottom of the plot:
```
;numbers=1 0 0 1
```

2. Numbers at all axis:
```
;numbers=1 1 1 1
```

3. Numbers left, right and at the bottom:
```
;numbers=1 0 1 1
```

5.7.8.40 OverflowDelete

```
;OverflowDelete=<Number>
```

This command is used in style files for the SE 401 in-situ ellipsometer to drive the queuing of data. For the plot program itself this command has no influence.
For the SE 401 MAXCOUNT is the maximum number of data displayed during data collection. If your computer is slower a value of 200 may be a good choice. Fast computers may work with 1000 data points. The parameter of this command can be an integer number from 100 to 2000. If the number of data exceeds the MaxCount value, the first N data are deleted (and saved to hard disk) where N is a value set by the OVERFLOWDELETE command.

Example:

```
;MaxCount=500
```

5.7.8.41 Part

```
;Part=<NoCellsY> <NoCellsX> <CellY> <CellX>
```

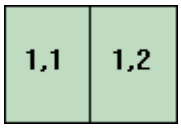
The whole plot area is divided into cells like a matrix of plots. You have a number of plots in horizontal direction <NoCellsX> and a number of cells in vertical direction <NoCellsY>. The second two parameters select the cell from the matrix defined with the first two parameters. The first cell is 1 for both directions and is the lowest most left cell of the matrix.
This definition sets the part of the whole drawing area, where the next plot is positioned. By means of multiple PART commands it is possible to change the matrix from plot to plot. This enables the user to overwrite parts of previous plots and care is required in using this command.
This command requires the multiple file mode (“;NoDraw=1”).

See also:
Plot, Range, Read, DrawScale

Example:

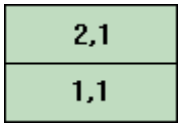
The following examples requires a line “;NoDraw=1” in the style file!

1. Define the following array with d1.dat to (1,1) and d2.dat to (1,2):



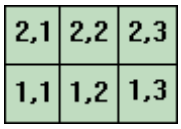

```
;part=1,2,1,1
;plot=d1.dat
;part=1,2,1,2
;plot=d2.dat
```

2. Define the same array vertically with d1.dat to (1,2) and d2.dat to (1,1):



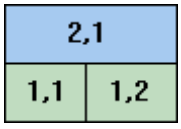

```
;part=2,1,2,1
;plot=d1.dat
;part=2,1,1,1
;plot=d2.dat
```

3. The next example may give a crucial display but works good for landscape printing (set the font sizes to lower values such as 10 or 8 pts.). The top row should display d1.dat, d2.dat and d3.dat (from left to right), the bottom row d4.dat, d5.dat and d6.dat.




```
;part=2,3,2,1
;plot=d1.dat
;part=2,3,2,2
;plot=d2.dat
;part=2,3,2,3
;plot=d3.dat
;part=2,3,1,1
;plot=d4.dat
;part=2,3,1,2
;plot=d5.dat
;part=2,3,1,3
;plot=d6.dat
```

4. The last example demonstrates the combination of suitable matrix arrangements. The blue cell should contain d1.dat while the green (1,1) is for d2.dat and green (1,2) is for d3.dat:




```
;part=2,1,2,1
;plot=d1.dat
;part=2,2,1,1
;plot=d2.dat
;part=2,2,1,2
;plot=d3.dat
```

5.7.8.42 Pattern

A pattern describes the line style. You can select solid or dotted lines or any other style. The default line style is a solid line. A pattern can be up to 30 characters long.

***	solid line
--*	dotted line
*****--*--	dash dot line
*******---------	dashed line

Each "*" is a solid segment of the line with a length of the line width. Each "-" describes an empty segment. The command is a typical array command since it refers to single curves. This command works only if the draft mode is disabled (see "draftmode").

Example:

```
;Pattern=*                all curves have solid lines
;Pattern[2]=*-            column 2 is dotted
;Pattern[3]=***---        column 3 is dashed
;Pattern[3,5..6]=***---   column 3 and 5 to 6 are dashed
```

5.7.8.43 Plot

```
;Plot=<filename>
```

This command draws a whole file into a selected rectangle. This command requires to switch to multiple file mode by "NoDraw=1". The default rectangle is the whole drawing area.

See also:
Range, Read, Part, DrawScale

Examples:

The following examples requires a line ";NoDraw=1" in the style file!

1. This axamples should draw a single file:

```
;plot=c:\temp\sample1.dat
```

2. Two data files should be plotted with horizontal adjustment. The PART command is used to split the draw are into 1 piece in y-direction and 2 pieces in x-direction and to select cell 1 for y and cell 1 for x direction. This is the lower left cell. The plot command draws the first file. The second PART command selects the same cell sizes but the lower right cell. A second PLOT command draws the second file:

```
;part=1 2 1 1
;plot=c:\temp\filter1.dat
;part=1 2 1 2
;plot=c:\temp\filter2.dat
```

2. It should be mentioned, that all style elements could be changed during this plot. For example the titles could be set (modified example 1):

```
;title=Filter No. 1
;part=1 2 1 1
;plot=c:\temp\filter1.dat
;title=Filter No. 2
;part=1 2 1 2
;plot=c:\temp\filter2.dat
```

3. A second type of modification is to change the displayed columns. This example uses the same cell adjustments but the left plot should show the first and the right plot the second column:

```
;title=Column 1
;part=1 2 1 1
;row=1
;plot=c:\temp\filter.dat
;title= Column 2
;part=1 2 1 2
;row=2
;plot=c:\temp\filter2.dat
```

5.7.8.44 Range

```
;Range=0|1,<filename>
```

This command is used together with DRAWSCALE and READ to retrieve the floating point range of a file. For multiple file operations the first parameter is a flag whether the file to scan is the first file or not. If you want to scan a single file this parameter should always be 1 otherwise the first file has 1 and all following files require a 0. This flag must be followed by a colon (“,”) and a filename.
This command requires the multiple file mode (“;NoDraw=1”).

See also:
Plot, Read, Part, DrawScale

Example:

The following examples requires a line “;NoDraw=1” in the style file!

This sequence combines the use of several multiple file commands. There are four files d1.dat, d2.dat, d3.dat, d4.dat to display in two plots. The two plots should be vertically stacked. The following comments should not be included in the commands:

```
;Part= 2 1 2 1      Two cells above each other and select the top cell
;range=1,d1.dat     Get the floating point range for plot no. 1 from d1.dat
;range=0,d2.dat     Expand this range with d1.dat
;drawscale          Draw the scales
;read=d1.dat        Draw the data of d1.dat
;read=d2.dat        Draw the data of d2.dat
;Part= 2 1 2 2      Two cells above each other and select the lower cell
;range=1,d3.dat     Get the floating point range for plot no. 2 from d3.dat
;range=0,d4.dat     Expand this range with d4.dat
;drawscale          Draw the scales
;read=d3.dat        Draw the data of d3.dat
;read=d4.dat        Draw the data of d4.dat
```

5.7.8.45 Read

```
;Read=<filename>
```

The read command is used together with DRAWSCALE and RANGE. It draws the lines and markers of a data file into the plot. This allows to draw multiple files into the same scale.
This command requires the multiple file mode (“;NoDraw=1”).

See also:
Plot, Range, Part, DrawScale

Example:

The following examples requires a line “;NoDraw=1” in the style file!

This sequence combines the use of several multiple file commands. There are four files d1.dat, d2.dat, d3.dat, d4.dat to display in two plots. The two plots should be vertically stacked. The following comments should not be included in the commands:

```
;Part= 2 1 2 1      Two cells above each other and select the top cell
;range=1,d1.dat     Get the floating point range for plot no. 1 from d1.dat
;range=0,d2.dat     Expand this range with d1.dat
;drawscale          Draw the scales
;read=d1.dat        Draw the data of d1.dat
;read=d2.dat        Draw the data of d2.dat
;Part= 2 1 2 2      Two cells above each other and select the lower cell
;range=1,d3.dat     Get the floating point range for plot no. 2 from d3.dat
;range=0,d4.dat     Expand this range with d4.dat
;drawscale          Draw the scales
;read=d3.dat        Draw the data of d3.dat
;read=d4.dat        Draw the data of d4.dat
```

5.7.8.46 RightGraphSkip

```
;RightGraphSkip=<Value>
```

The distance between the right of the plot window and the numbers at the right is set by this command in pica points. The value can be either positive or negative. The default layout has the value 0.

See also:
TopGraphSkip, BottomGraphSkip, LeftGraphSkip, XAxisSkip, YAxisSkip

Example:

```
;RightGraphSkip=1
```

5.7.8.47 Row

```
;row=<No>|<range>[,<no>|<range> ...]
```

The format of a text line read from data files is

<d0>,<d1>,<d2> ....

The standard display uses d0 as x-axis and d1 as y-axis. Curves are separated by lines that do not contain valid data or have a ";" as first character. One of the most important tasks of the style file is to choose the columns used for x- and y-axis. The ROW command selects the columns that are displayed. This can be any number of columns. If the data do not exist in the selected column no data are drawn. If you load a data file and see no pictures you have a wrong "row" / "xrow"-command or automatic scaling is not active while the scale command works outside the data range.

Note: The maximum supported row number is 30. You may have more data columns, but you need to separate it into individual data sets (use SpectraRay "Trim" command to create a copy of individual columns).

Examples:

1. Standard display for (x,y)-files:
```
;row=1
```

2. Display to columns d1,d2:
```
;row=1,2
```

3. Display the columns 4..6:
```
;row=4..6
```

4. Display 1 and 4..6:
```
row=1,4..6
```

5.7.8.48 Sample

```
;Sample=<String>
```

If you check “Use frame for plots” a standard frame is drawn around the plot area containing several elements of text. One of these elements is the sample description set by this command.

See also:
Date, User

Examples:

```
;Sample=15-0000-37
;Sample=VR 271 B
;Sample=
```

5.7.8.49 Scale

```
;Scale=<XNum> <Xtick> <XDig> <Xcolon> <YNum> <Ytick> <YDig> <YColon>
```

The manual scaling requires this command to set the positions for numbers and ticks. The parameters are two identical groups for the x and y axis. Each group has the following data:

Num	Interval for numbers
Tick	Interval for ticks
Dig	Digits for the number (1 is good for all cases)
Colon	Digits displayed after the colon

See also:

Autoscale, FloatWindow

Example:

A manual scaling should display data within 0..10 for x and 7..9 for y. The x-axis numbers should be 0, 2..10, the ticks should be at 0, 0.5, 1, .. 10. The y-axis numbers should be 7, 7.5..9, the ticks should be at 7, 7.1, 7.2, .., 9. The full command sequence would be the following:

`;autoscale=0`	disable automatic scaling
`;floatwindow=0 7 10 9`	set the desired floating point range
`;scale=2 0.5 1 0 0.5 0.1 1 1`	set the differences and 0 and 1 digits after the colon

5.7.8.50 Spectrum

```
;Spectrum=0|1
```

The data that are to display cover a certain floating point range. The automatic scaling normally extends the x- and y-axis to start at suitable numbers for scaling. In this mode the left edge of the x axis contains the first scaling number and the right edge contains the last number. This default mode is useful for free curves in the xy-plane and ensures a certain distance to top, left, right and bottom.
In many cases this behavior creates a gap between the first and last x-values and the start end of the scaled axis. In such cases the automatic extension of the x-axis should be disabled by this command. Its name describes the type of curves for which disabling is useful.
See also:

LockYMin, LockYMax

Examples:

1. Disable the automatic x-axis extension for spectrum like curves:
```
;Spectrum=1
```

2. Enable the automatic x-axis extension for free curves in the xy-plane:
```
;Spectrum=0
```

5.7.8.51 StopAtMax

This command is useful for large amounts of data. This enables the program to stop reading, when the scanned or zoomed maximum of the x-axis is reached. You should use this command for data of the spectrum type, not for free curves. Free curves could have parts that return to lower x-values. If your dataset consists of subsequent datasets you should reset this flag.
For the case of large datasets with sorted x-values this flag accelerates zooming and displaying parts of the dataset.

Example:

```
;StopAtMax=0        disables the stop of reading at maximum
;StopAtMax=1        enables the stop of reading at maximum
```

5.7.8.52 Subtitle

```
;Subtitle=<Text>
```

The plot can contain a header consisting of a title and subtitle. The command subtitle sets the sub-header part of the plot. You can use the multiple font feature to create text output.

Examples:

```
;subtitle=Operator John Little
;subtitle=Measured with single wavelength ellipsometer at \symbol=12\l\arial=12\=633 nm
```

5.7.8.53 Text

```
;Text=<intHeight>,<Align>,<Font>,<Text-String>
```

This command allows text output to be added to a plot. The text relates to the current plot-window in floating point coordinates. It assumes the position set by a preceding MOVETO command.

intHeight	font size in Pica points
Align	Text-Alignment: 1 - left 2 - right 4 - centered
Font	Font-ID: 1 - Times 2 - Swiss 4 - Symbol 8 - Courier
Text	String of up to 200 characters, multi-font is allowed

See also:

MoveTo, Co_Text

Examples:

1. At the floating point (10,12) a text “Maximum” should be added centered (4) in 12 pts. Arial (i.e. Swiss:2):

```
;moveto=10,11.2
;text=12, 4, 2,Maximum
```

5.7.8.54 Ticks

```
;Ticks=<LongLen> <ShortLen>
```

The length of the ticks could be set by this command. It is possible to select the ticks inside, outside or no ticks. The parameter LongLen is the length of the ticks at numbers on the scaling axis in pica points. The parameter ShortLen describes the tick length between the numbers in pica points. Both values can be a negative or positive numbers.

Examples:

1. Ticks inside:
```
;ticks=4 2
```

2. Ticks outside:
```
;ticks=-4 -2
```

3. Tick inside, only at numbers:
```
;ticks=4 0
```

5.7.8.55 Title

```
;Title=<Text>
```

The plot can contain a header consisting of a title and subtitle. The command title sets the header part of the plot. You can use the multiple font feature to create text output.

Examples:

```
;Title=This is a title
;Title=Photoresist on Silicon
;Title=Oil on H\oy=-2\2\oy=0\O
```

The latter example uses the multiple font feature and describes oil on water.

5.7.8.56 TopGraphSkip

```
;TopGraphSkip=<Value>
```

The distance between the subtitle and the numbers at the top of the plot is set by this command in pica points. The value can be either positive or negative. The default layout has the value 0.

See also:
BottomGraphSkip, LeftGraphSkip, RightGraphSkip, XAxisSkip, YAxisSkip

Example:

```
;topgraphskip=1
```

5.7.8.57 UpdateFrequency

```
;UpdateFrequency=<number>
```

When a plot is drawn the program first scans the whole file to retrieve the floating point range of data. The next step draws the scaling axis and the third step draws the curves. During the third step the display is actualized periodically. This update is executed every N-th line, where N is 100 as default and set by this command. If you set N to higher values the reading will be faster while lower values slow down the reading but show earlier more information.

Examples:

```
;updatefrequency=200
```

5.7.8.58 User

```
;User=<String>
```

If you check “Use frame for plots” a standard frame is drawn around the plot area containing several elements of text. One of these elements is the user name set by this command.

See also:
Date, Sample

Examples:

```
;User=UR
;User=Micheal
;User=
```

5.7.8.59 Wrap360

```
;Wrap360=0|1
```

Ellipsometry measures the so called ellipsometric angles PSI and DELTA in degrees. Delta is periodical. This means values of 359° are identical to -1°. When measuring around DELTA=0° (or 360°) it would be convenient to have a zero crossing line and no sharp changes between 0° and 360°. This special feature converts all data x>180° to 360°-x.

Examples:
1. Enable wrapping data:
```
;wrap360=1
```

2. Disable wraping data:
```
;wrap360=0
```

5.7.8.60 XAxis

```
;xaxis=<Text>
```

The title of the x-axis is written at the bottom of the plot. The text can be a multiple font text. If text is empty, no axis description will be plotted and the plot will be larger.
Examples:

```
;xaxis=Angle of incidence [°]
;xaxis=Process time [min]
```

5.7.8.61 XAxisSkip

```
;XAxisSkip=<Value>
```

The distance between the numbers and the title of the x-axis is set by this command in pica points. The value can be either positive or negative. The default layout has the value 0.

Example:

Increase the distance by 10 pts.:

```
;xaxisskip=10
```

5.7.8.62 XRow

```
;xrow=<No>
```

The format of a text line read from data files is

<d0>,<d1>,<d2> ....

The standard display uses d0 as x-axis and d1 as y-axis. Curves are separated by lines that do not contain valid data or have a ";" as first character. One of the most important tasks of the style file is to choose the columns used for x- and y-axis. The XROW command selects the column used for the x-Axis.

Examples:

1. Standard display for (x,y)-files:
```
;xrow=0
```

2. The second column contains the x-axis (for example for data like <counter>, <time>, <meas. values>:
```
;xrow=1
```

5.7.8.63 Xunit, Yunit

```
;xunit=<Text>
```

The text written at the number positions during scaling the axis can contain text defined by these commands. The general format for this multiple font text is

<Text1>##<Text2>

The output written to the axis ticks consists of a piece of text written before and a second text write after the number. The position of the number is detected by the "##". If no "##" is used the full text is appended to the number. If numbers only should be used the <Text> should be empty.

Examples:

1. Use no additional text:
```
;xunit=
```

2. Add seconds (the space after "=" is used to separate the number and the seconds):
```
`;xunit= s
```
3. Use the pattern "t= 1 s":

```
;xunit=t= ## s
```

4. Add powers of ten to signal a factor used:

```
;xunit=\arial=12\*10\oy=5,arial=8\-4
```

5.7.8.64 YAxis

```
;yaxis=<Text>
```

The title of the y-axis is written at the left side of the plot. The text can be a multiple font text. If text is empty, no axis description will be plotted and the plot will be larger.

Examples:

```
;yaxis=Psi [deg] \arrow\
;yaxis=\symbol=12\D\arial=12\ [deg] \arrow=20\
```

5.7.8.65 YAxisSkip

```
;YAxisSkip=<Value>
```

The distance between the numbers and the title of the y-axis is set by this command in pica points. The value can be either positive or negative. The default layout has the value 0.

Example:

Increase the distance by 10 pts.:

```
;yaxisskip=10
```

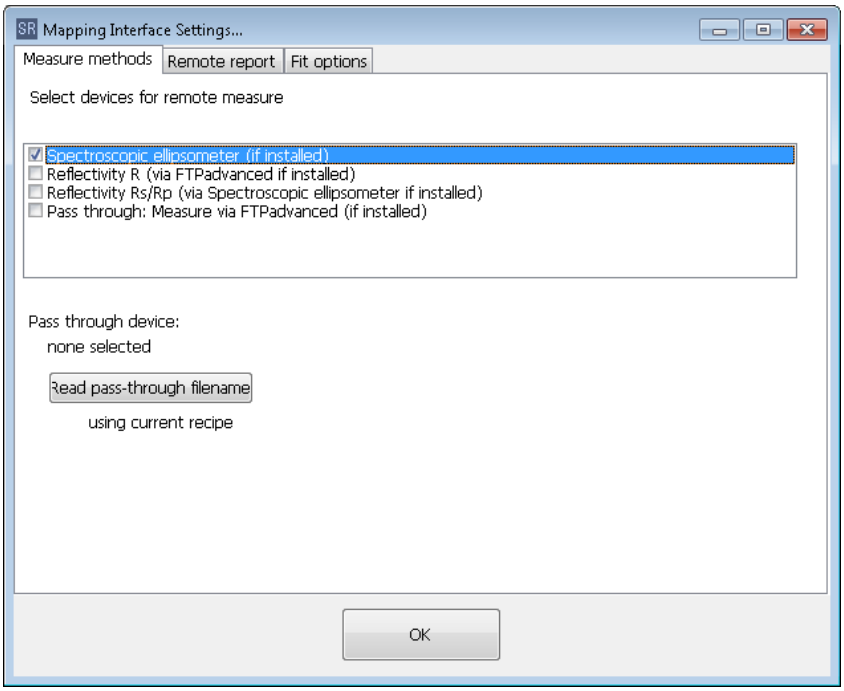
5.8 Measurements via Mapping Interface

The SE-Advanced module can be used as a device driver for the Mapping module.
In the Mapping Manual it is described how to configure SE-Advanced as a device driver for Mapping.

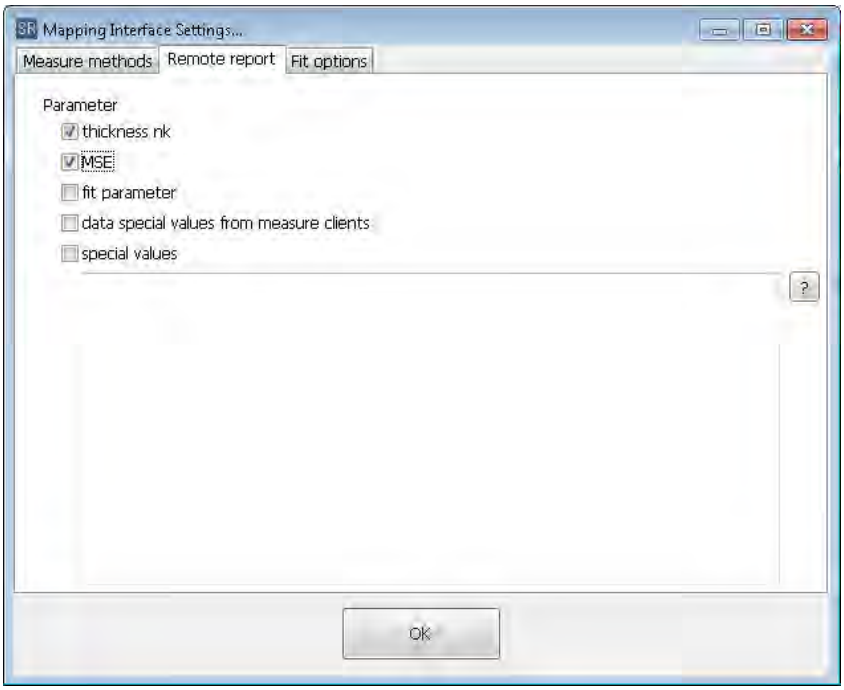
Every change in the recipe must be saved because the Mapping module reloads the recipe every time when the mapping is started.

To configure the SE-Advanced recipe it is necessary to open the “Mapping Interface Settings” dialog.
This is in the Menu Options located.

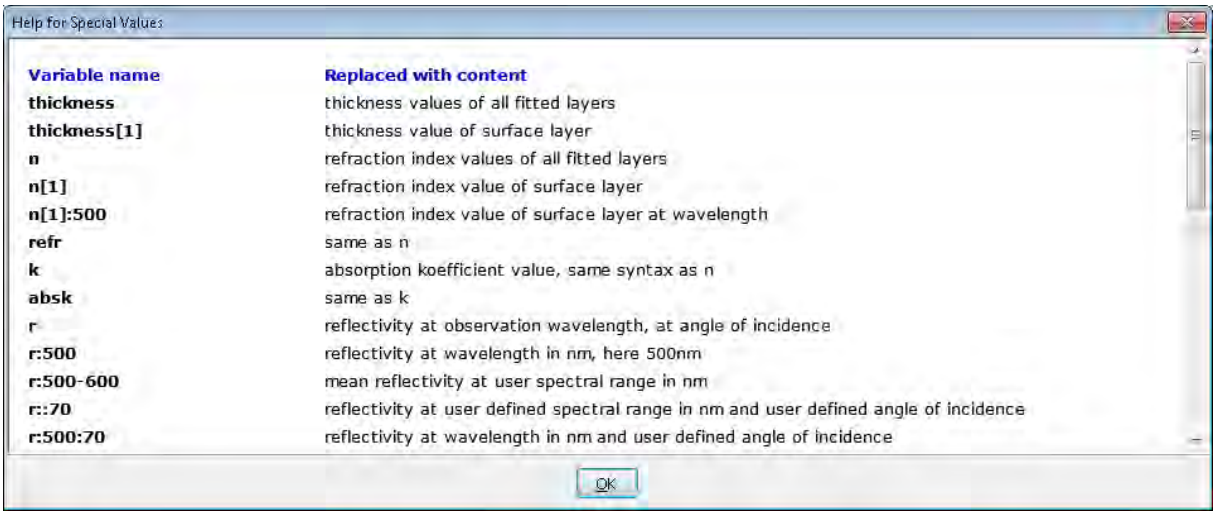
On the first tab the measurement method can be selected. It is possible to select more than one, if any selected is not a “pass through” entry. Every entry requires the necessary equipment.
The first three entries use the settings of the Measurement page (see chapter 5.1.1). The pass through device uses only the settings defined in the device. For the pass through device it is mandatory to specify the filename, this can be done by clicking on the button. This file is read and restored if the mapping begins.



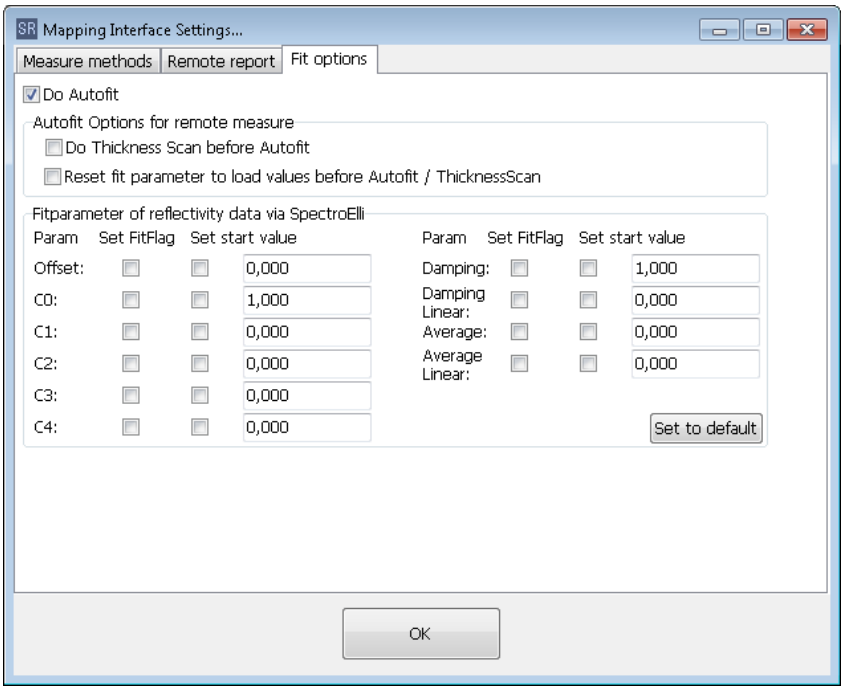
The parameters returned to mapping are specified on the second tab. There are some predefined parameters.
In addition some special values can be specified in the text box.



A detailed help for the special values can be opened by clicking on the question mark.



On the third tab some fit options can be defined.
For reflectivity measurements the stray light parameters can be selected for fit and the start value can be defined.


Mapping Interface Settings...
Measure methods
Remote report
Fit options
Do Autofit
Autofit Options for remote measure
Do Thickness Scan before Autofit
Reset fit parameter to load values before Autofit / ThicknessScan
Fitparameter of reflectivity data via SpectroElli
Param
Set FitFlag
Set start value
Offset:
0,000
C0:
1,000
C1:
0,000
C2:
0,000
C3:
0,000
C4:
0,000
Param
Set FitFlag
Set start value
Damping:
1,000
Damping Linear:
0,000
Average:
0,000
Average Linear:
0,000
Set to default
OK

6 SE-Advanced in-situ module

The SE-Advanced in-situ module is a powerful software package designed for measuring data with in-situ ellipsometers, handling of these data and evaluation of these data. The functionalities of this module are described in the following chapters. As the SE-Advanced in-situ view is similar to the standard SE-Advanced view see chapter 5 for more details as they may not be repeated in the following paragraphs.

6.1 Access to the in-situ view

The in-situ view is embedded in the SpectraRay application frame. It can be accessed by clicking on the entry 'SE-Advanced - Insitu' in the menu at the top or on the tab selector at the bottom.

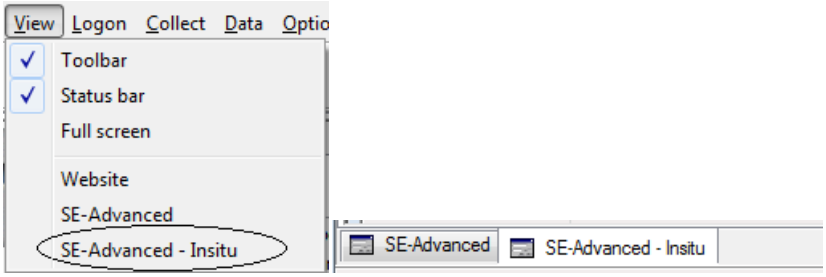


Fig. 6-1 Access to the in-situ view

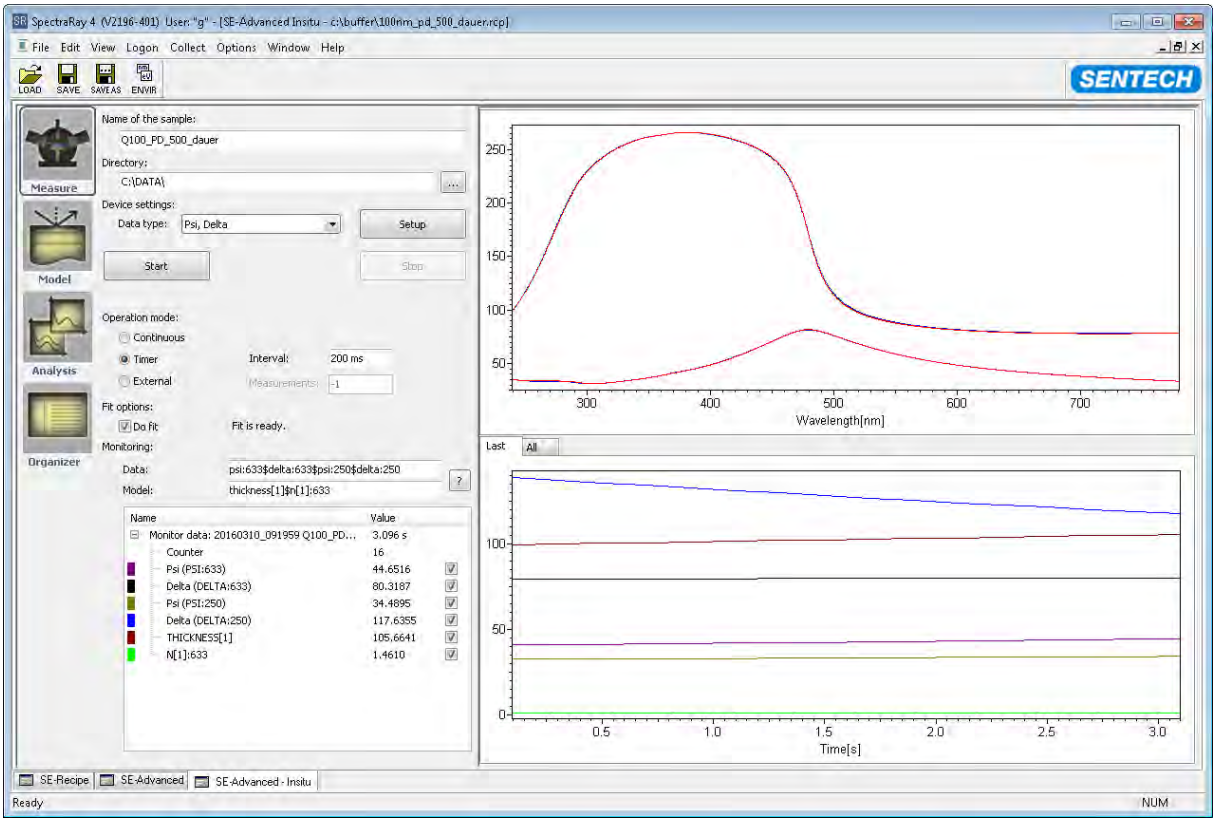


Fig. 6-2 Insitu main view

As the SE-Advanced in-situ view and the standard SE-Advanced view (described in chapter 5) interact, for example for handling and saving data, it may be practical to see both views. The option 'Window / Tile / Vertical' in the main menu (as shown in Fig. 6-3) places both views in the application frame simultaneously as shown in Fig. 6-4.

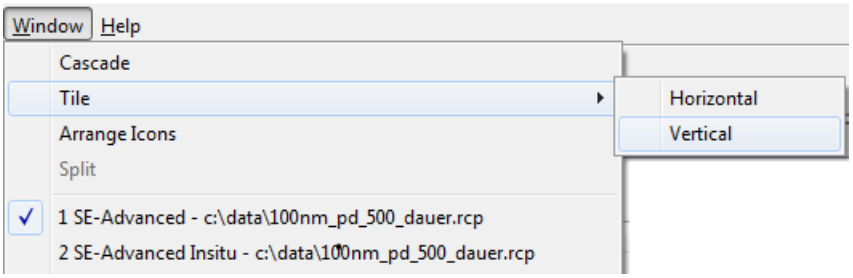


Fig. 6-3 Show views simultaneously

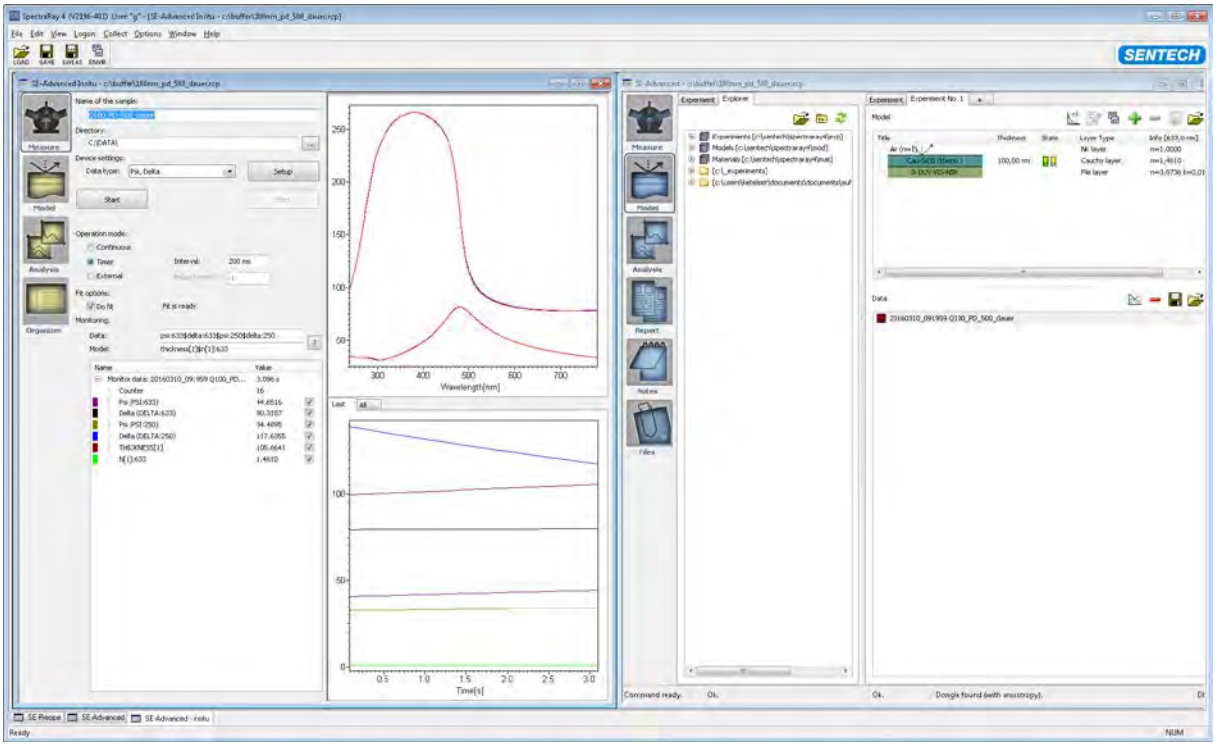


Fig. 6-4: In-situ view (left) and standard view (right)

The toolbar on the left side of the in-situ view gives access to the dialogs and functions described in the next paragraphs.

6.2 Menu of the in-situ view

Each view in the application frame has its own main menu and toolbar in the top part of the application frame. To access the desired menu it is necessary to activate the respective view by clicking with the mouse.

As shown in Fig. 6-5 the toolbar consists mainly of functions to load and save recipes (*.rcp). These files contain the settings for a measurement sequence including measurement settings, device driver settings, model settings etc. It is practical to define certain recipes for certain tasks which can then be started easily.
Further details are similar to the file loading and saving in the SE-Advanced standard view and are described there.

The 'Environment' for the in-situ measurement can be accessed by clicking the 'Envir' button in the toolbar. The function is described in chapter 5.2.6.

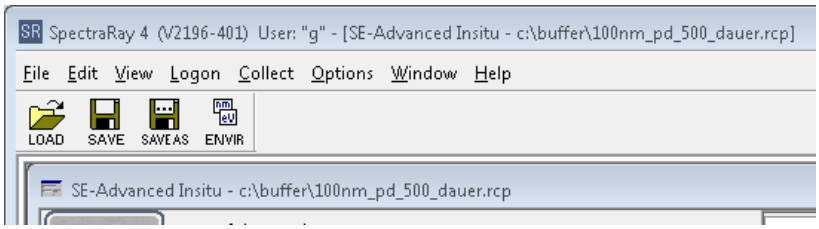


Fig. 6-5 Menu and toolbar of the insitu view

6.3 In-situ measurements

Clicking on 

in the tool bar on the left side opens the in-situ measurement window as shown in Fig. 6-6. The dialog offers the options which are explained in the following paragraphs:

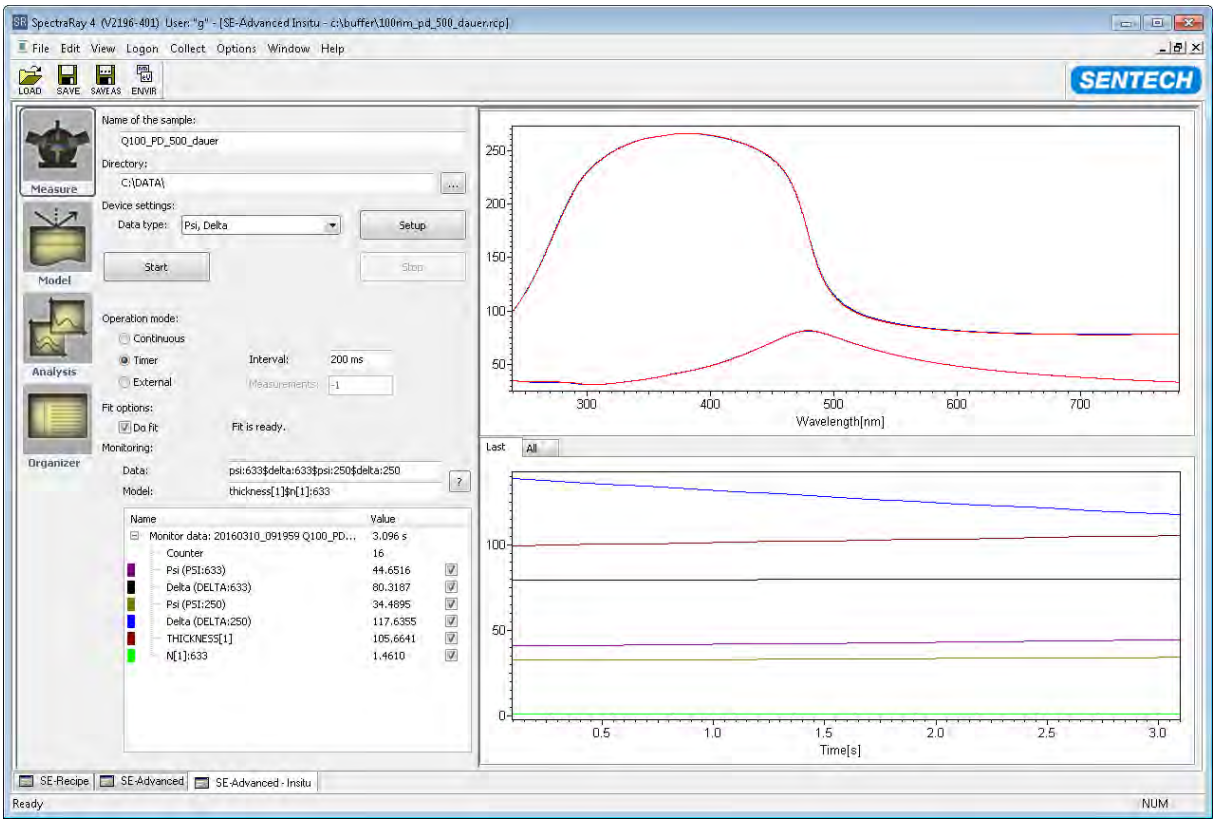
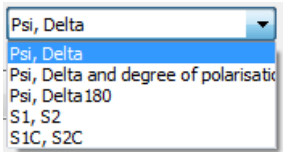


Fig. 6-6 In-situ measurement settings

6.3.1 Data file names

The name of the sample can be entered in the edit field at the top. The target directory for the data files can be entered in the next edit field.
The resulting filename will be created automatically from the given directory, the date and time of measurement and the given filename.
For example the entries shown in Fig. 6-6 will lead to the following filenames
c:\data\20140722_183605_Q100_PD_500_dauer.dob and
c:\data\20140722_183605_Q100_PD_500_dauer.control.dob
The first of these files (*.dob) will hold the spectral raw data and may become very large in case of high measurement rate over a longer period of time.
The second file (*.control.dob) will contain so called 'control lines' or 'time lines'. For example the Psi value at a certain wavelength versus time and the fitted film thickness versus time.

6.3.2 Measurement type

The desired measurement type can be selected in the list data type box 

.

For usual applications Psi, Delta and S1,S2 are the mostly used selections.
The measurement type Psi, Delta offers highest accuracy of the resulting data and the high sensitivity of the Delta value in the case of thin layers.
The measurement type S1,S2 offers fastest measurements, as no mechnical movement of a retarder takes place. This measurement mode may be helpful with fast in-situ process monitoring.

6.3.3 Driver settings

The button 

allows to open the device driver where many detailed settings can be made to customize the measurement.
See chapter 7 for details.
Note that settings are different for the SE-Advanced standard measurement and the SE-Advanced in-situ measurement.

For in-situ measurements discussed here the following settings may be especially important:

Depending on the spectrometer used in the ellipsometer it is possible to use the 'Fastmode' for data collection in addition to the 'Standard step scan' mode. During fastmode the polarizing element rotates continuously which results in much faster measurements. The speed should be chosen according to the desired time resolution and the signal to noise ratio of the measurement data.

The fastmode can be selected in the device driver settings as explained in chapters 7.1.3 and 7.1.4.

The fastmode speed can be selected in the intensity viewer described in chapter 0.

The fastmode becomes especially useful in connection with the measurement type s1,s2 as highest data rate can be reached here.

6.3.4 Operation mode

The measurement sequence can be defined by the following operation mode settings:

Fig. 6-7 Operation modes

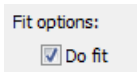
The option 'Continuous' will measure as fast as possible according to the selected measurement type and the device driver settings.

The option 'Timer' will measure in the given interval. The interval should of course be larger than the time needed for one measurement according to the selected measurement type and the device driver settings.

The option 'External' allows to start the measurement after an electrical trigger signal. This feature may be useful to integrate the in.situ ellipsometer for example into the sequence of a deposition process.

Details about the electrical interface can be found in the electronics documentation of the specific instrument. The edit 'Measurements' takes a number of measurements to be made after the trigger signal. A value of -1 means continuous measurement as long as the trigger signal is on.

6.3.5 Fit of measured data

The option 

allows to select the fit of the measured raw data during the data collection. A suitable model has to be present and suitable fit parameters have to be selected as described in chapter 6.4.

The fit will be performed during the data collection process. In order not to lose any measured data the data collection has higher priority. In case of very fast data collection or complex modelling the fit may be too slow. In this case the fit will be skipped for 1 or more measurements and the values will be kept from the last successful fit. The raw measurement data will be saved anyway It is possible to re-calculate all data after the process - so all measurements can be evaluated. See chapter 6.5 for details.

6.3.6 Defining control data (time lines)

The monitoring options allow to define so called control data or time lines.

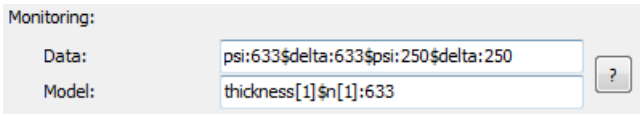


Fig. 6-8 Monitoring options

The first edit field allows to enter a string which defines the data for the control lines. Here it is possible to extract certain values from the measured raw data without further calculation. In the example the following values will be extracted from each measurement:

Psi at 633nm
Delta at 633nm
Psi at 250 nm
Delta at 250 nm

The second field allows to monitor the results from the fit of the measurement data to the given model.
In the example the following values will be monitored for each measurement:

Thickness of the first layer
Refractive index of the first layer at 633nm

A click on 

opens a list of possible values, as shown in Fig. 6-9.

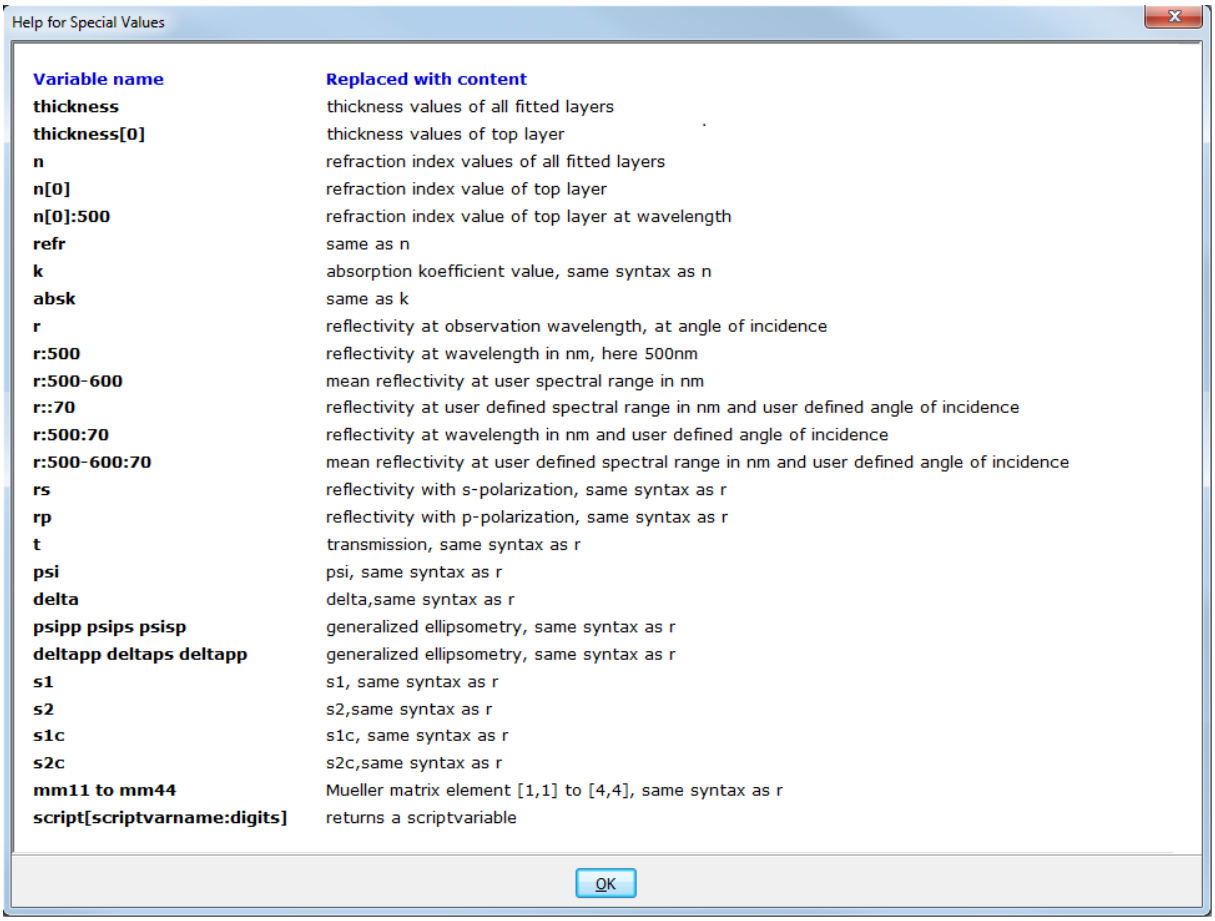


Fig. 6-9 Monitoring special values

6.3.7 Start / stop measurement

The buttons 

and 

allow to start and stop a measurement sequence according to the current settings.

6.3.8 Display during measurement

During a measurement sequence the measured spectra will be displayed in the upper right diagram. Usually (Psi, Delta) or (s1,s2) versus wavelength. If the fit option is active the fitted spectra are also displayed in red color. See for example Fig. 6-10.

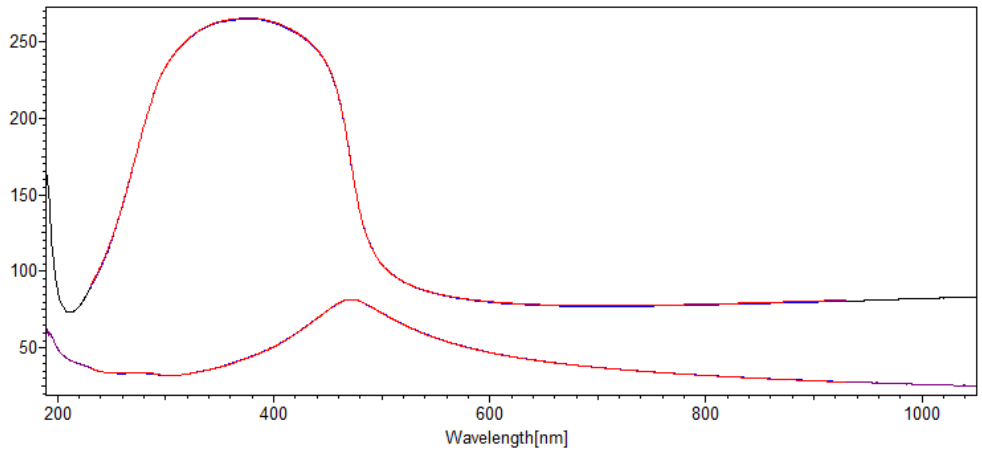


Fig. 6-10 Psi and Delta spectra with fit in online view during measurement

The control data according to the current selection (see chapter 6.3.6) are displayed in the lower right diagram versus time.
The legend is shown in the lower left box. See for example Fig. 6-11.
It is possible to select certain control line for display by clicking the check boxes.

The name of the current data file and the time and index (counter) of the current measurement are shown as well.

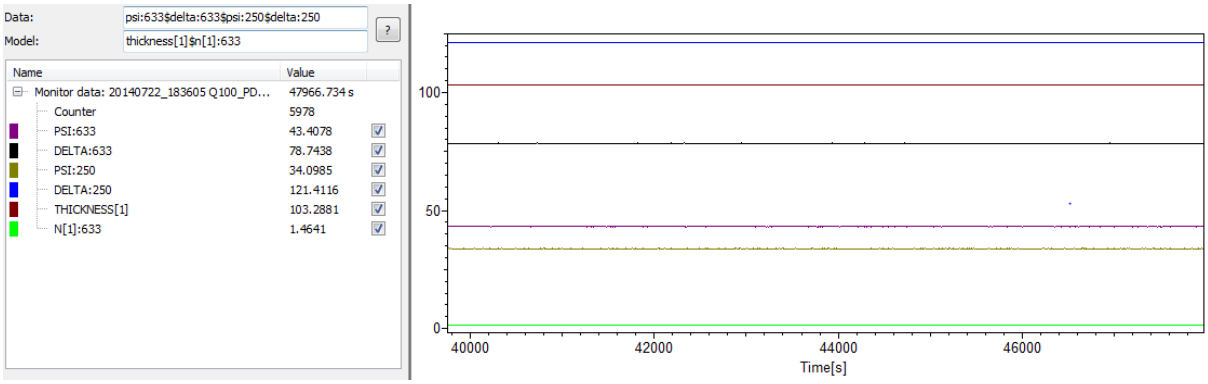


Fig. 6-11 Control lines during measurement

6.3.9 Data storing during measurement

The data are stored during the measurement procedure as shown in Fig. 6-12.

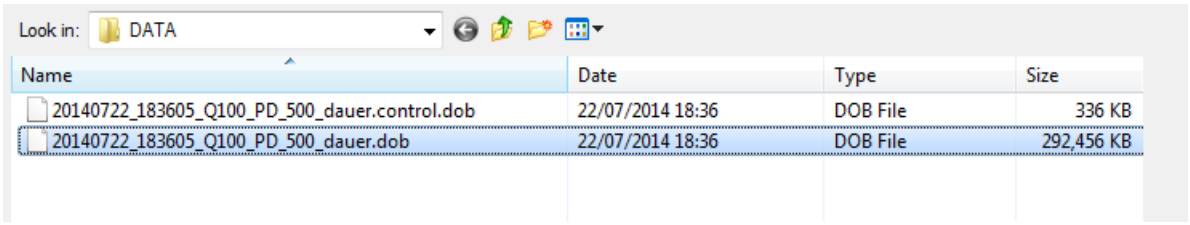


Fig. 6-12 Data file storage during measurement

6.3.10 Data loading after measurement

6.3.10.1 Loading control data into standard view

When the measurement sequence is finished the control data are automatically loaded into the data box (lower right corner) of the SE-Advanced standard view, see Fig. 6-13.

It is also possible to load the control data from the explorer like file selection box on the left side of the standard view. The file (*.control.dob) can be selected and copied by drag-and-drop to the data box.

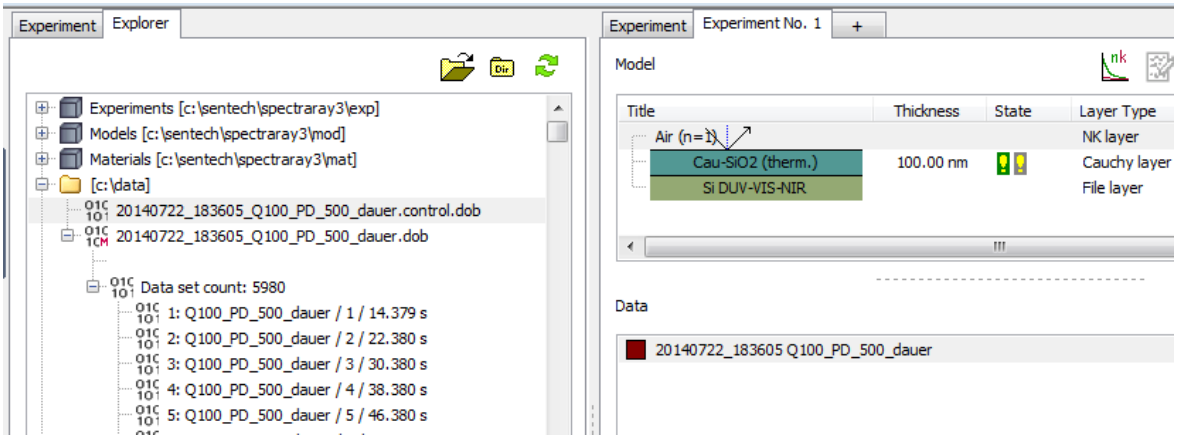


Fig. 6-13 Control data file in the data box of the standard view

6.3.10.2 Loading in-situ raw data into standard view

The measured in-situ raw data can also be loaded into the data box of the standard view. The file (*.dob) can be selected in the explorer like box on the left side as shown in Fig. 6-14. The file consists of subfiles with all the measured spectra. They are shown under the file name with their index and the time of measurement. Each sub-file can be selected individually and copied by drag-and-drop to the data box. In the example the 4th and 9th measurement are selected into the data box for further processing.

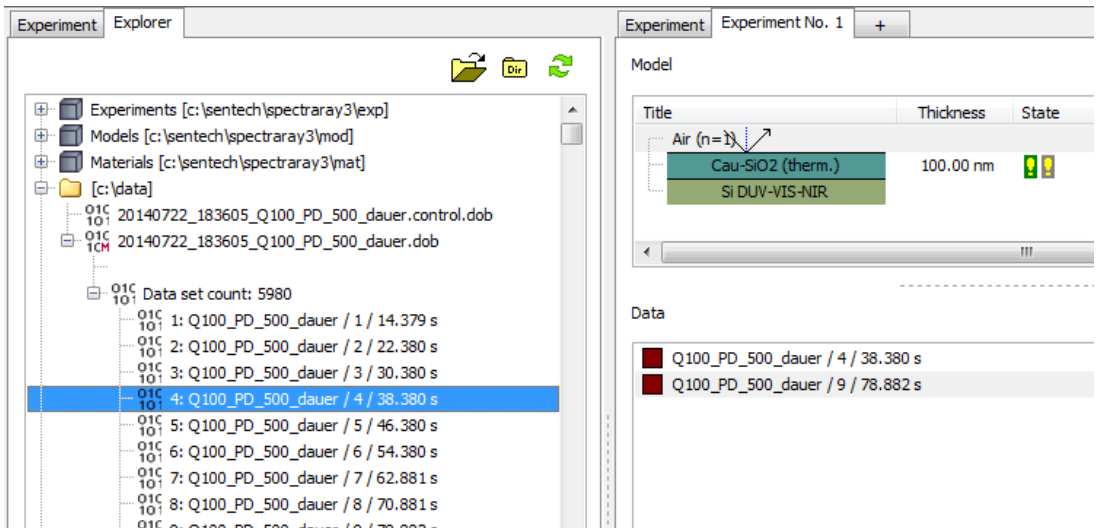


Fig. 6-14 In-situ raw data file in the data box of the standard view

6.4 In-situ model

Clicking on 

in the tool bar on the left side opens the in-situ model window as shown in Fig. 6-15.

The in-situ model view presents the same functionality as the standard model view, therefore see chapter 5.2 for details which are not repeated here.

The example shows a model taken from the explorer-like directory tree on the left side. The model can be inserted by drag-and-drop operation, also single layers can be defined be inserting individual materials from models or from the materials data base.

Double click a layer in the in-situ model view to open the details as shown in Fig. 6-15. Select and edit details of the fit parameters as described in chapter 5.2.

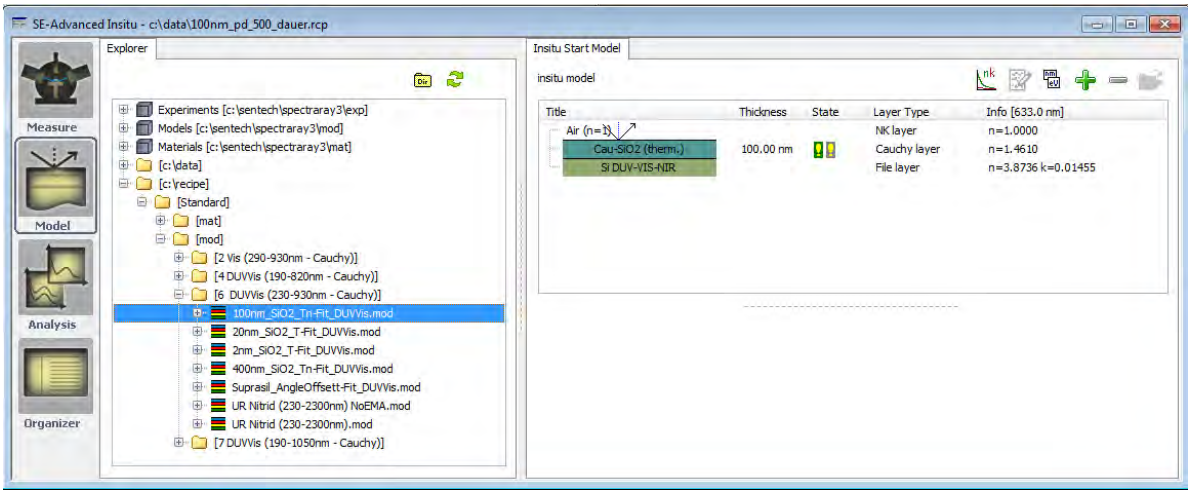


Fig. 6-15 In-situ model view

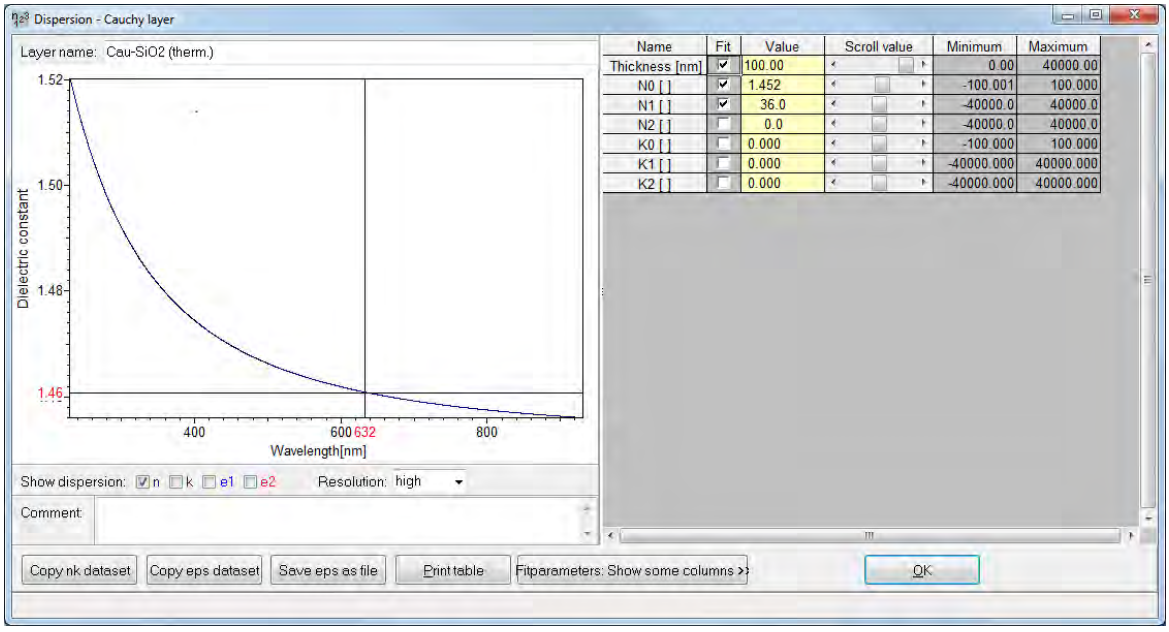


Fig. 6-16 Layer details, Cauchy layer as example

6.5 In-situ analysis

Clicking on 

in the tool bar on the left side opens the in-situ analysis window as shown in Fig. 6-17. The analysis view allows to fit and re-analyse in-situ data.

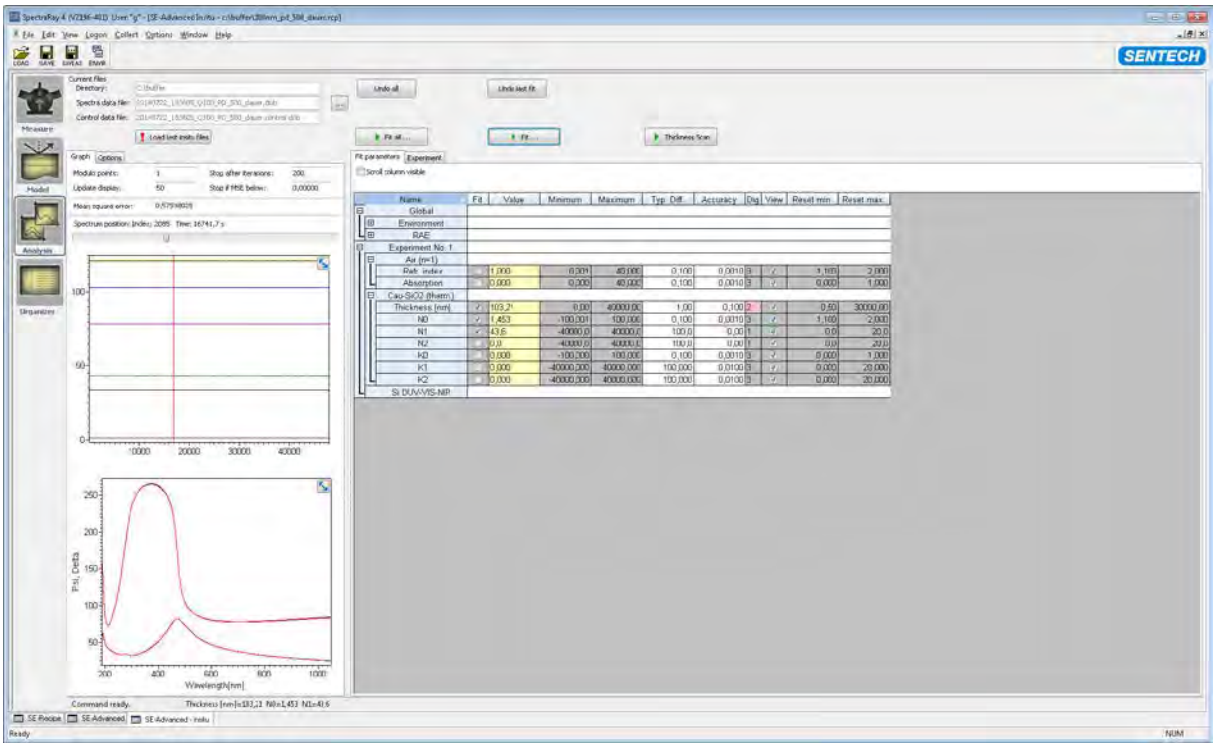


Fig. 6-17 In-situ analysis view

6.5.1 Loading data into the analysis view

The data which is to be handled can be loaded into the organizer by the  button in top part of the dialog. A file selection box shown in Fig. 6-18 allows to select the raw data file (*.dob). This file and the corresponding *.control.dob file are then shown as the currently active files in the name fields shown in Fig. 6-19.

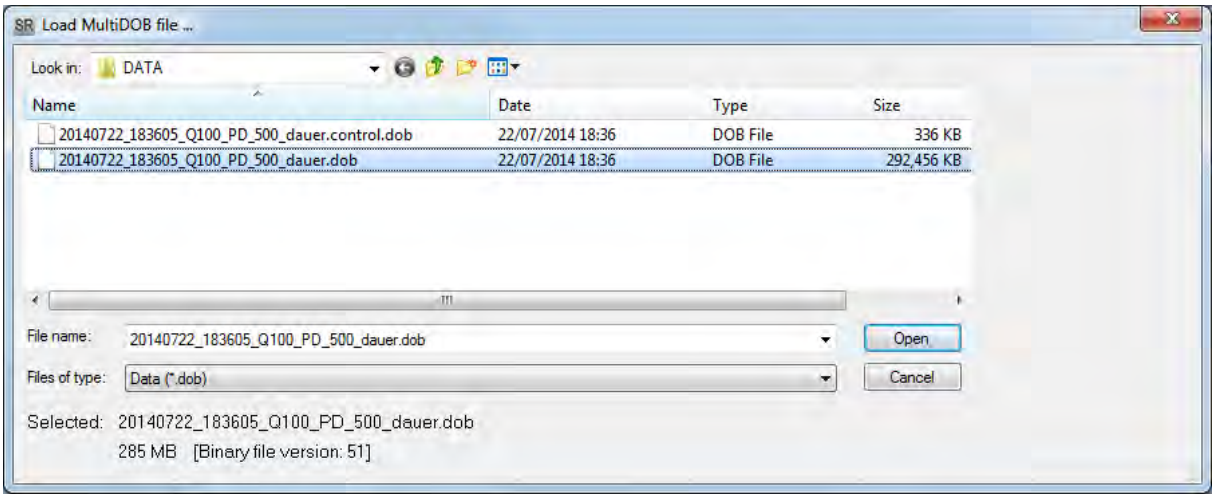


Fig. 6-18 Selection of raw data file for the organizer

Fig. 6-19 Currently selected files

6.5.2 Viewing control data

The control data are shown in the upper left diagram. The legends can be opened by moving the vertical separation bar with the mouse. The checkboxes allow to select the desired curves.

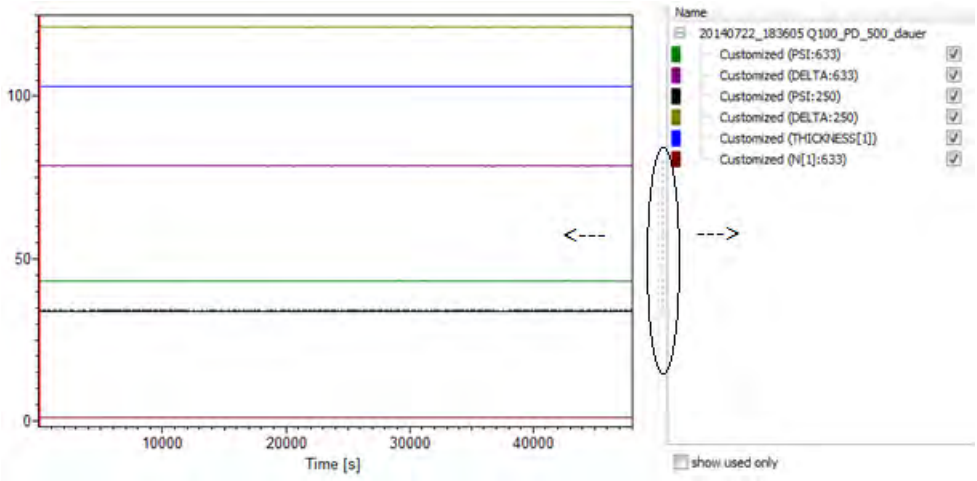


Fig. 6-20 Control data in the upper left diagram. Open legends by moving the vertical separation bar.

The diagram can be zoomed using the mouse in the usual way.

Fig. 6-21 Spectral position of current selection

A slider above the diagram can be activated as shown in Fig. 6-21. It can be used to select a certain measurement.
The arrow can be clicked by the mouse and moved to select a certain measurement at a certain time. This selection is shown by the red cursor line.
When the slider is selected it is also possible to move the cursor by the left (<---) and right (--->) arrow keys on the keyboard.
The index and process time of the currently selected measurement are also shown.

6.5.3 Viewing spectral data and fitted data

The raw data of the currently selected measurement is shown in the diagram on the lower left side. As shown in Fig. 6-22 the display shows the measured data and the fitted data according to the current setting of the model and the fit parameters. The given example shows data before and after a fit with a suitable model.

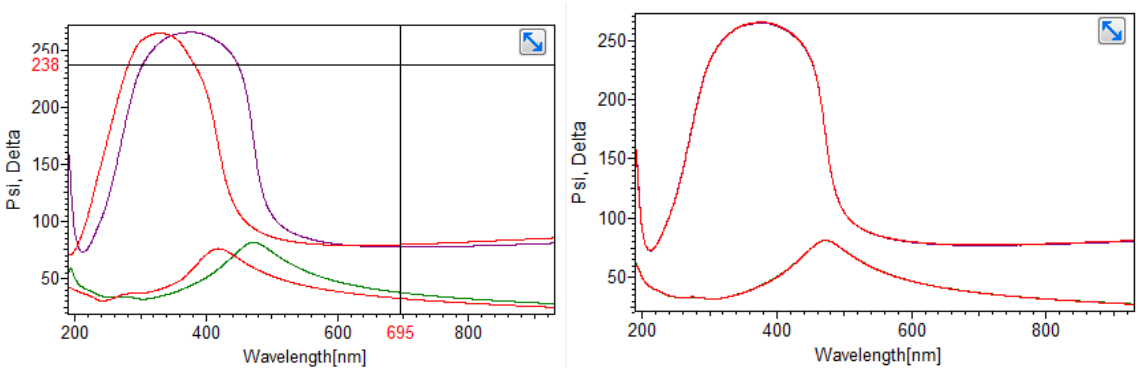


Fig. 6-22 Selected spectra with fitted (theory) spectra. Left side: before fit, Right side: after fit

As shown in Fig. 6-23 the display can be modified using the optional settings.

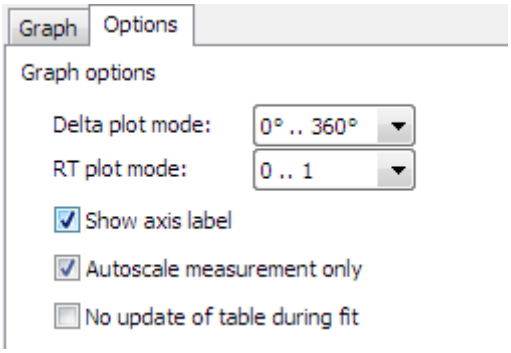
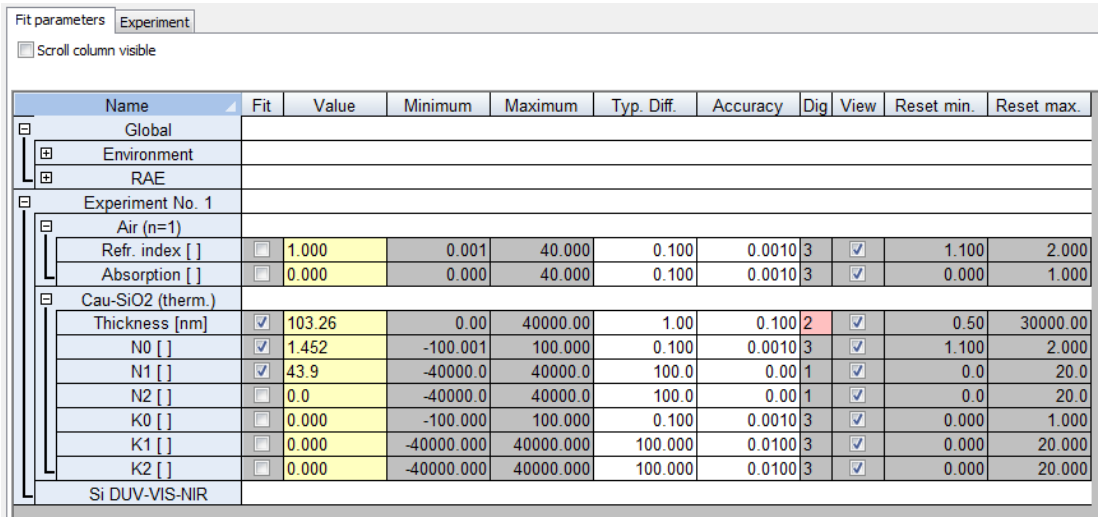


Fig. 6-23 Options

6.5.4 Fit parameters

The current model for the analysis of the data has to be set up as decribed in chapter 6.4. The fit parameters can then be set in the table on the right side as shown in Fig. 6-24.

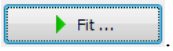
The details about fit procedures and setting up suitable parameters are given in chapter 5.6 and are not repeated here.



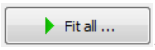
Name	Fit	Value	Minimum	Maximum	Typ. Diff.	Accuracy	Dig	View	Reset min.	Reset max.
Global										
Environment										
RAE										
Experiment No. 1										
Air (n=1)										
Refr. index [ ]	☐	1.000	0.001	40.000	0.100	0.0010	3	☑	1.100	2.000
Absorption [ ]	☐	0.000	0.000	40.000	0.100	0.0010	3	☑	0.000	1.000
Cau-SiO2 (therm.)										
Thickness [nm]	☑	103.26	0.00	40000.00	1.00	0.100	2	☑	0.50	30000.00
N0 [ ]	☑	1.452	-100.001	100.000	0.100	0.0010	3	☑	1.100	2.000
N1 [ ]	☑	43.9	-40000.0	40000.0	100.0	0.00	1	☑	0.0	20.0
N2 [ ]	☐	0.0	-40000.0	40000.0	100.0	0.00	1	☑	0.0	20.0
K0 [ ]	☐	0.000	-100.000	100.000	0.100	0.0010	3	☑	0.000	1.000
K1 [ ]	☐	0.000	-40000.000	40000.000	100.000	0.0100	3	☑	0.000	20.000
K2 [ ]	☐	0.000	-40000.000	40000.000	100.000	0.0100	3	☑	0.000	20.000
Si DUV-VIS-NIR										

Fig. 6-24 Fit parameter settings of currrent in-situ model

6.5.5 Performing a fit and a recalculation

After a suitable model and suitable fit parameters are set up a fit procedure can be started by clicking 

. The fit will use the currently selected data set.

A recalculation of all data can be started by clicking 

. All data sets in the currently loaded data file are recalculated. If the model is only suitable for a part of the data it is possible to trim (select) the desired part into another file using the organizer described in chapter 6.6.
The result of the recalculation is saved to the given result file with the suffix and a n automatically increased number.

The recalculation may be used for detailed evaluation of measured data after the in-situ process. It is also possible to re-calculate the data in case the fit procedure has not been active during the process or if the fit procedure was not fast enough for all measurement during a fast measurement, see chapter 6.3.5.

Options for the recalculation can be set as shown in Fig. 6-25.

“Thickness scan” initiates a thickness scan by searching the best agreement for thicknesses between minimum and maximum

"Monitoring values" The currently extracted monitoring values are shown

"New monitoring values" New monitoring values can be defined in roder to create new controla data lines.

"Safe filename suffix" The optional suffix is appended to the new filename

"Autosave to file" Automatically saves results of the recalculation to a new file

"Copy to experiment" Control data lines a re automatically copied to the data box of the standard view.

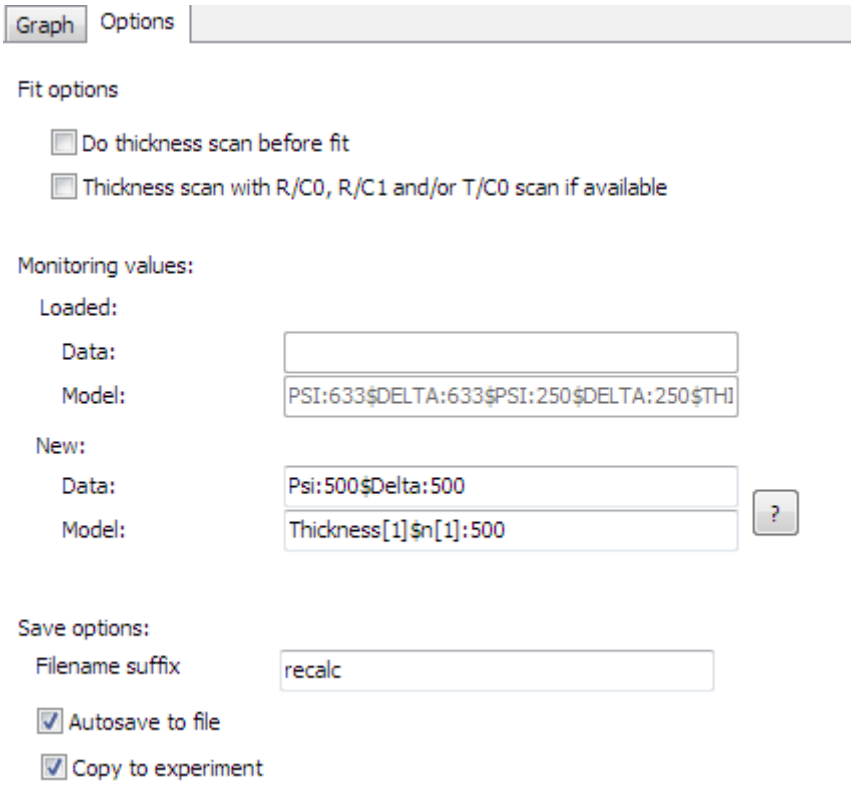


Fig. 6-25 Options for fit and recalculation

During the recalculation the results may of course change due to the selection of other control parameters or other model settings.

The lower diagram in Fig. 6-26 shows the current measured spectra and the current fitted spectra. The display can be used to check if the recalculation process works well.

The previous monitoring data are shown in the upper diagram in Fig. 6-26. According to the settings for the new reults additional monitoring lines are added during the reclaculation process.

If the arrow in the upper left corner are clicked the display is enlarged and the legends for all curves are shown on the right side in Fig. 6-27.

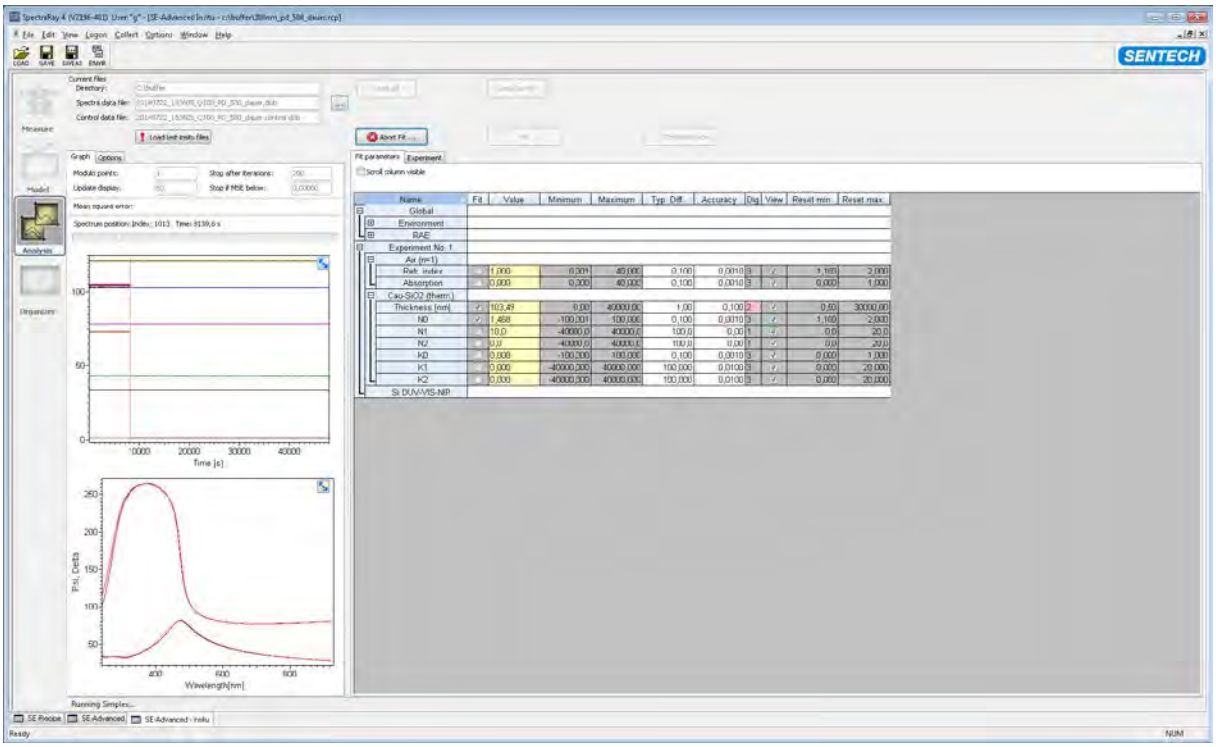


Fig. 6-26 Recalculation in progress

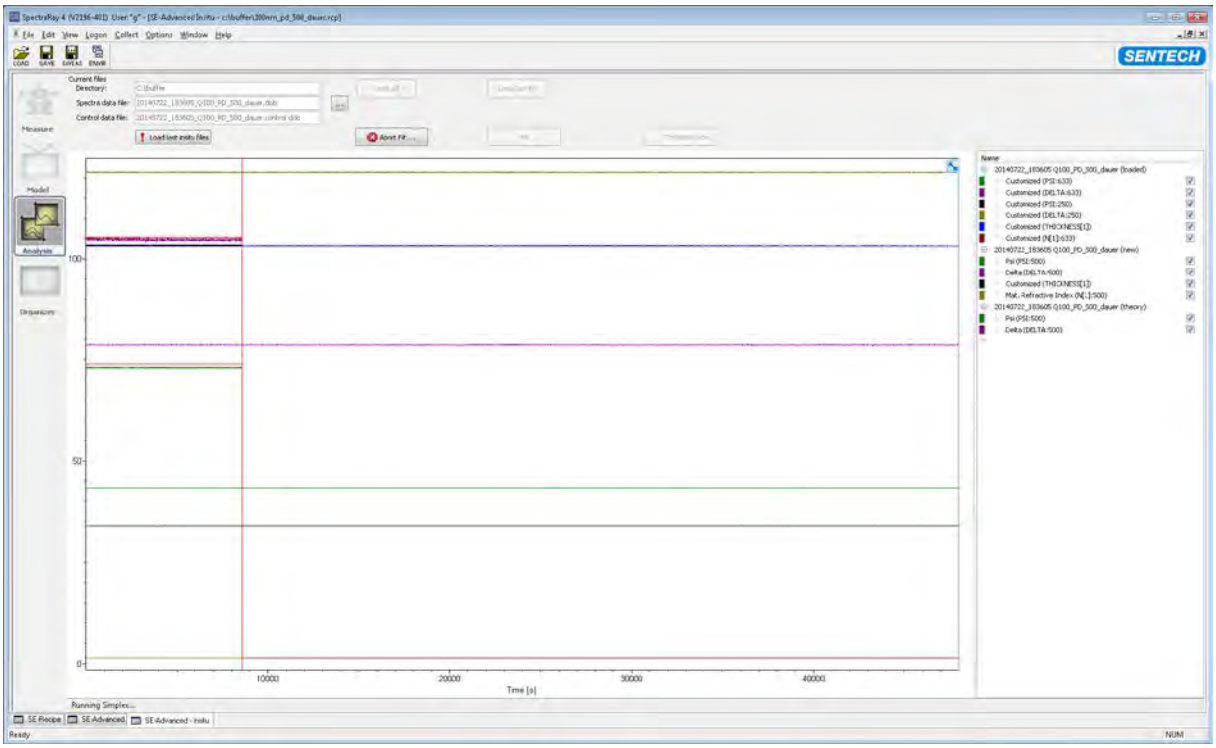


Fig. 6-27 New results from recalculation in enlarged display

6.6 In-situ organizer

Clicking on in the tool bar on the left side opens the in-situ organizer window as shown in Fig. 6-28. The organizer view allows to handle files with in-situ data and provided functions to show, trim and cut large amounts of data.

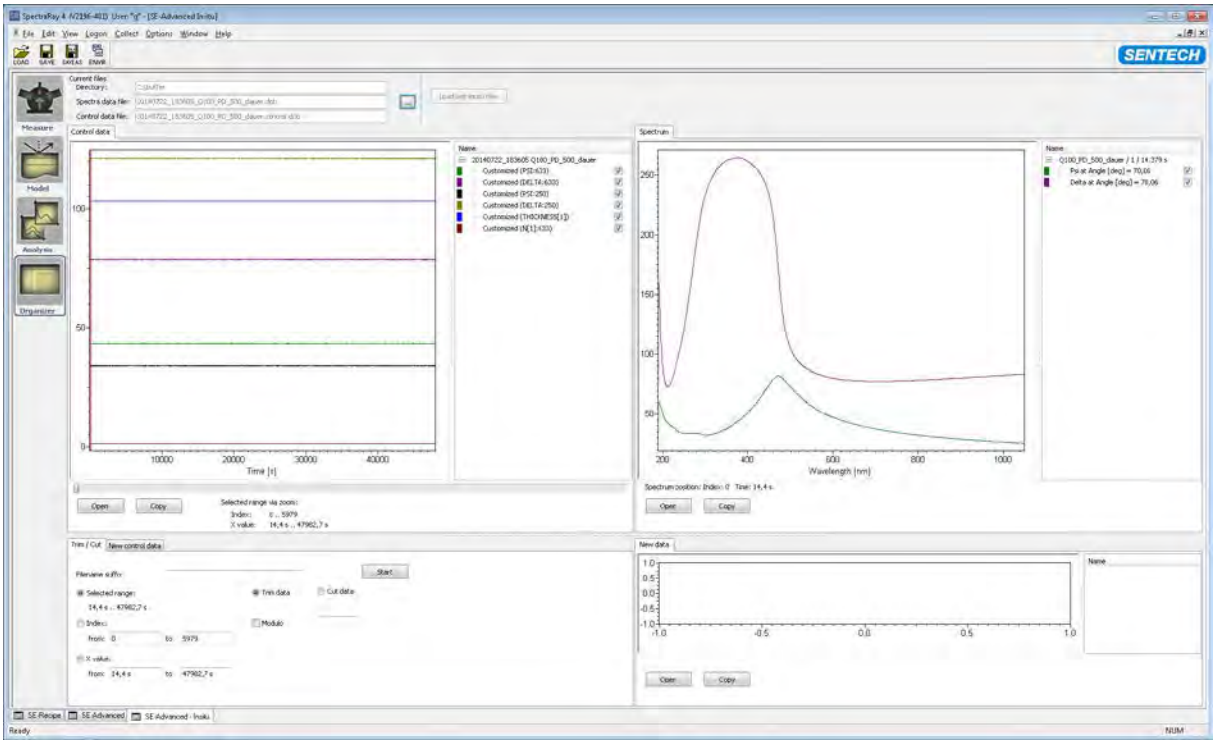


Fig. 6-28 In-situ organizer view

6.6.1 Loading data into the organizer

The data which is to be handled can be loaded into the organizer by the  button in top part of the dialog. A file selection box shown in Fig. 6-29 allows to select the raw data file (*.dob). This file and the corresponding *.control.dob file are then shown as the currently active files in the name fields shown in Fig. 6-30.

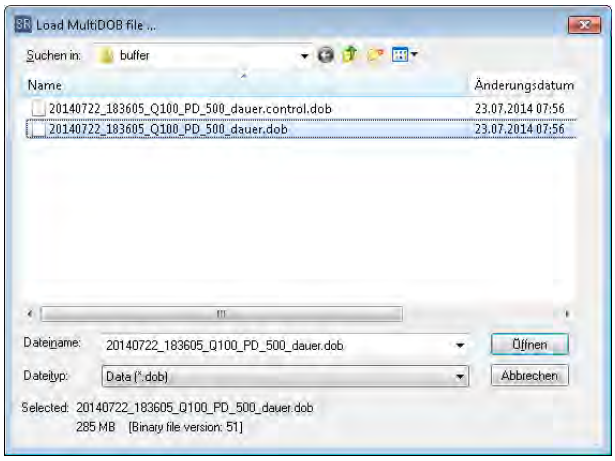


Fig. 6-29 Selection of raw data file for the organizer

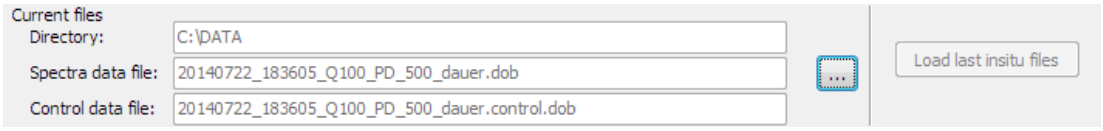


Fig. 6-30 Currently selected files

6.6.2 Viewing control data

The control data are shown in the upper left diagram. The legends can be opened by moving the vertical separation bar with the mouse. The checkboxes allow to select the desired curves.

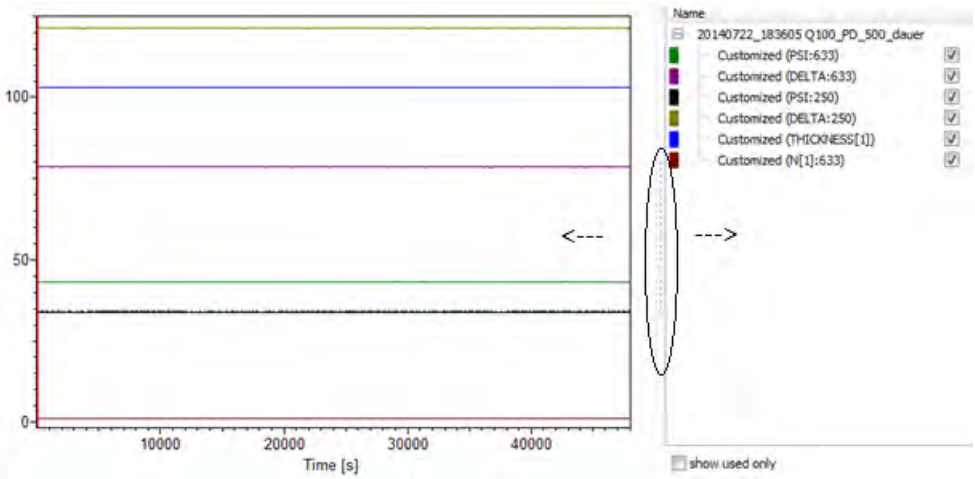


Fig. 6-31 Control data in the upper left diagram. Open legends by moving the vertical separation bar.

The diagram can be zoomed using the mouse in the usual way. Fig. 6-32 shows an example of a zoomed part of the control data.
The minimum and maximum indices and times of the selected range are shown below the diagram.

A slider below the diagram can be activated as shown in Fig. 6-33. The blue range indicates the selected part of the data set.
The arrow can be clicked by the mouse and moved to select a certain measurement at a certain time. This selection is shown by the red cursor line.
When the slider is selected it is also possible to move the cursor by the left (<---) and right (--->) arrow keys on the keyboard.

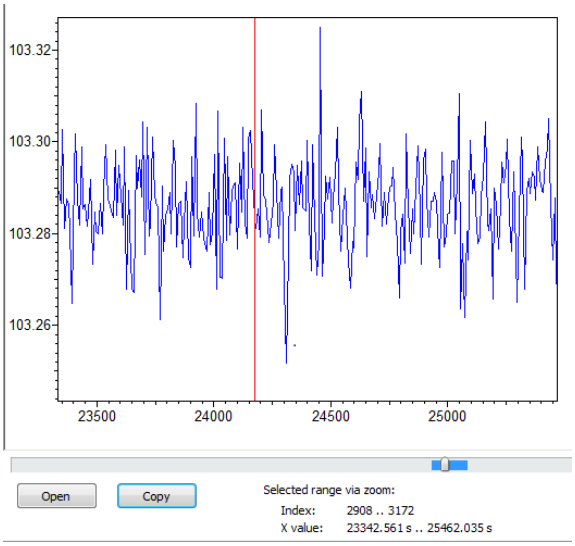


Fig. 6-32 Zoomed part of the data with slider (arrow on blue range indicator) and cursor (red line)

Fig. 6-33 Slider showing zoomed range of the data and cursor for selection

The button Open allows to view details of the control data file currently displayed as shown in Fig. 6-34. The data viewer is described in more detail in chapter 5.5.2.
The description given in the field y-Axis detail should not be changed as they are used in the recalculation procedure.

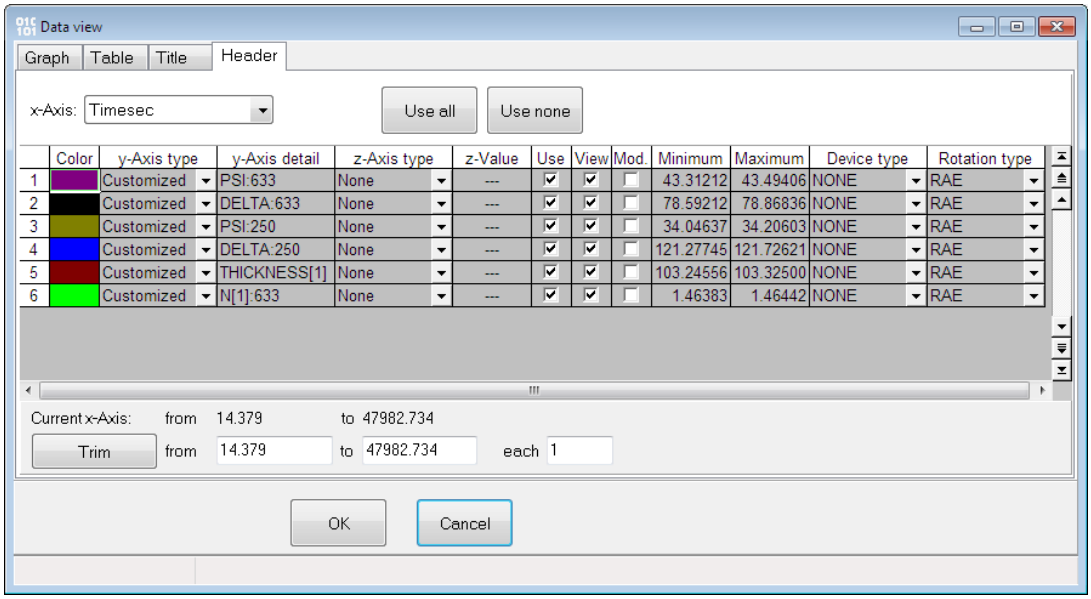


Fig. 6-34 Details of the currently displayed control data file

The button Copy allows to copy the currently displayed control data into the data box of the standard view, an example is shown in Fig. 6-35. The data can be used further processing there.

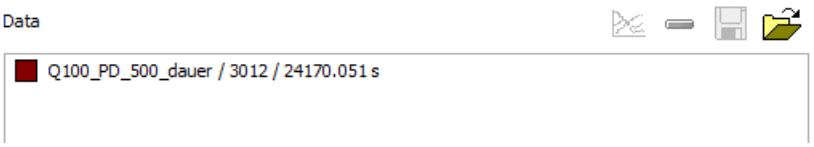


Fig. 6-35 Copied control data in the data box of the standard view.

6.6.3 Viewing raw data spectra

As shown in the previous chapter the individual measurements can be selected from the control data file. The corresponding raw data spectra are shown on the upper right diagram. The 'position' of the spectrum is shown below the diagram indicated by the index of the spectrum in the file and the time of measurement. The diagram is automatically updated when according to the selection by the cursor in the control data diagram on the upper left side.
The legend shows the type of data and the checkboxes can be used to select certain spectra for display.

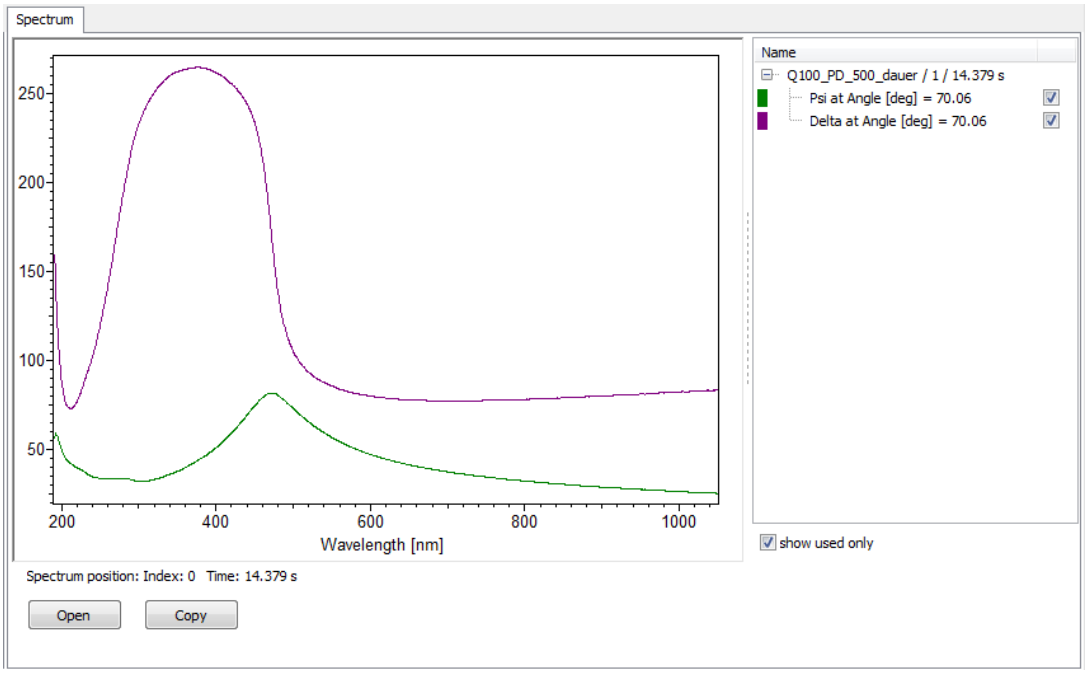
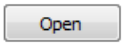


Fig. 6-36 Raw data spectra display.

The button 

allows to show details of the spectra.
Fig. 6-37 shows the name, date, index and time of measurement and other information.
Fig. 6-38As shown in The type of data can be shown.

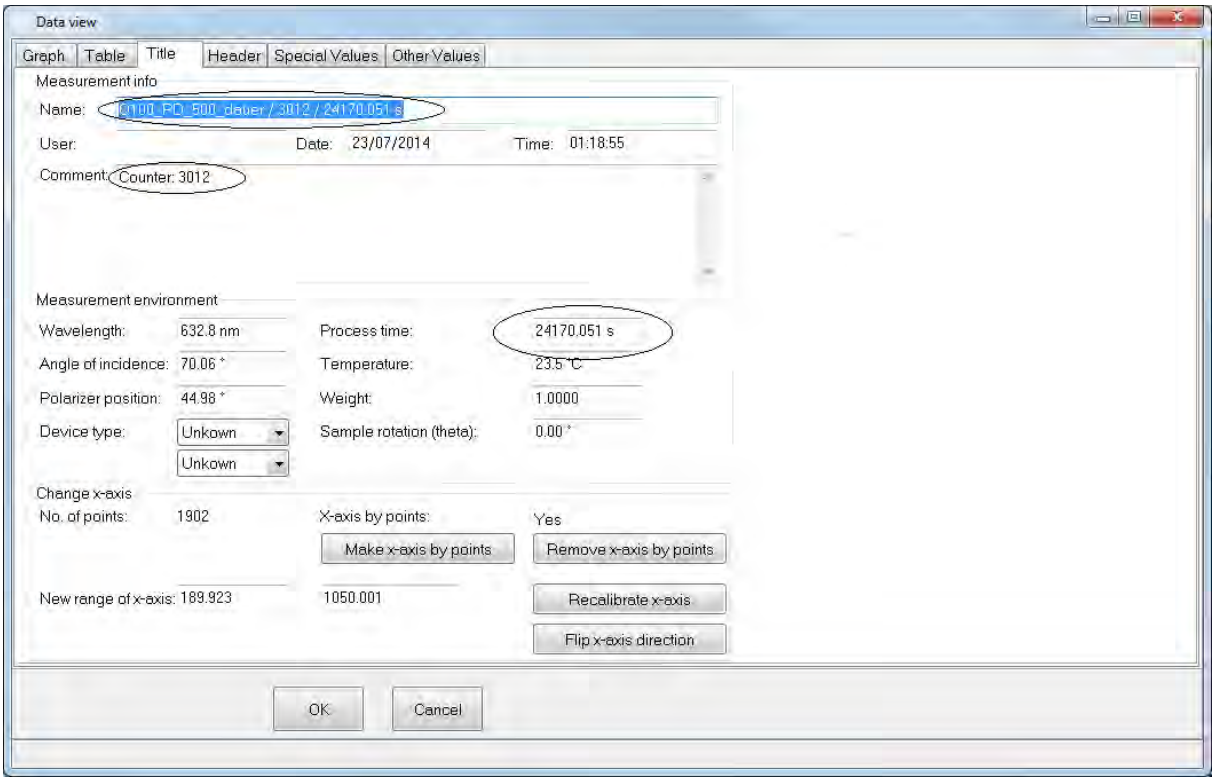


Fig. 6-37 Name, index, time of measurement of selected spectra

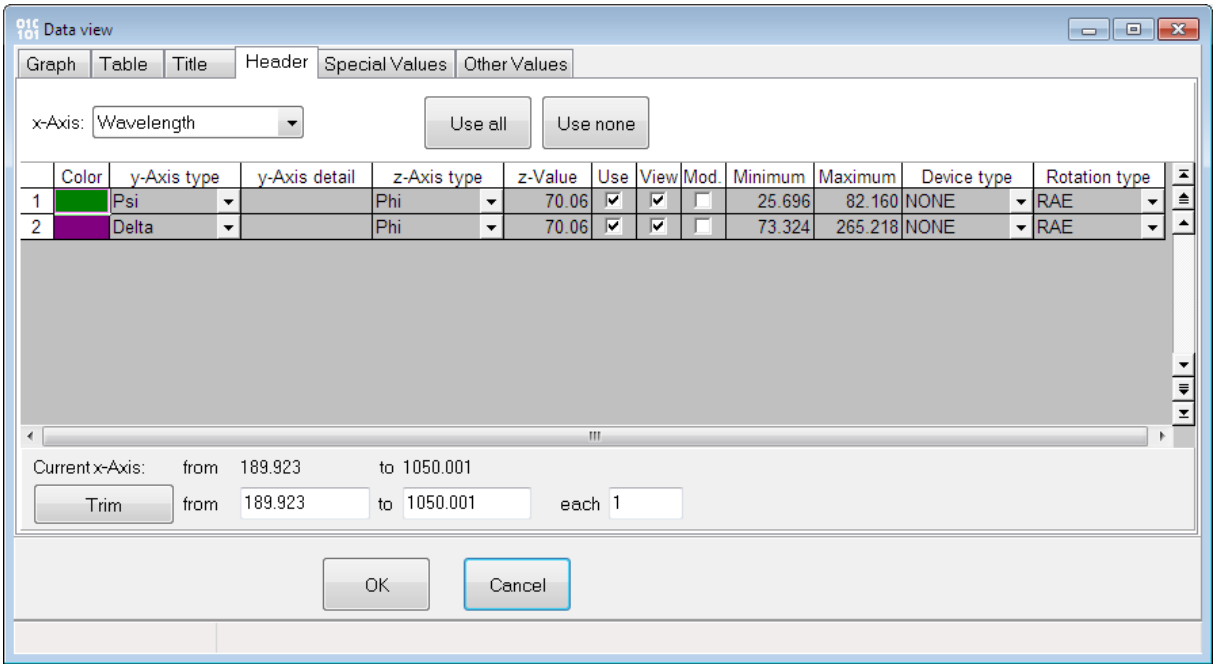


Fig. 6-38 Data types of selected spectra

The button Copy below the diagram allows to copy the currently displayed raw spectra to the data box of the standard view. An example is shown in Fig. 6-39. The data can be used further processing there.

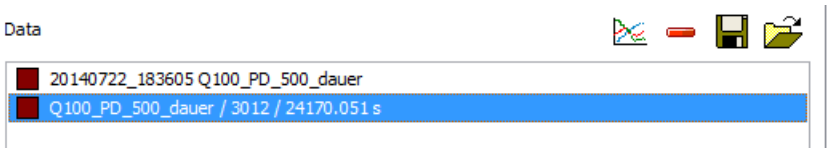


Fig. 6-39 Copied raw data spectrum in the data box of the standard view

6.6.4 Trim and cut data

During in-situ measurement processes a large amount of data may be collected and it may be necessary to reduce the amount of data afterwards. For example the interesting part of a deposition process has to be extracted or certain events like closed shutters result in bad measurements which have to be removed. The trim and cut section on the lower left side of the organizer allows to perform this type of data selection.

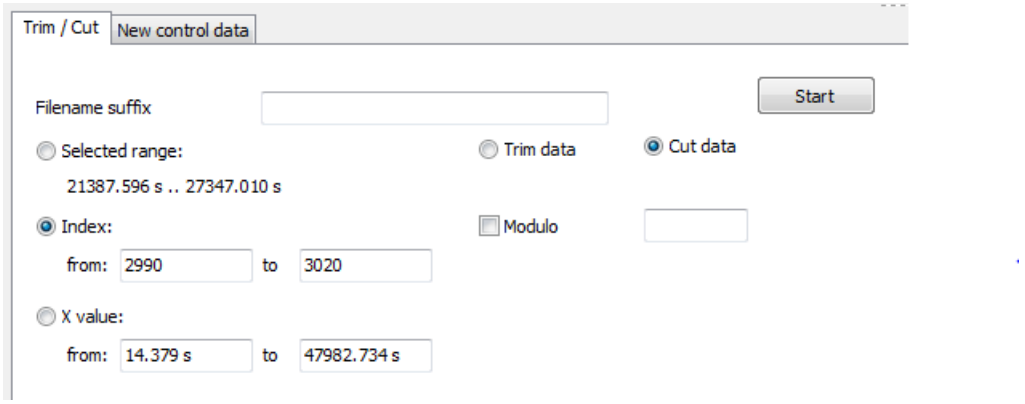


Fig. 6-40 Trim and cut settings

The example shown in Fig. 6-40 allows to select the desired actions:

The range of action can be selected

- from the currently selected range in the control data diagram above or
- from the minimum and maximum index given in the edit field or
- from the minimum and maximum measurement time.

The type of action can be

Trim: which means that the data in the specified range will be kept and data on the left and right side will be removed or

Cut: which means that the data in the specified range will be removed and the rest will remain.

In addition the option Modulo allows to take every x-th measurement and remove the others.

When the trim or cut action takes place both data file (*.dob) and (*.control.dob) are changed in the same way in order to get matching data sets again.
The original files are not overwritten, instead new files are stored in the same location but with modified filenames. As a standard the suffix '_trim' is added to the filename. The optional filename suffix may be used to give another suffix instead.

The trim or cut action is started by the button 

.
A progress bar

indicates the advance. Even in the case of large amount of data the action is quite fast due to efficient file structure.

6.6.4.1 Example for cutting data

An example for cutting data is shown in Fig. 6-41. A typical application would be to remove a part of the measurement which is known to be disturbed.

The filenames of the currently loaded data are shown. A certain part of the data is selected for display. Note that the X-axis is always shown as process time and not as measurement index.

A cut operation is selected in the range from measurement index 2990 to index 3020.

Fig. 6-42 shows the result after the operation. The desired part of the measurement is removed. The suffix is added to the filenames.

The new files are saved to the disc as shown in

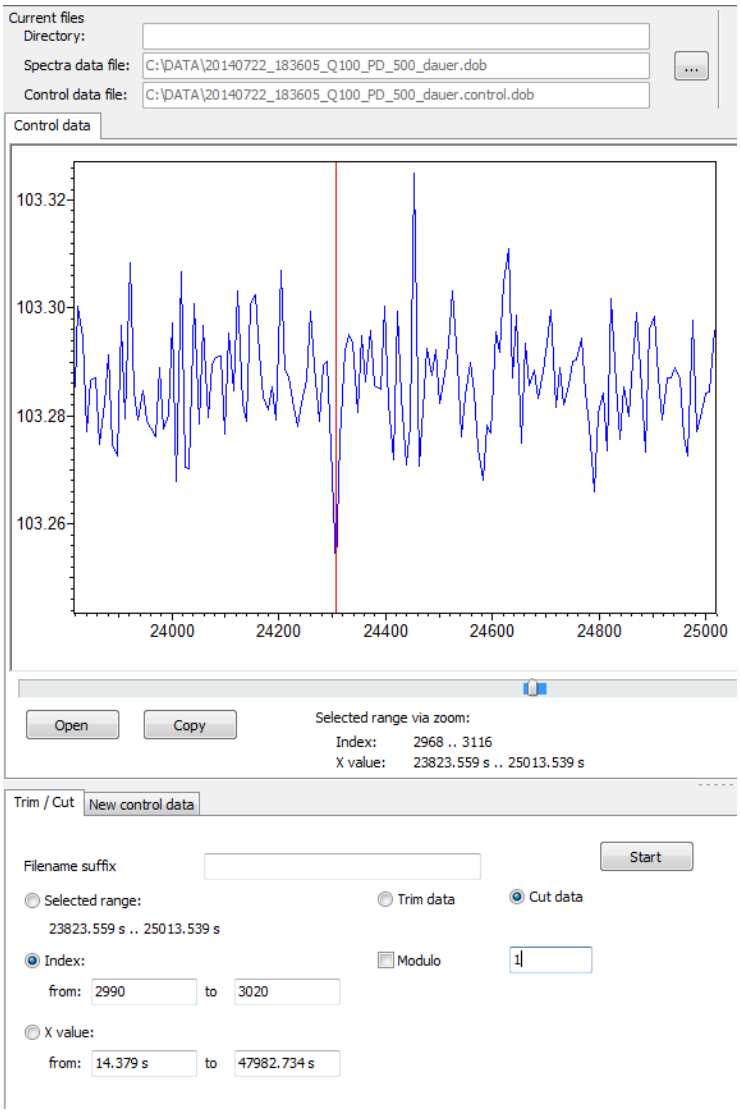


Fig. 6-41 Example before cut operation

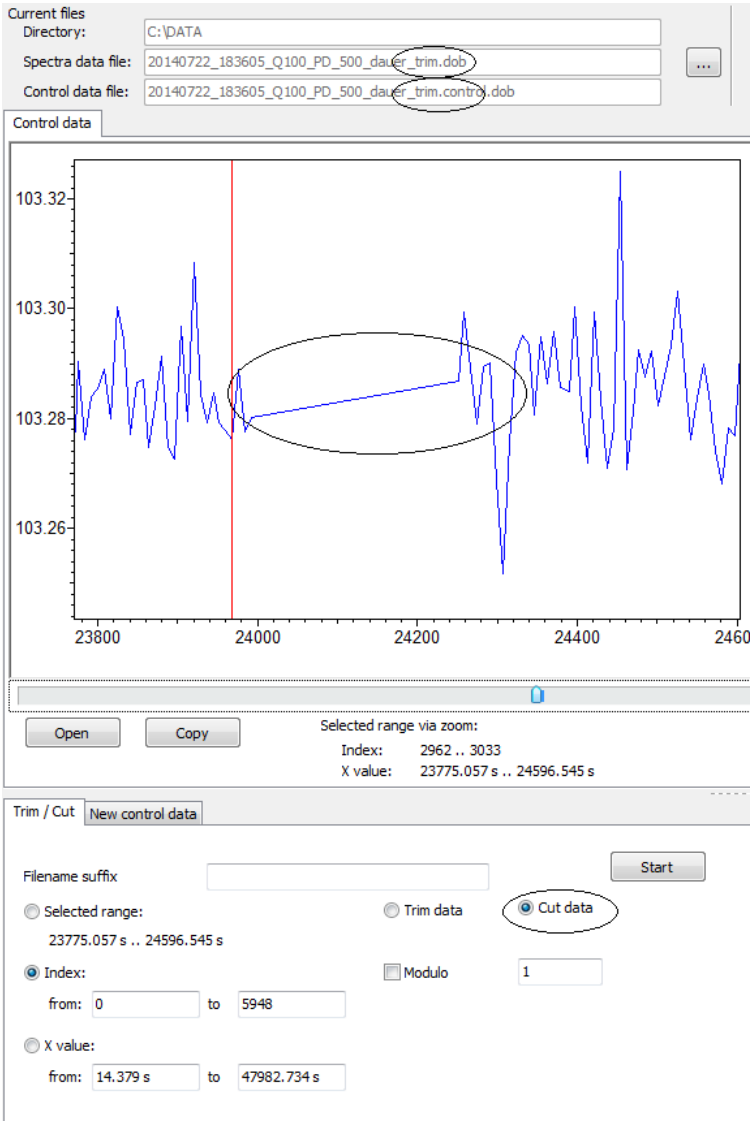


Fig. 6-42 Example after cut operation

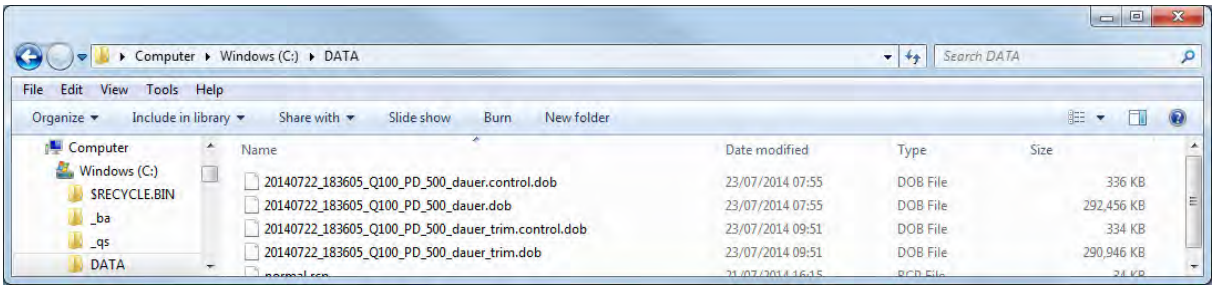


Fig. 6-43 New data files saved on the disc

6.6.4.2 Example for trimming data

An example for trimming data is shown in Fig. 6-44. A typical application would be to extract an interesting part of a measurement sequence and remove the part before and after the desired range.

The filenames of the currently loaded data are shown. The whole data range is displayed. Note that the X-axis is always shown as process time and not as measurement index.

A trim operation is selected in the range from measurement process time 1200 s to 22000 s.
The modulo option is set to 5 which means that the data will be thinned out to every 5th measurement.
A customized sufix for the filename is selected.

Fig. 6-45 shows the result after the operation. The desired part of the measurement is extracted. The suffix is added to the filenames.

The new files are saved to the disc as shown in Fig. 6-46.

The button Open allows to show details of the new files. As shown in the data table in Fig. 6-47 the start and end process time in the trimmed data set now corresponds to the selected range.

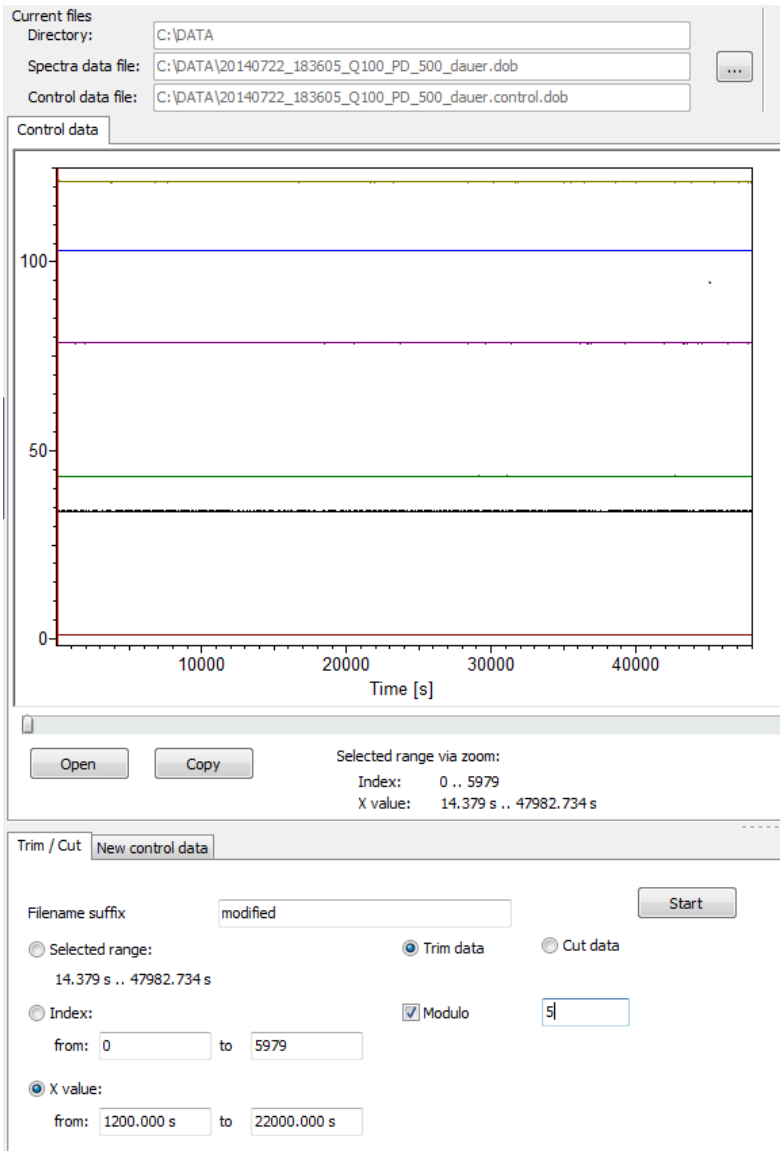


Fig. 6-44 Example before trim operation

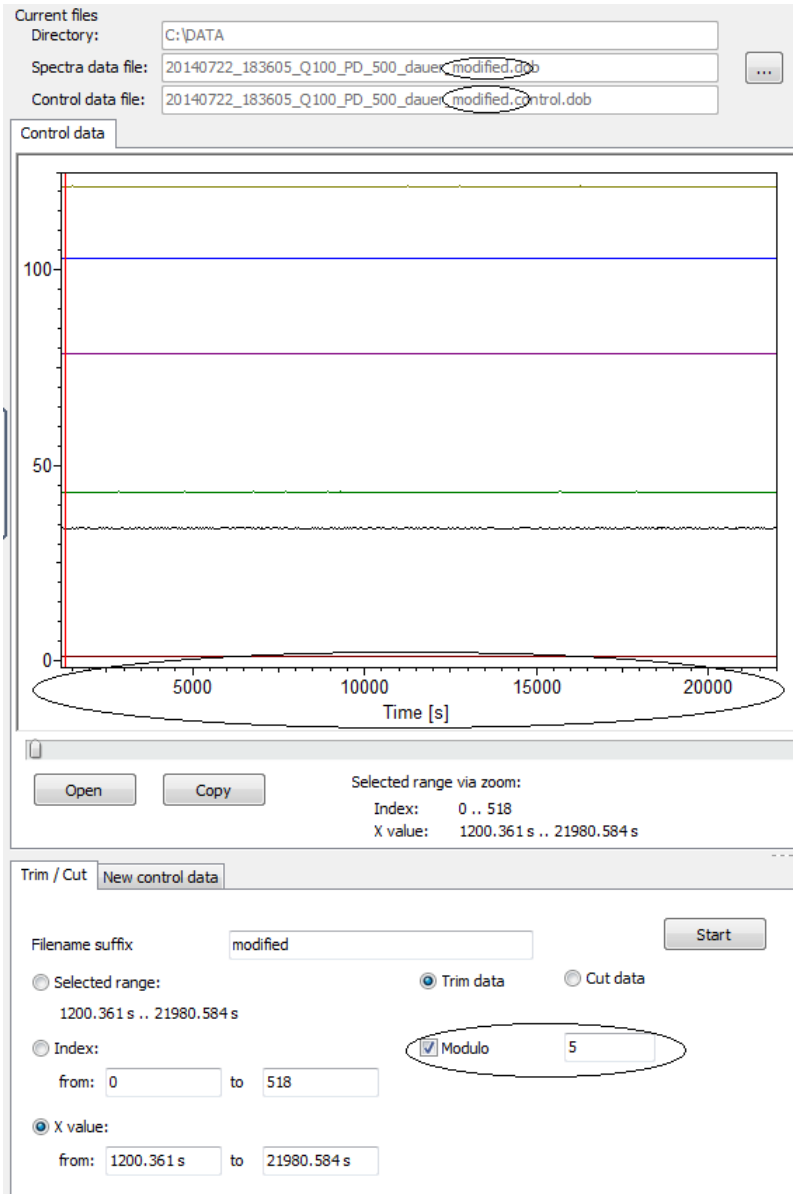


Fig. 6-45 Example after trim operation

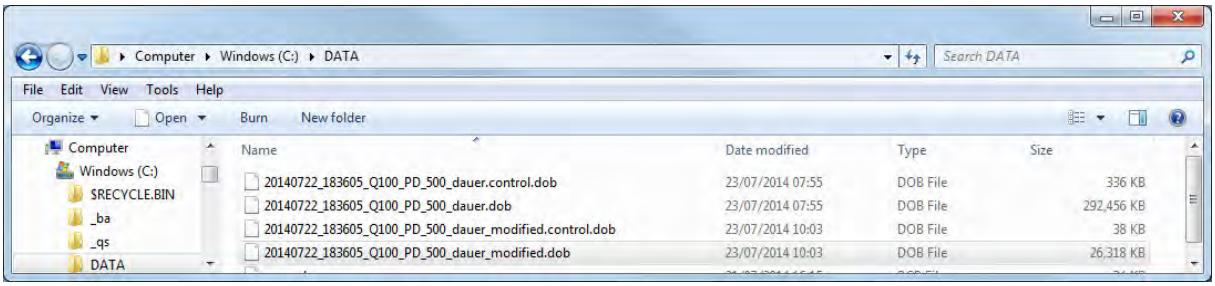


Fig. 6-46 New files saved on the disc

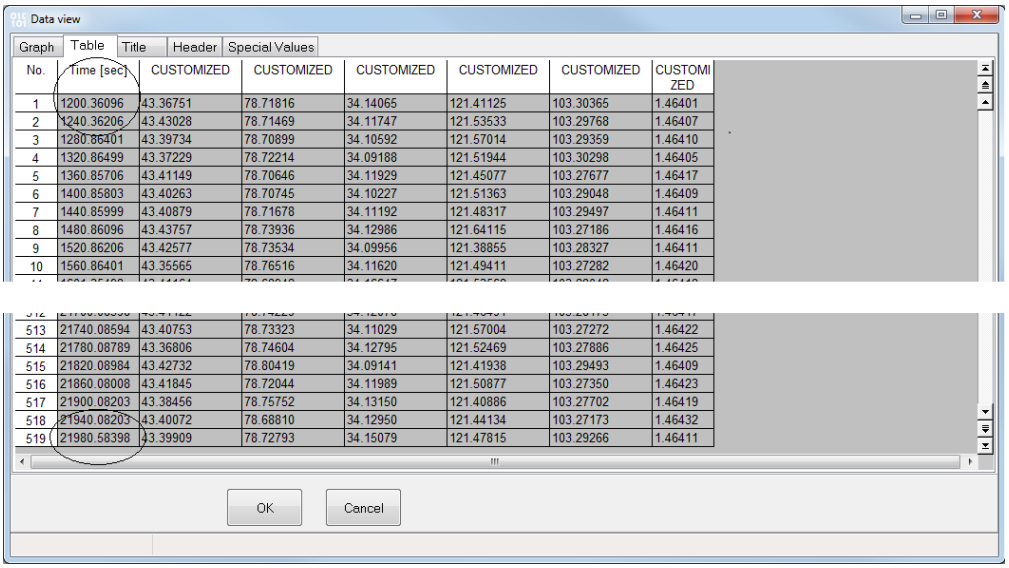


Fig. 6-47 Data table of trimmed file. Start and end time shown in the data view.

6.6.5 Creating new control data

The dialog 'New control data' allows to create new control data (time lines) from a raw data file. This may be interesting if for example the Psi value or the Delta value at a certain wavelength turns out to be sensitive to a certain physical effect.

As shown in Fig. 6-48 the new desired type of control data can be entered in the edit field. The syntax is the same as shown in chapter 6.3.6. The table for all commands can be opened by clicking ?. The table is shown in Fig. 6-9.

The button Create starts the extraction of the desired values. The resulting curves are shown in diagram on the right side.

The button Open allows to view details of the dataset and the button Copy allows to copy the new dataset to the data box of the standard view.

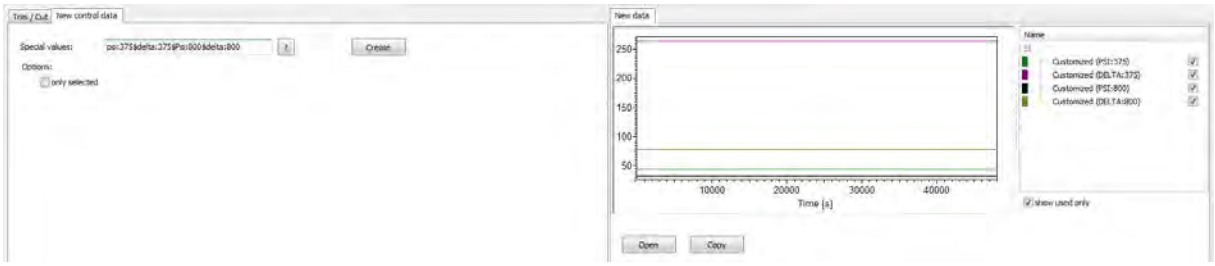


Fig. 6-48 Create new control data

7 Device driver

7.1 Main window

The main window as shown in Fig. 7-1 consists of a toolbar and up to five different tabs for global measurement settings and the configuration of the different spectral ranges.

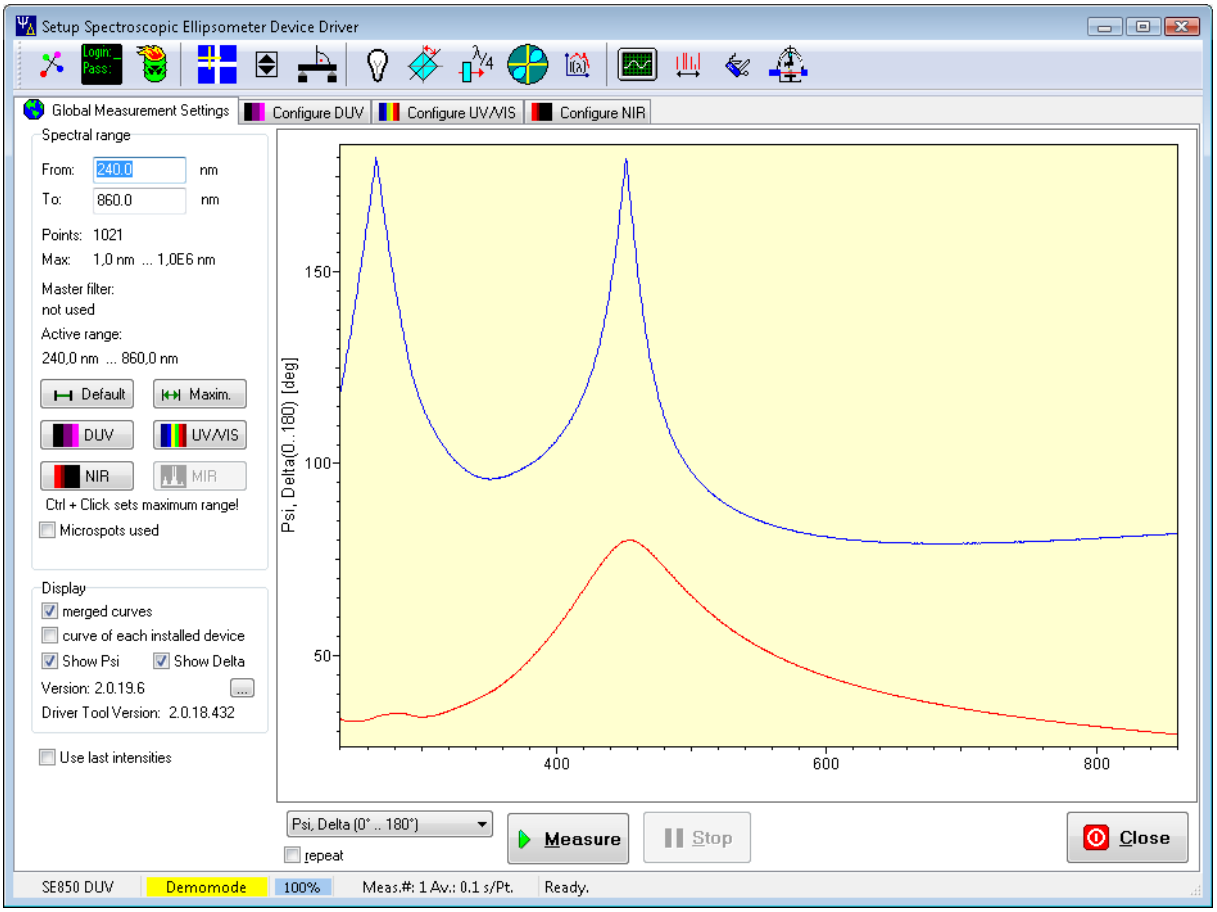


Fig. 7-1 The main window of the device driver

7.1.1 Toolbar

The toolbar gives fast access by instructive icons to the most often used functions of the device driver.

Fig. 7-2 The toolbar of the device driver window

The toolbar consists of 15 icons:

- Installed equipment 
- Controller access 
- Initialize the hardware again (reset all components) 

- Automatic sample alignment 
- Move sample stage (xyz) 
- Move sample stage (tilt and height) 
- Setup Xenon light source 
- Polarizer and analyzer setup 
- Calibration viewer 
- Polar graph 
- Intensity viewer 
- Server for SE800 calibration tool 
- Spectral calibration 
- General tools 
- Calibration at 90 degree 

Each icon is described in detail in the following sections.

7.1.1.1 Installed equipment

Clicking on  opens a window with 8 different tabs (Fig. 7-3). The “Installed equipment” window allows setting the settings for the installed hardware and the demo mode.

These settings should only be changed by advanced/introduced users.

7.1.1.1.1 General

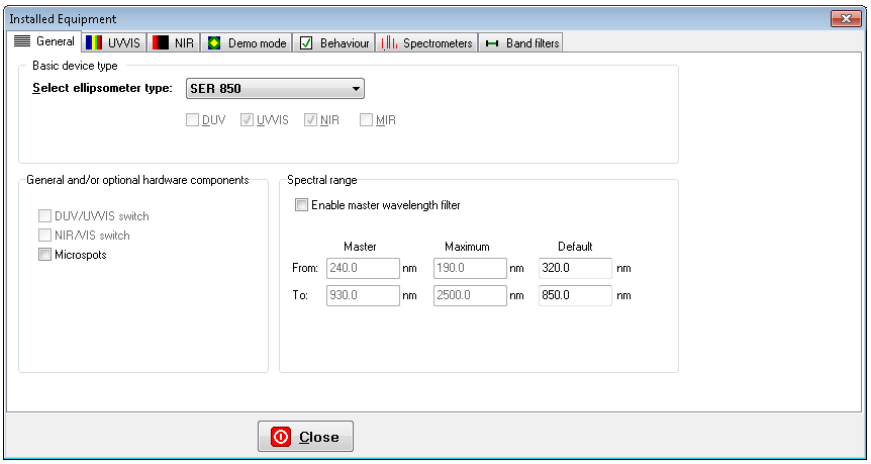
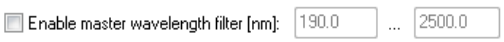


Fig. 7-3 Installed Equipment - General

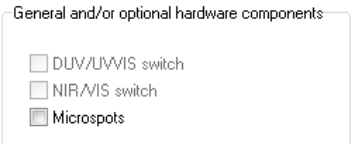
Here you can choose the installed measurement device.

Depending on the selected device the checkboxes for the spectral ranges are checked or unchecked. Note, that if you change this selection you apply presets to new selected spectral ranges. Change this setting only BEFORE alignment of the device (you may also backup the configuration file “SpelliAdv.Config.xml” to ensure that you do not cause damage).

The “Enable master wavelength filter” allows setting a wavelength in a defined spectral range.



In “General and/or optional hardware components” you may edit the list of optional components. The list has grayed items which are not available for the selected machine and enabled items for optional components. If you check an option, it will be used – otherwise it is ignored.



7.1.1.1.2 DUV

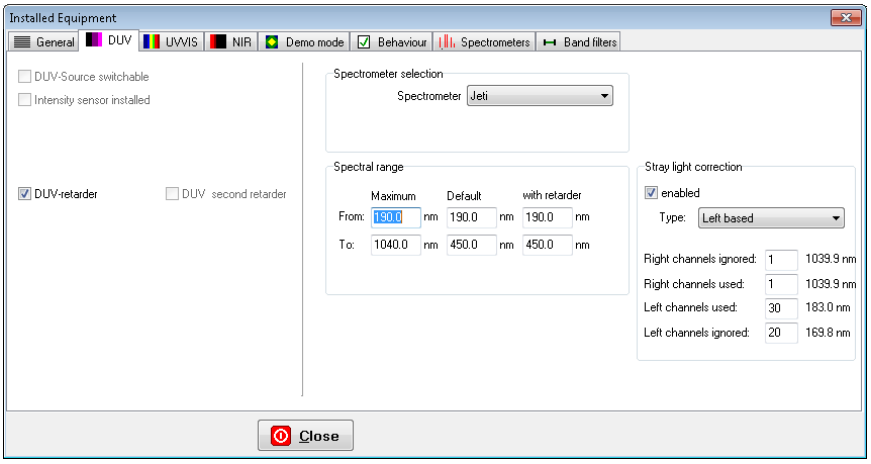
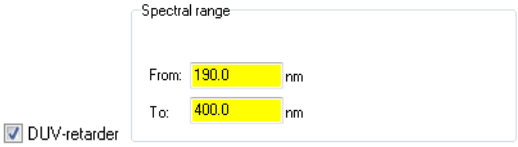
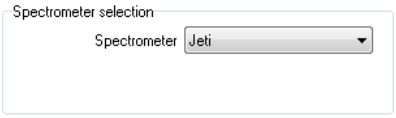


Fig. 7-4 Installed Equipment - DUV

In the DUV-tab you have to choose the right settings for the DUV spectral range like the minimum and maximum wavelength for the DUV and if there is DUV-retarder installed.



Also you have to choose one of the installed spectrometers.



7.1.1.1.3 UV/VIS

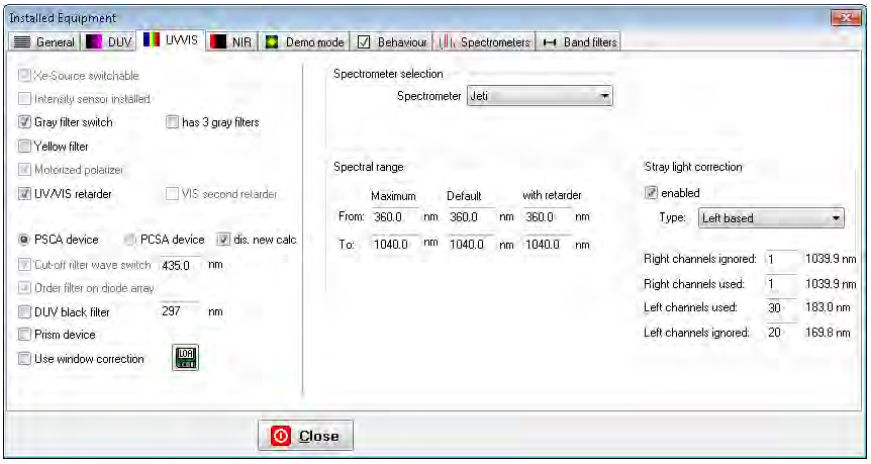


Fig. 7-5 Installed Equipment – UV/VIS

In the UV/VIS-tab you have to choose the right settings for the UV/VIS spectral range, similar to the DUV-tab. On the left side there are some additional general options to set like filters or the correct device (PSCA or PCSA). Do not change these settings without reason, the list must reflect the hardware installed in your system. This list is intended to assist the device setup during the device alignment and may be used as information source for service purposes.

7.1.1.1.4 NIR

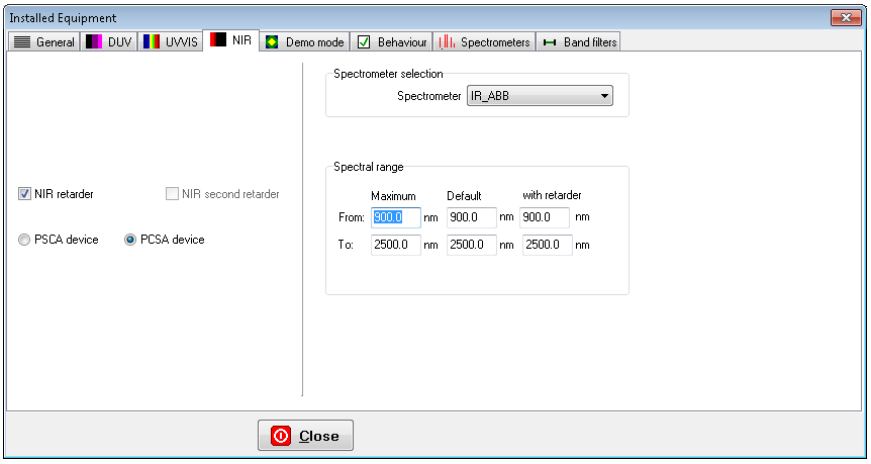


Fig. 7-6 Installed Equipment - NIR

In the NIR-tab you have to choose the right settings for the NIR spectral range like the minimum and maximum wavelength for the NIR and if there is NIR-retarder installed.
Also you have to choose one of the installed spectrometers just like in the DUV-tab.

7.1.1.1.5 Demo Mode

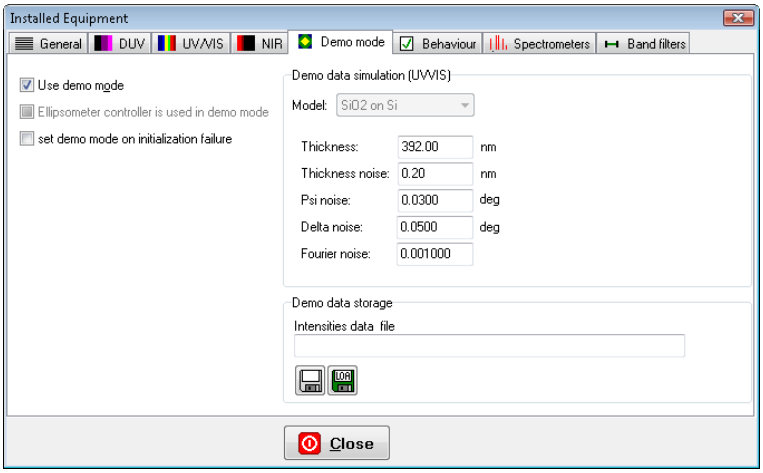
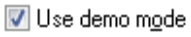
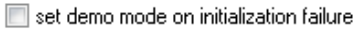


Fig. 7-7 Installed Equipment – Demo mode

If there is no hardware connected to the computer you can activate the demo mode of the software.

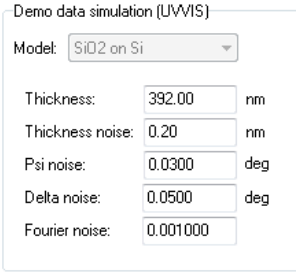


You can choose whether the demo mode should be activated automatically on initialization failure.

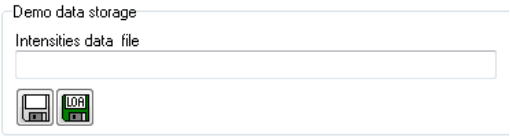


If you want to test the software without having a controller, you may also force the interface to the controller to run in demo mode (this is intended for service purposes, users should never enable this switch).

In demo mode the software generates simulated data based on the settings in this tab when you want to measure.



For reporting the system status, the following function allows to save all raw spectra involved in the measurement of ellipsometric spectra. This service function can be used to report the current state of the light source, beam adjustment and spectral intensity distribution. You may save a file here and send this XML file to the SENTECH service (usually you will be requested to do so by our service, this service function is not intended for typical users).



7.1.1.1.6 Behavior

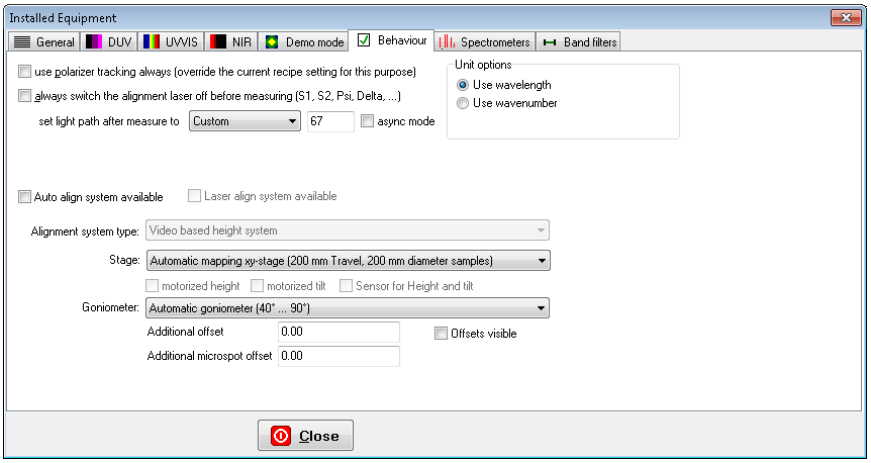
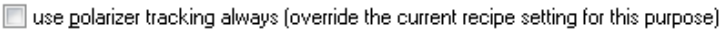
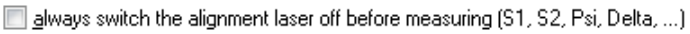


Fig. 7-8 Installed Equipment - Behavior

In this tab you can set the behavior of some hardware components.

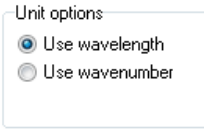


If this option is checked the polarizer tracking will be activated, also the option is not set in the recipe.

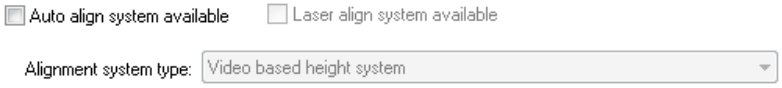


If this option is checked the alignment laser (if available) is always switched off before a measurement.

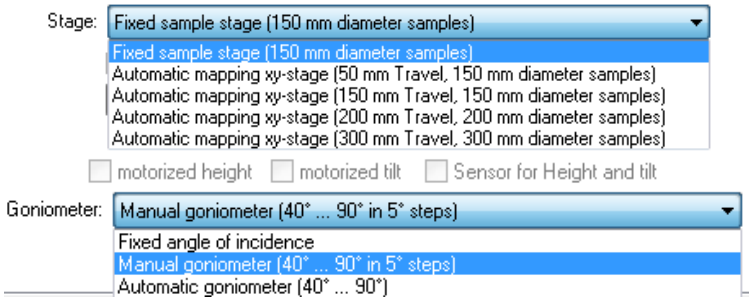
Here you can choose a light path like UV/VIS or NIR. After each measurement this light path will be set. The number to the right is the symbolic digital I/O-number of the controller which will be set.



Here you can choose the unit for the wavelength.



These settings display the installed alignment system.



These settings display the installed hardware (sample stage and goniometer).
Additional offsets for the angle of incidence for the goniometer and/or the installed microspots can be defined here, too.

7.1.1.1.7 Spectrometers

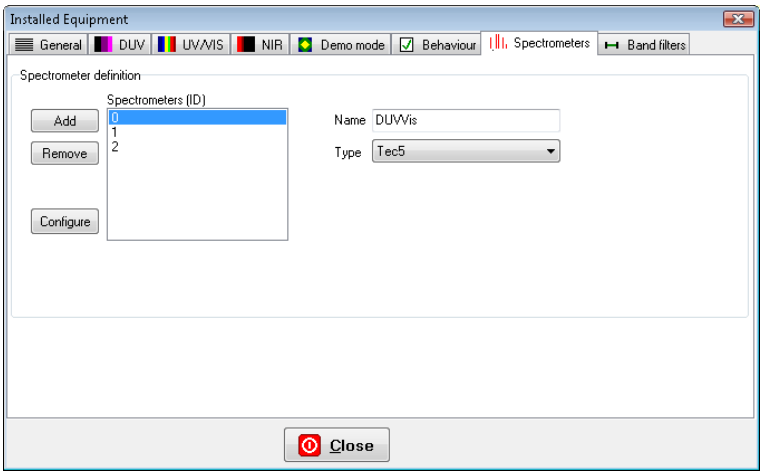


Fig. 7-9 Installed Equipment - Spectrometers

The tab “Spectrometers” shows the installed spectrometers. You can add additional spectrometer or remove spectrometers. The following types of spectrometers can be controlled by the software:

7.1.1.1.8 Band Filters

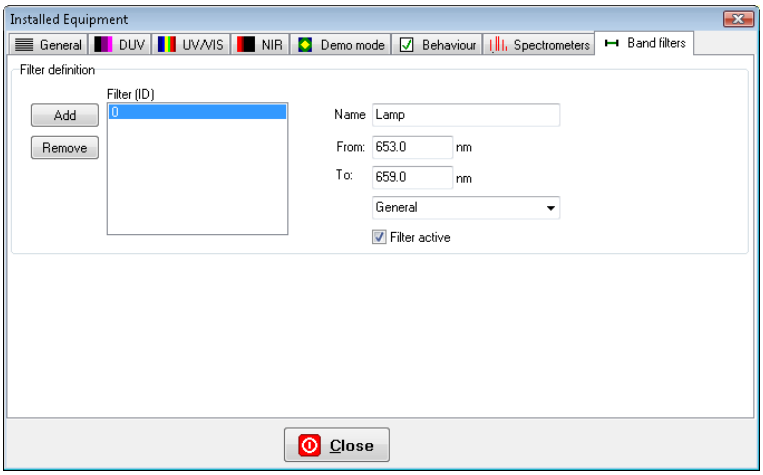


Fig. 7-10 Installed Equipment – Band filters

The tab allows creating additional “software” band filters. This means that the spectra are manipulated by the software. The spectral points between 653nm and 659nm in this case are not displayed and not used for the calculation of the measured values (like Ψ and Δ). You can activate, deactivated, add or remove band filters. These filters are useful for minimizing the influence of sharp peaks in spectrum of the light source.

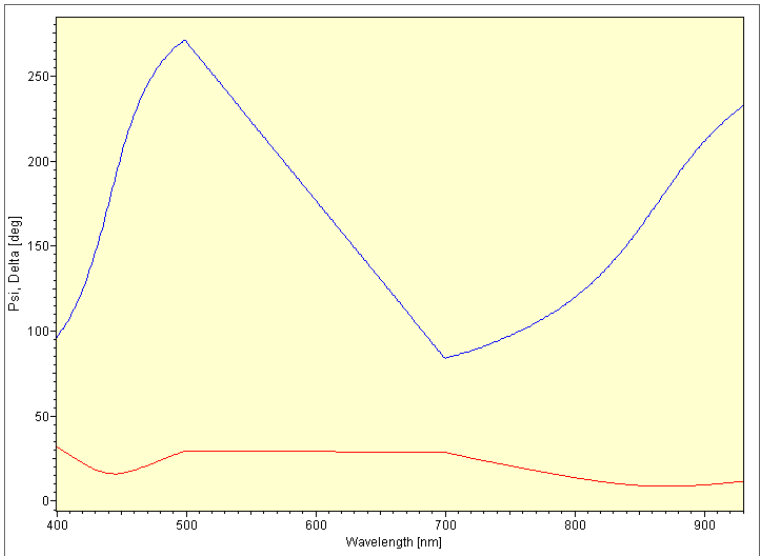


Fig. 7-11 Example for activated filter (500nm-700nm)

7.1.1.2 Controller access

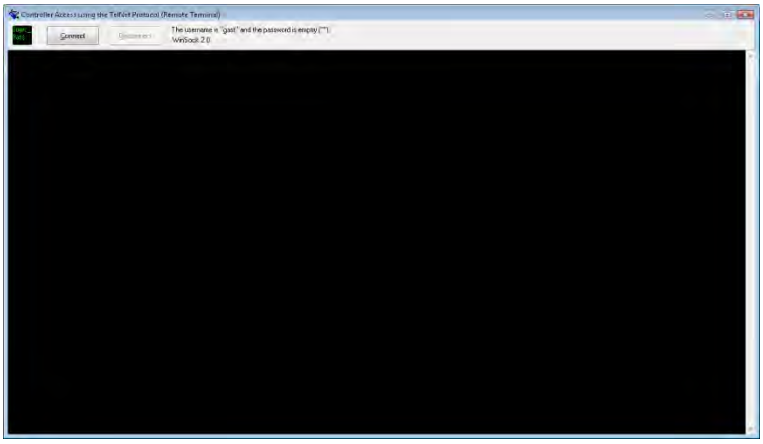


Fig. 7-12 The controller access window

Clicking on 

opens a connection to the ellipsometer controller using the Telnet protocol. This is a useful tool for updating or looking at the logging outputs of the controller software. This tool should only be used by advanced users.

7.1.1.3 Initializing the hardware

Clicking on  resets all hardware components. This causes a complete restart of the ellipsometer driver: Switches lamps on and off, initializes polarizer and analyzer (home function) and sets all the I/O's as apertures and retarder. You should only need this function during service, when you manually work on or move the components.

7.1.1.4 Automatic sample alignment

This function allows running the autofocus and autotilt function directly from the driver. You may align the sample by clicking on this icon. Please note, that the function may work only on devices equipped with autofocus and/or autotilt hardware.

7.1.1.5 Move sample stage

Similar to the alignment this function allows to move the automatic sample stage in x,y and z-axis (height). You must have a mapping stage and/or a height stage installed for proper operation.

7.1.1.6 Alignment

This function resembles the alignment button but is intended to allow the tilt angles of the sample stage manually. Use this function for special purposes (samples that are complicated to align) or for service purposes. Note that you need to have an automatic tilt stage installed in your device (e.g. as it is standard in the SENDURO ellipsometer).

7.1.1.7 Setup Xenon light source

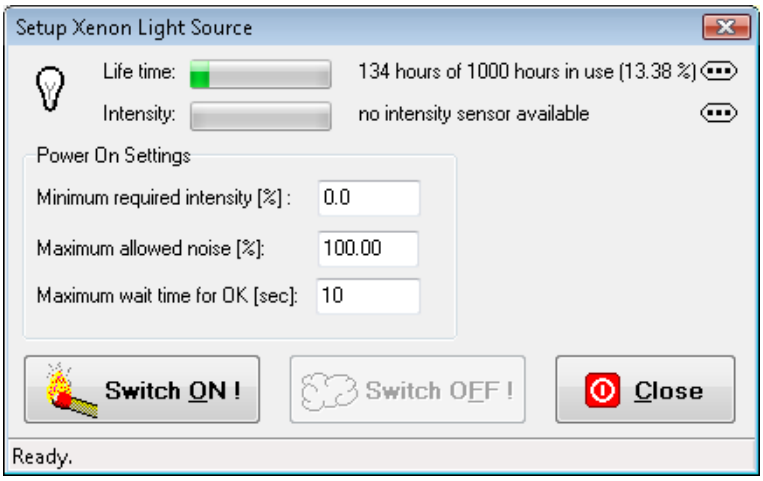


Fig. 7-13 Xenon light source setup

Fig. 7-13 shows the setup window for the Xenon light source. If there is a switchable light source available you switch it on/off and the lifetime and intensity is displayed.

Note: If the lifetime of a lamp is exceeded, you need to reset the lifetime counter. There is a small utility “LifeTime.exe”, which is available in the program folder of SpectraRay which assists you for this function.

Note: this function may also be used for other types of lamps, for example a deuterium lamp.

7.1.1.8 Polarizer and analyzer setup

The polarizer and analyzer setup allows to set the measurement position of the polarizer and the calibrated offsets of the polarizer and the analyzer.

Note: It is important NOT to change the settings in this dialog except for a good reason as the settings are important calibration data of the ellipsometer.

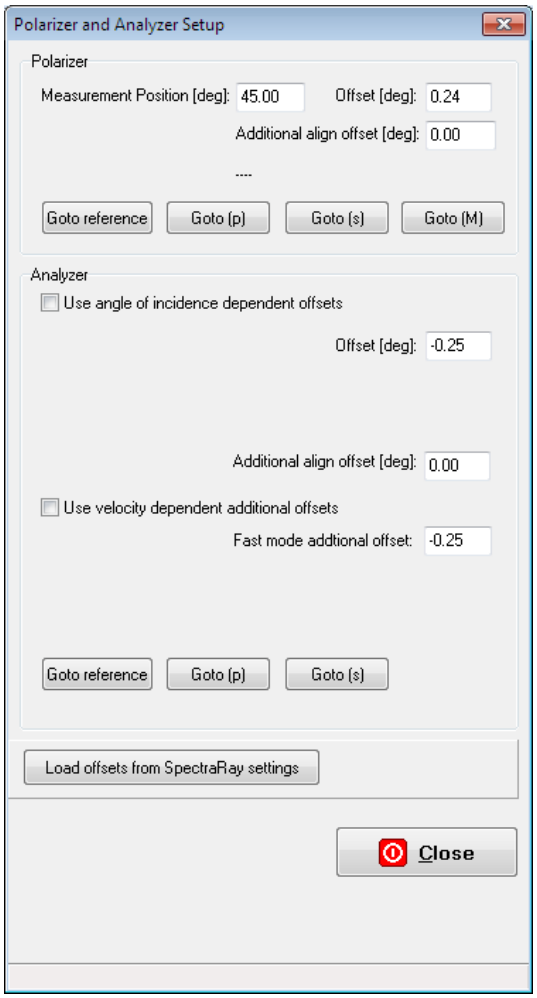


Fig. 7-14 Polarizer and analyzer setup

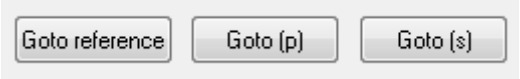
The position of the analyzer for measurements is set in the field

and it is usually set to 45° for most applications.
The analyzer measurement position may be set to other values between approx. 20° and 70° in case of samples that require a changed individual setting for higher measurement accuracy.

The polarizer can be referenced and moved individually by the buttons

where (p) denotes the direction of p-polarization and
(s) denotes the direction of s-polarization and
(M) denotes the measurement position.
Of course it is assumed that the correct offset is already given for a correct positioning.

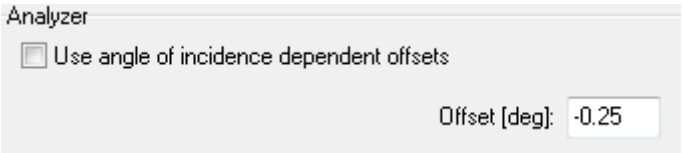
The analyzer can be referenced and moved individually by the buttons



where (p) denotes the direction of p-polarization and
(s) denotes the direction of s-polarization.
Of course it is assumed that the correct offset is already given for a correct positioning.

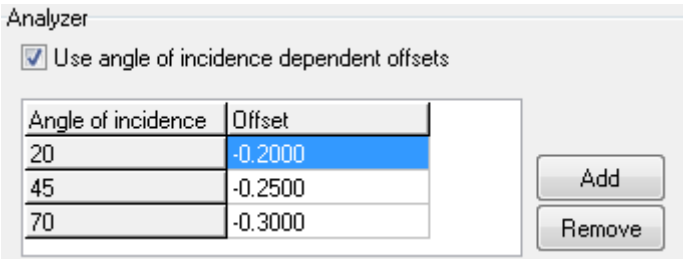
The offsets for the analyzer and polarizer are given in the fields

and

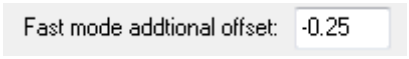


These entries are used to define the offset between the mechanical reference and the optical coordinate system.

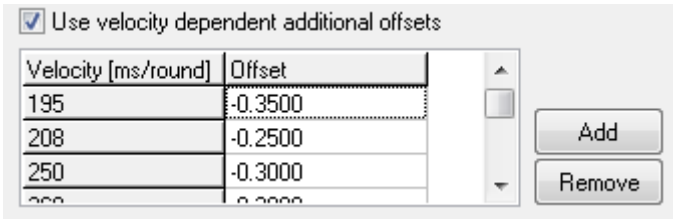
In certain cases calibration valuesfor the analyzer are dependent from the angle of incidence. In this case the option 'Use angle of incidence dependent offset may be checked and a table of offsets may be entered using the 'Add' and 'Remove' button.



For analyzers used in the optional 'fast mode' (which means continuous rotation) an additional offset is given in the field



which is valid for all rotation velocities.
It may be necessary to set different offsets for different rotation velocities. This can be done by checking the option 'Use velocity dependent additional offsets'. A table of offsets may then be entered using the 'Add' and 'Remove' button.



For upgrades from earlier SpectraRay software versions which used the file spelli.ini for the configuration settings (instead of the file spelliadv.config.xml which is currently used) it is possible to import the old values by clicking 

and selecting the correct file 'spelli.ini' in a file selection box.

7.1.1.9 Calibration viewer

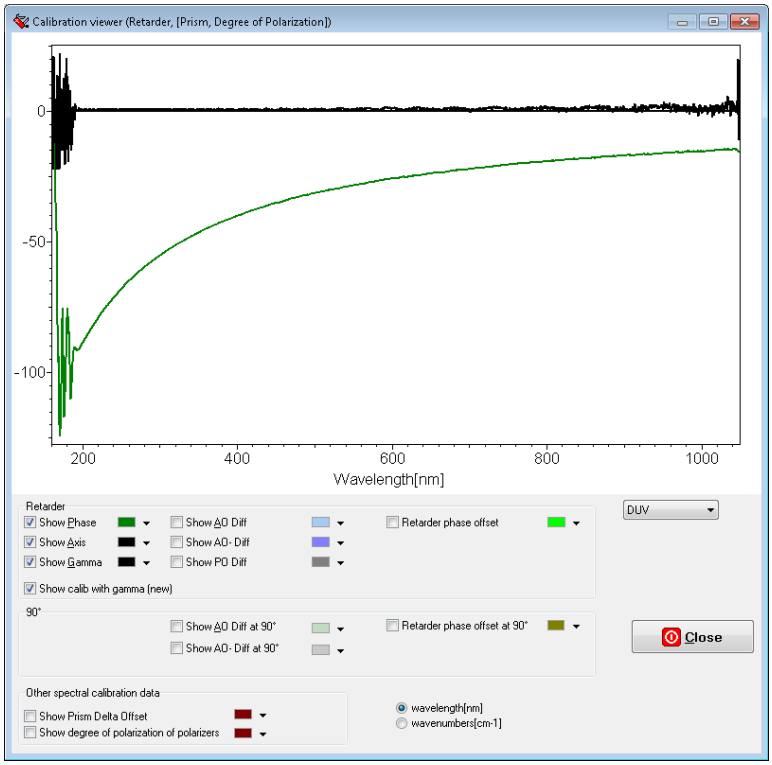
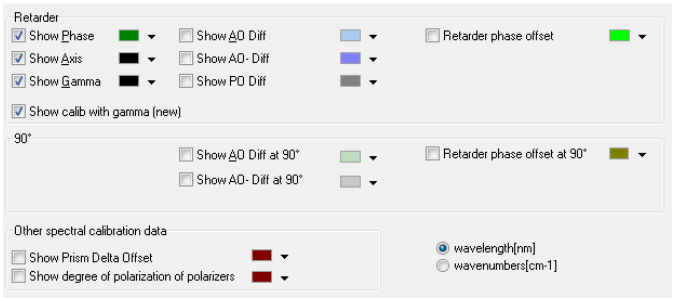


Fig. 7-15 Calibration viewer window

In the calibration viewer window all calibrated values (like retarder phase and axis,…) are displayed. You can choose the spectral range

and the calibrated value



which should be displayed in the graph. You cannot change the calibration in this dialog.

7.1.1.10 Polar graph

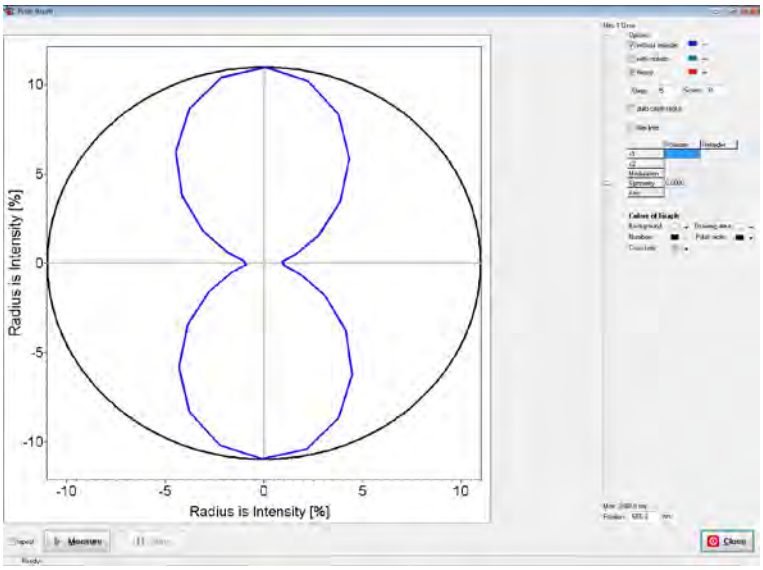
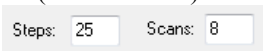


Fig. 7-16 Polar graph window

The polar graph window allows measuring the polar diagram of the intensities for the spectral range chosen in the main menu (see Fig. 7-1). The polar diagram can be measured with and/or without retarder and a theory can be displayed too.

You can choose the count of analyzer positions (for resolution) and scans (for averaging).



For detailed information the values of s1, s2, modulation, symmetry and axis the polarizer and retarder measurement are displayed too.

	Polarizer	Retarder
s1		
s2		
Modulation		
Symmetry	0.0000	
Axis		

The slider on the right side allows setting the wavelength for which the polar diagram should be displayed.

7.1.1.11 Intensity viewer

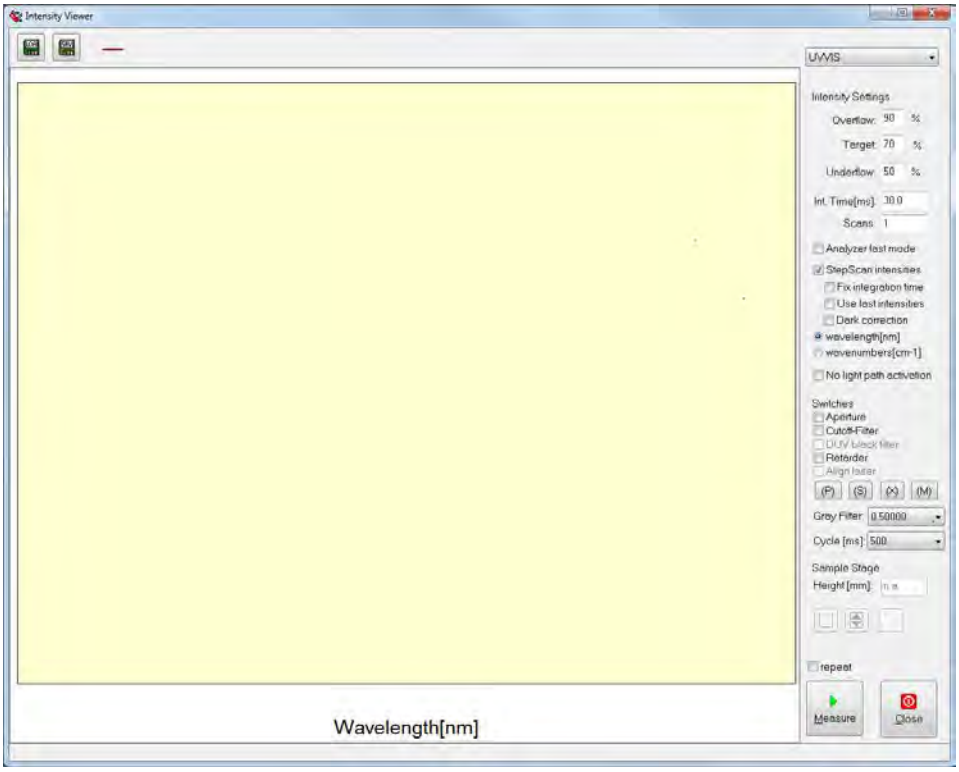


Fig. 7-17 Intensity viewer

The intensity viewer allows measuring, saving and loading spectra. It is mostly used for testing and setup. Clicking on the button  in the upper left corner opens a file dialog for saving the actual spectrum as XML or ASCII-file. Clicking on the button  opens a file dialog for reloading a spectrum (only XML-files).

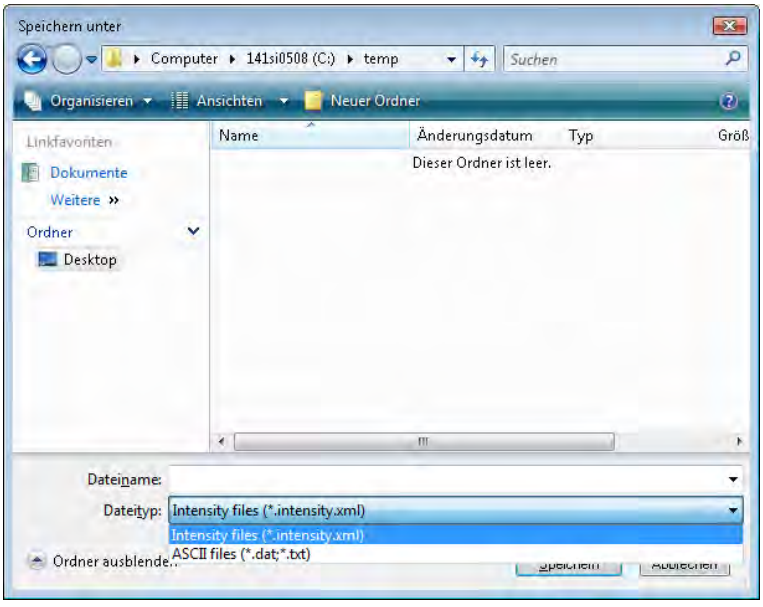
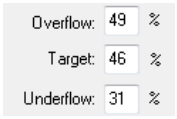


Fig. 7-18 “Save”-dialog

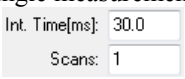
Just above the spectrum the maximum and average intensity in percent as well as “underflow” (or “overflow”) is displayed.

The “underflow” message appears when the maximum intensity is lower than the underflow setting on the right side. The “overflow” message appears when the maximum intensity is greater than the overflow setting.

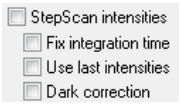


If the integration time is not fixed, it will be adjusted, so that the maximum intensity is in the range of the target intensity.

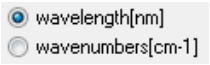
This option allows choosing the spectral range for the measurement and sets the correct spectrometer for the selected spectral range (see section 7.1.1.1.7).
Here you can set a fixed integration time for a single measurement and the number of scans for averaging:



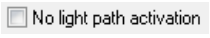
If you want to compare the spectra for different analyzer positions you have to check the option “StepScan intensities”. The number of analyzer positions is set in the “Configure XXX”-tab for the chosen spectral range. Here you can use a fixed integration time for all analyzer positions. If “Use last intensities” is checked the spectra of the last ellipsometry measurement will be displayed. If “Dark correction” is checked a dark correction will be made.



It also possible to switch between wavelength and wavenumbers.



If “No light path activation” is unchecked the correct light path (fiber switch,…) for the selected spectral range will be set automatically when you click “Measure”. If “No light path activation” is checked the actual light path will not be changed even if it is the wrong one.

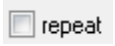


Checking the switches “Aperture”, “Retarder” and “Align laser” bring the aperture/retarder into the light path or make the right settings for the laser alignment. Clicking on (P), (S), (X) or (M) will bring the polarizer and the analyzer to p-, s-polarization or crossed to each other and in the case of (M) into the standard polarizer position.

The optional gray filters can be selected by the list. The value is the approximate reduction factor of the intensity. In case of ellipsometric measurements the optional grayfilters are set automatically according to the light level. The display will then be updated accordingly.

If the spectrometer and electronics is capable of fastmode the cycle time can be selected from the list. The value gives the time of a whole rotation of the continuously rotating polarizing element.

Clicking on 

will start a single measurement or if 

is checked will measure the whole time until “repeat” is unchecked again.

7.1.1.12 Server for SE800 calibration tool

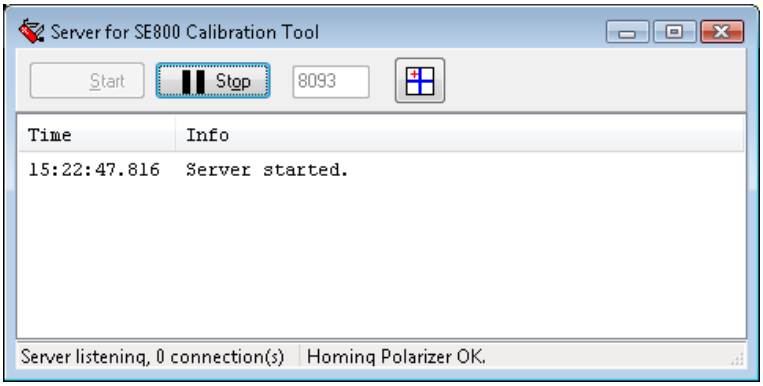


Fig. 7-19 Calibration server

Clicking on  will open the calibration server window. This is intended for insitu calibration or calibration of the ellipsometer at fixed angles of incidence (when the 90 degree position is not available). Please read the manual of the “SE800 Calibration Utility” for further information.

7.1.1.13 Spectral calibration

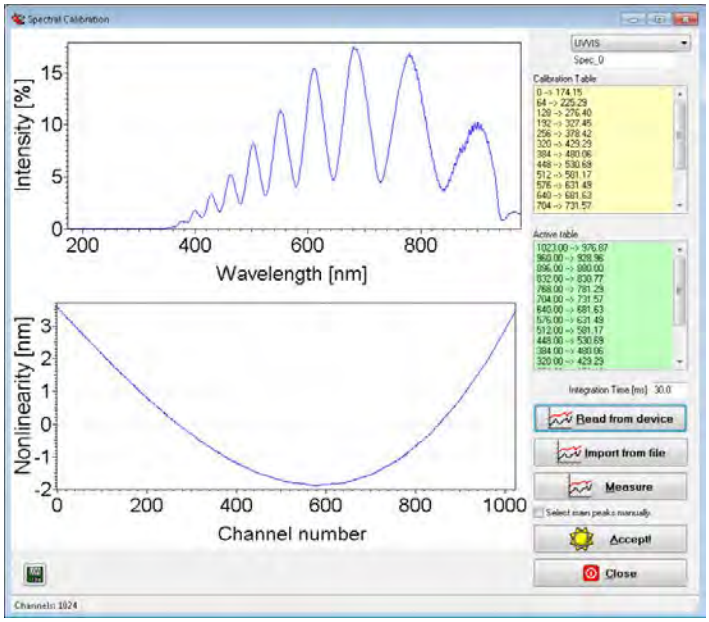


Fig. 7-20 Spectral calibration window

The spectral calibration window allows calibrating the spectrometer. You can read the spectral calibration from the spectrometer itself, import it from a file or make a manual calibration. Clicking on “Accept” will change the configuration for future measurements.
This “readout” function is available typically for spectrometers attached to the USB port. If you have an internal spectrometer within the controller, you need to attach a spectral line lamp (available from our service) and make an intensity measurement. After a measurement the software automatically searches specific line positions and finds the spectral calibration. You may check within the display whether the lines found are correct and you may accept the new calibration by pressing the “Accept” button. This should tell you, that your spectral calibration is not change unless you press “Accept”.

7.1.1.14 General tools

Fig. 7-21 General tools

This tool allows communicating with the ellipsometer controller by means of a Telnet, FTP or XML-connection if connected to the controller. The controller used is a small computer running a Linux operating system. With “Telnet” you may directly “work” on the controller. With FTP you can read/write files from and to the controller. The latter function is mainly intended for servicing. Telnet is a preferred method to enabled extended diagnostics (by our service) and FTP allows to read the log files from the controller (our service may instruct you to read some files by using these tools). With “Comm” you may setup the TCP/IP connection to the controller.

A simple tool is “Initialize goniometer”. This function is a bit hidden because all high level function run the initialization automatically if required. Please note, this is again a function which mainly is intended for device setup or servicing purposes.

7.1.1.15 Calibration at 90 degree

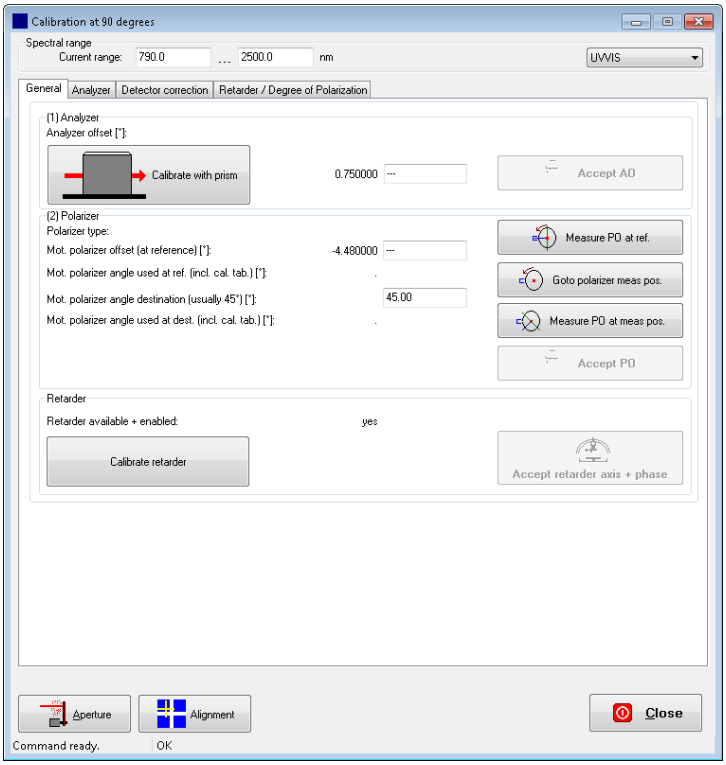
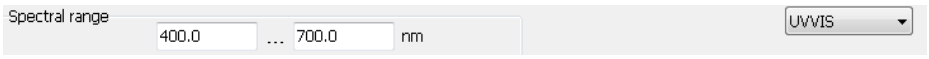


Fig. 7-22 Calibration at 90 degree - General

To perform a calibration of the ellipsometer you have to click  . The window shown below will be opened. Choose the spectral range for the calibration



and click on 

. The Analyzer-tab will be opened.

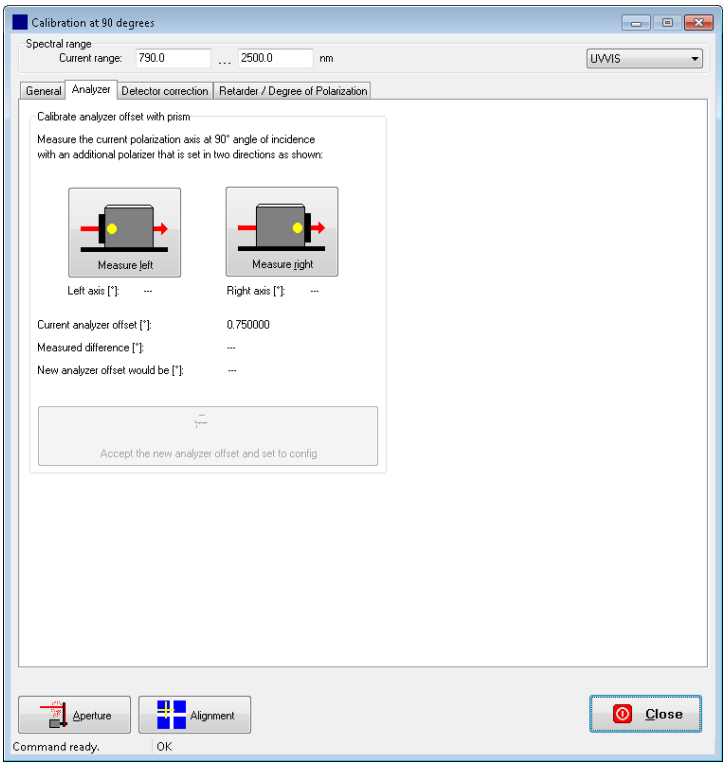
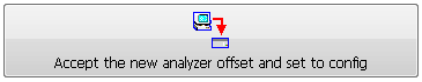


Fig. 7-23 Calibration at 90 degree – Analyzer

For the analyzer calibration you need a special prism, which has to be aligned on the sample stage in two positions as can be seen on the buttons.

For each position you have to make a measurement at an angle of incidence of 90 degree by clicking on the corresponding button. After that the new analyzer offset will be calculated and you can accept and save the new offset by clicking



.

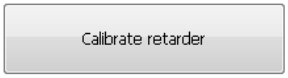
In second step return to the first tab and perform the polarizer calibration (without additional prism) by clicking

or

.

After accepting the new polarizer offset

you have to continue with the retarder calibration



.

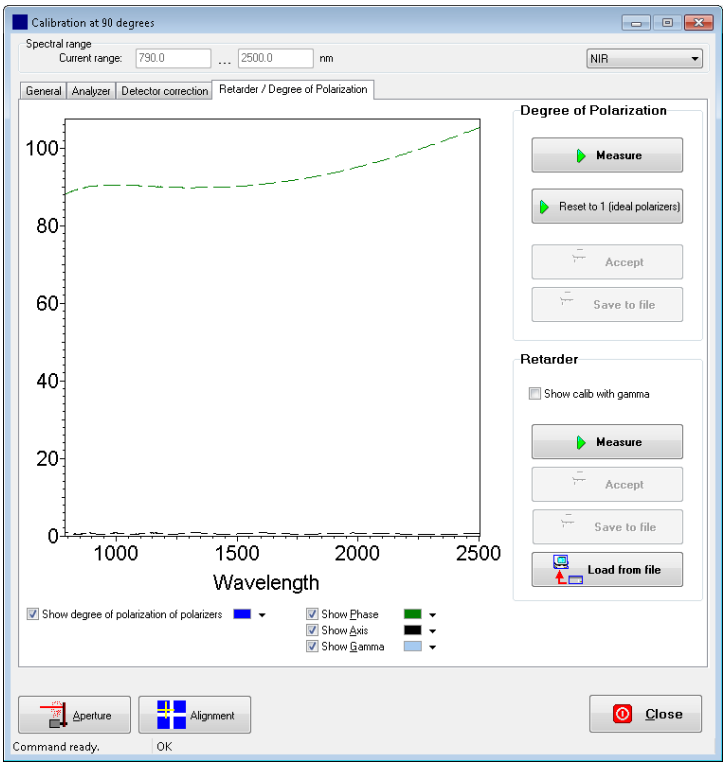


Fig. 7-24 Calibration at 90 degree – Retarder/Degree of Polarization

In the last step you have to calibrate the axis and phase of the retarder by clicking on “Measure” and “Accept”. The “Degree of polarization” is intended for infrared ellipsometers, where the polarizers have not that high extinction ration compared to UVVIS polarizers. In such case you may run this additional calibration which measures the extinction ratio from the degree of polarization (since we assume here a straight through setup, we can associate the virtual drop in the degree of polarization (should be always 1) to the polarizer/analyzer parameters.

7.1.2 Global measurement settings

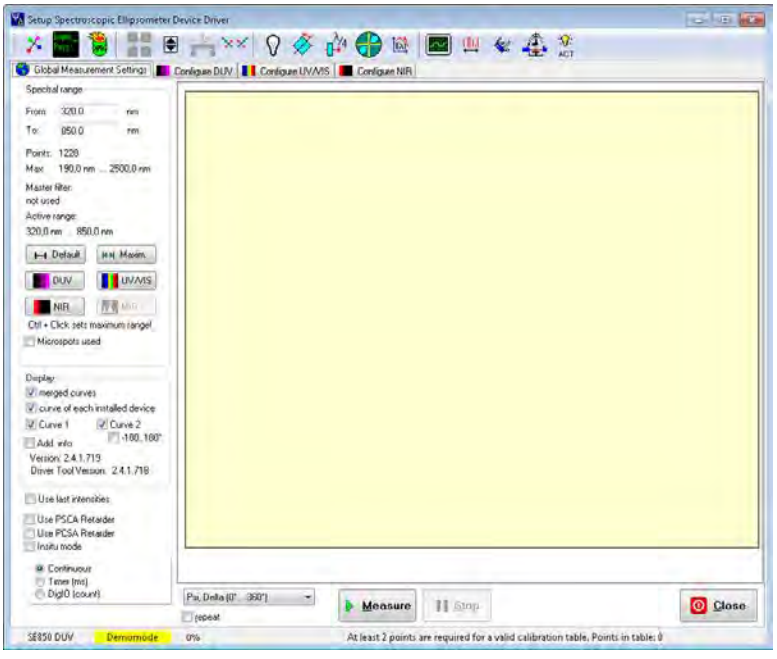
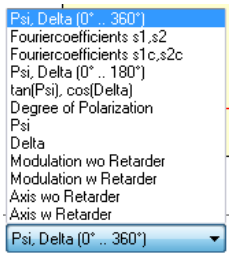
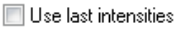


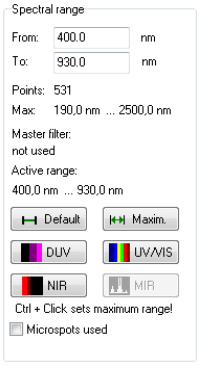
Fig. 7-25 Global measurement settings

The “Global measurement settings”-tab allows performing ellipsometry measurements by clicking on

Similar to the intensity viewer (see sec. 0)  allows repeated measurements until unchecked.
You can select different measurement tasks:

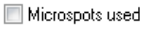


If  is checked the last measured spectra will be used to perform the actual measurement task without measuring new spectra.
In the “Spectral range”-frame

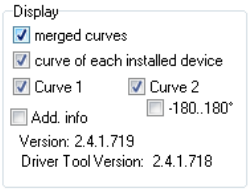


The spectral range for the measurement can be set. Clicking  will set a default spectral range, clicking  will set the maximum spectral range. Clicking  ,  or  will set the corresponding spectral range.

<u>If you have microspots attached</u> to your ellipsometer, you should check the following box. Please note, that the exact angle of incidence which is written to measured spectra is calibrated with specific angle offsets for measurements with and without microspot. **If you do not set the checkbox below properly this may affect the absolute result values of your ellipsometer!**



The following options allow to select the display of curves after measurement. “merged curves” and “curve of each …” are intended for combined spectral ranges as UVVIS and NIR. “Show Psi” and “Show Delta” select which of the two result spectra is displayed (this also applies to measurements of s_1, s_2).



7.1.3 Configure DUV

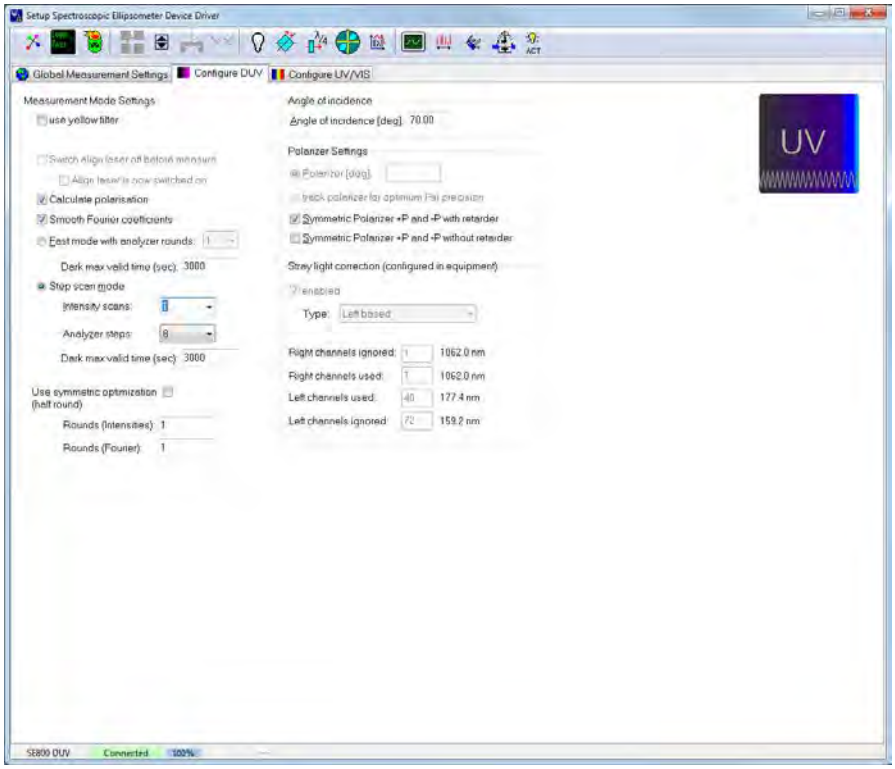
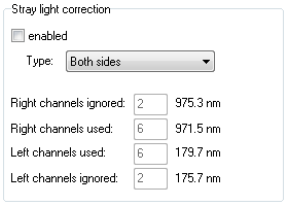


Fig. 7-26 Configure DUV settings

In the “Configure DUV”-tab all settings for the DUV spectral range can be changed. The settings which all spectral ranges have in common are summarized in the following table.

Setting	Recomm. settings	Explanation
Use yellow filter	Off	The optional yellow filter may be switched in to protect certain samples from short wavelength radition.
Calculate Polarization	On	Depolarization effects due to non-idealities of the sample (e.g. inhomogeneities, backside reflections or nano particles) will falsify the (Ψ, Δ) spectra. In combination with the compensator/retarder measurement this influence can be removed completely, so the (Ψ, Δ) spectra as measured on ideal samples.
Smooth Fourier coefficients	Off	A smoothing algorithm is applied to the Fourier coefficients s1, s2.
Fast mode	Off	This is contrary to step scan mode. Here the analyzer is rotating continuously. This is only available for in-situ option.
Fast mode rounds	1	Allows to accumulate 1 or more rounds during fast mode to enhance signal-to-noise ratio
Fast mode dark valid time (sec)	1000	Allows to determine how long the dark signal remains valid, so the measurement will not be interrupted. The dark signal becomes invalid anyway and has to be measured again if the rotation speed is changed.
Step scan mode	On	See explanation below
Intensity scans	1-3	Some spectrometers need much higher settings depending on their sensitivity.
Analyzer steps	8-16	
Step scan dark valid time (sec)	1000	Allows to determine how long the dark signal remains valid, so the measurement will not be interrupted. The dark signal becomes invalid anyway and has to be measured again if the integration time is changed.
Use symmetric optimization	Off	It should be switched on only when a high measurement speed is necessary (e.g. for mapping)
Rounds (intensities)	1	This averages the intensity spectra for n rounds. In case of strong intensity drifts of the light source, this setting shouldn't be used, the Rounds (Fourier) should be used instead.
Rounds (Fourier)	1-16	This setting averages the Fourier coefficients for n rounds. The Fourier coefficients are free of influences of the intensity drift of the light source. Therefore an arbitrary number of rounds can be averaged to increase the SNR.
Angle of incidence	-	It has no effect for measurements started from SpectraRay. Its value will be overwritten by the SpectraRay measurement window.
Symmetric Polarizer +P and -P	On	In some cases, when the Polarizer azimuth is P≠45 deg artifacts due to the compensator / retarder may occur. This setting removes these artifacts. It can also be switched on for P=45 deg.
Symmetric Polarizer +P and -P without retarder	Off	In some cases artifacts also occur in the measurement without the retarder. This setting can remove theses artifacts.

Tab. 7-1 Settings which all spectral ranges have in common



The “stray light correction”-frame allows applying a stray light correction of the detected intensities. This function is intended for SENTECH internal use, users should never change these settings (you may backup the file “spelliadv.config.,xml” to ensure that no settings can be lost.
In newer software versions the settings for the stray light have moved to the calibration section and are shown here for information only.

Ellipsometric measurement mode

SENTECH spectroscopic ellipsometers use the unique “step scan analyzer” mode. Here the analyzer is moved to designated analyzer azimuth positions. There it is stopped and the full spectral range is collected at one shot using either the spectrometer for the UV / VIS or the FTIR for the NIR / MIR spectral ranges.
Then the analyzer is moved to the next azimuth position and the next spectrum is collected. This procedure is repeated until a full round (or a half round) is finished.
At the end the ellipsometric (s1, s2) or (Ψ, Δ) spectra are calculated.

The number of analyzer positions, intensity spectra (collected at each analyzer position) and the total number of Fourier rounds determines the measurement speed and SNR.

7.1.4 Configure UV/VIS

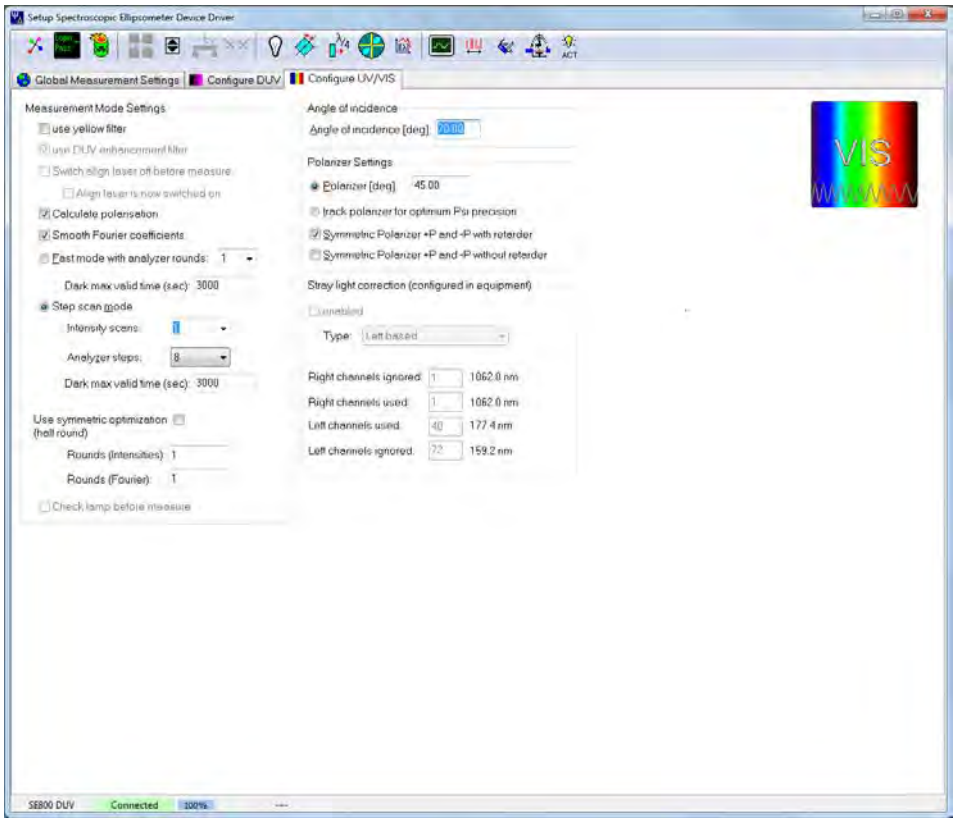


Fig. 7-27 Configure UV/VIS settings

In the “Configure UV/VIS”-tab all settings for the UV/VIS spectral range can be changed. The settings in the DUV-tab and the UV/VIS-tab are mostly identical.

7.1.5 Configure NIR

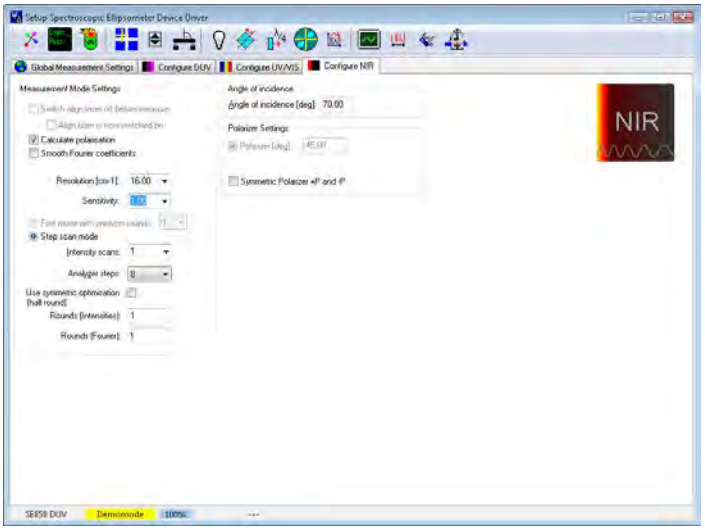
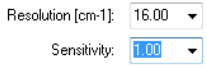


Fig. 7-28 Configure NIR settings

In the “Configure NIR”-tab there are some different options. For the FTIR used for measuring in the NIR spectral range you can set the Resolution (1-32 cm^{-1}) and the sensitivity (1-16).



In the NIR spectral range no stray light correction is necessary. The other settings are identical to the DUV- and UV/VIS-tab.

8 SE-Advanced tutorial

8.1 Basic operation of the SE-Advanced client

8.1.1 Starting the SpectraRay software

The SpectraRay software is started by double clicking the SpectraRay icon on the desktop  .

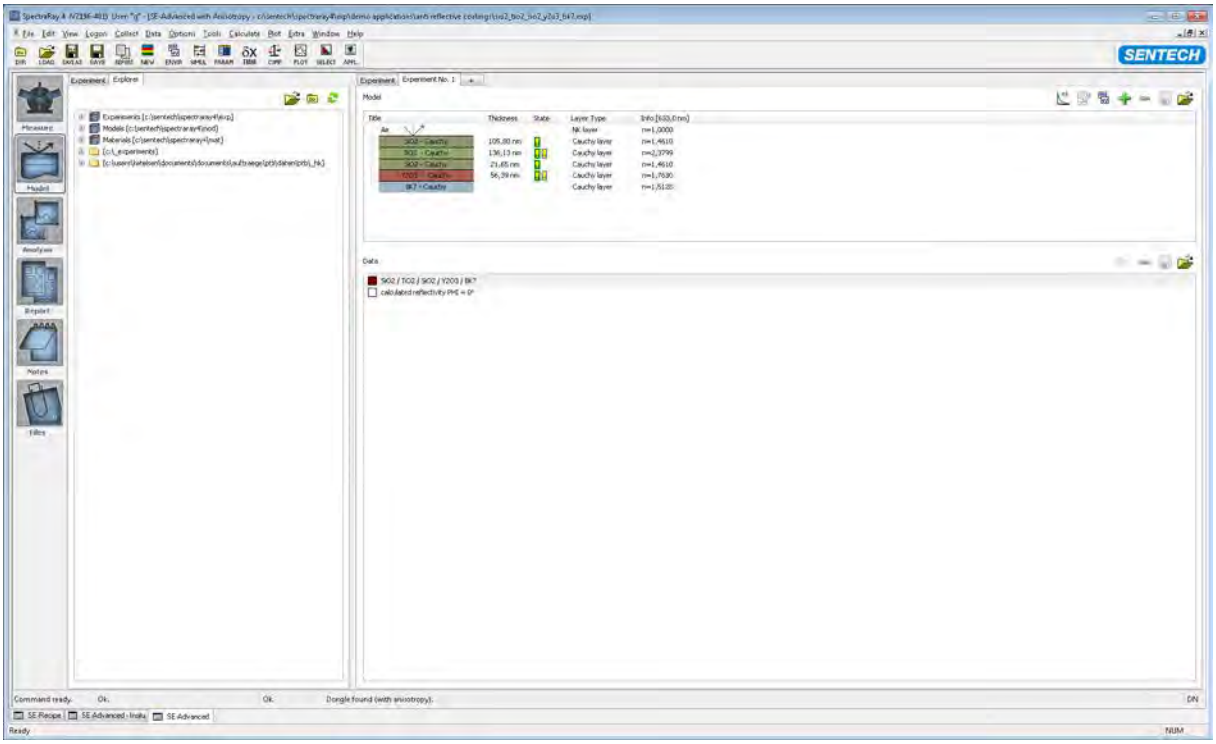


Fig. 8-1 SE-Advanced client

8.1.2 SE-Advanced main window at a glance

The SE-Advanced main window consists of the menu bar, icon bar, tool bar and sub-windows.

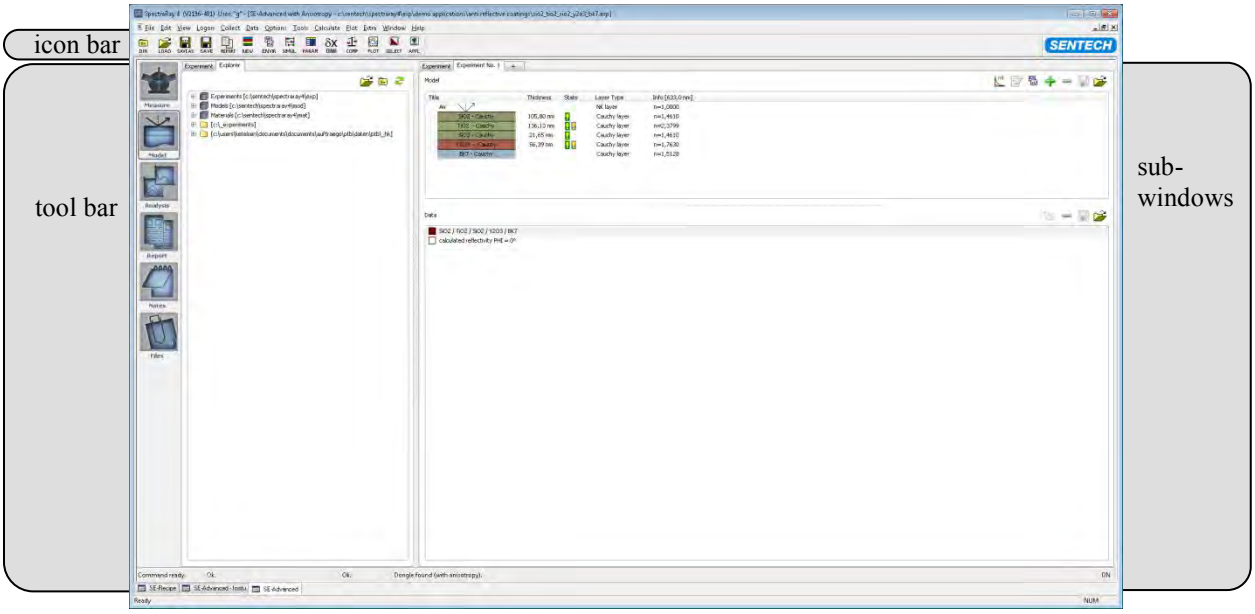


Fig. 8-2 Main window

Icon bar:

The icon bar contains buttons for loading, saving and windows for important settings like the environmental parameters ENVIR and fitting parameters PARAM.

Tool bar:

The most important functions of SE-Advanced are represented in the icon bar for fast access like the measurement window Measure, fitting window Analysis or modeling window Model.

Sub-windows:

The appearance of the sub – windows depends on the task you have chosen in the tool bar.

Model:

When you open SE-Advanced the model-window will appear as shown in Fig. 8-2. In this case there are three sub-windows, the explorer/experiment, the model and the data. This window is used to build up the optical model which is describing the optical behavior of the sample layer stack. Here is defined, which parameters are used for the fitting procedure.
New layers can be inserted into to optical model or existing layers can be deleted from the optical model at any time during the modeling process. There is practical no upper limit for the amount of layers in the optical model.

Measure:

The measurement-window you can see in Fig. 8-3. The measurement-window consists of 4 sub-windows for measurement settings, display of measured data and datasets.

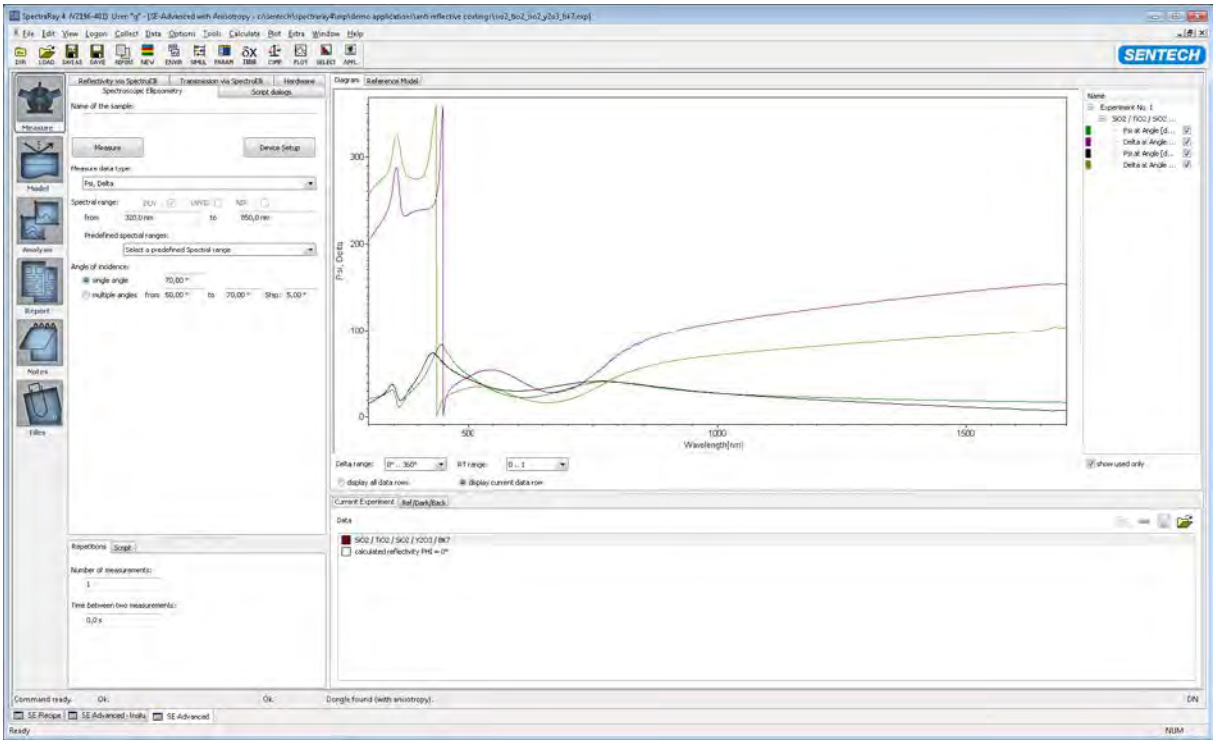


Fig. 8-3 Measurement window

Analysis:

This window is used for fitting the measured data. On the left hand side the measured and fitted curves are displayed. On the right hand side the fit-parameters are listed. Here you can select the parameters used for fitting and change their start values and ranges.

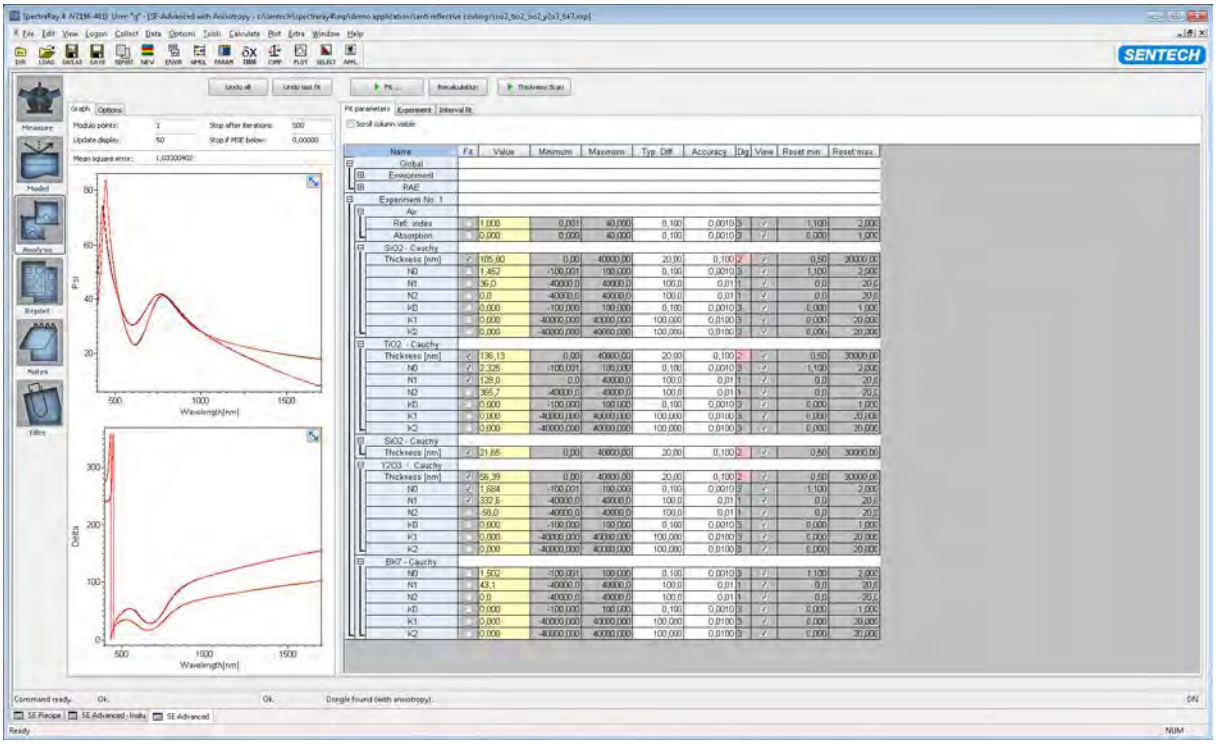


Fig. 8-4 Analysis window

Report:

Here you can report your results and export them into a WORD™-file.

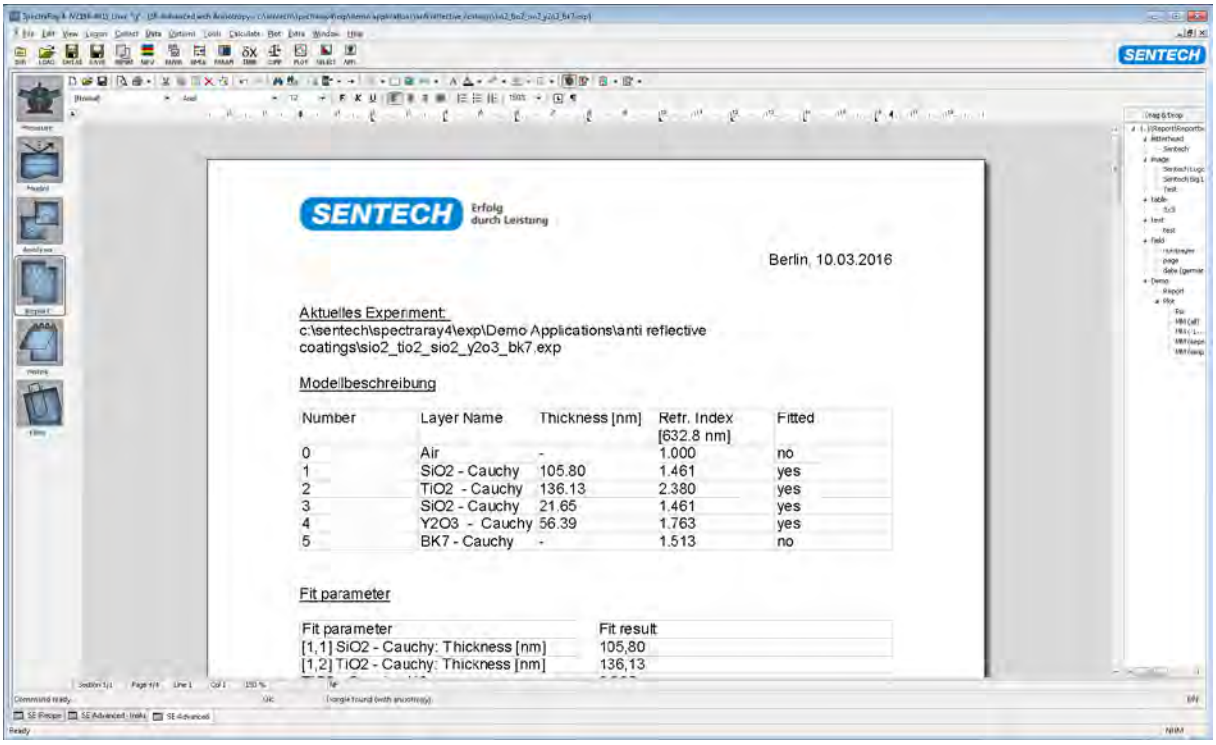


Fig. 8-5 Reporting

Notes:

Here you can write down notes for the current experiment. These notes are saved within the experiment.

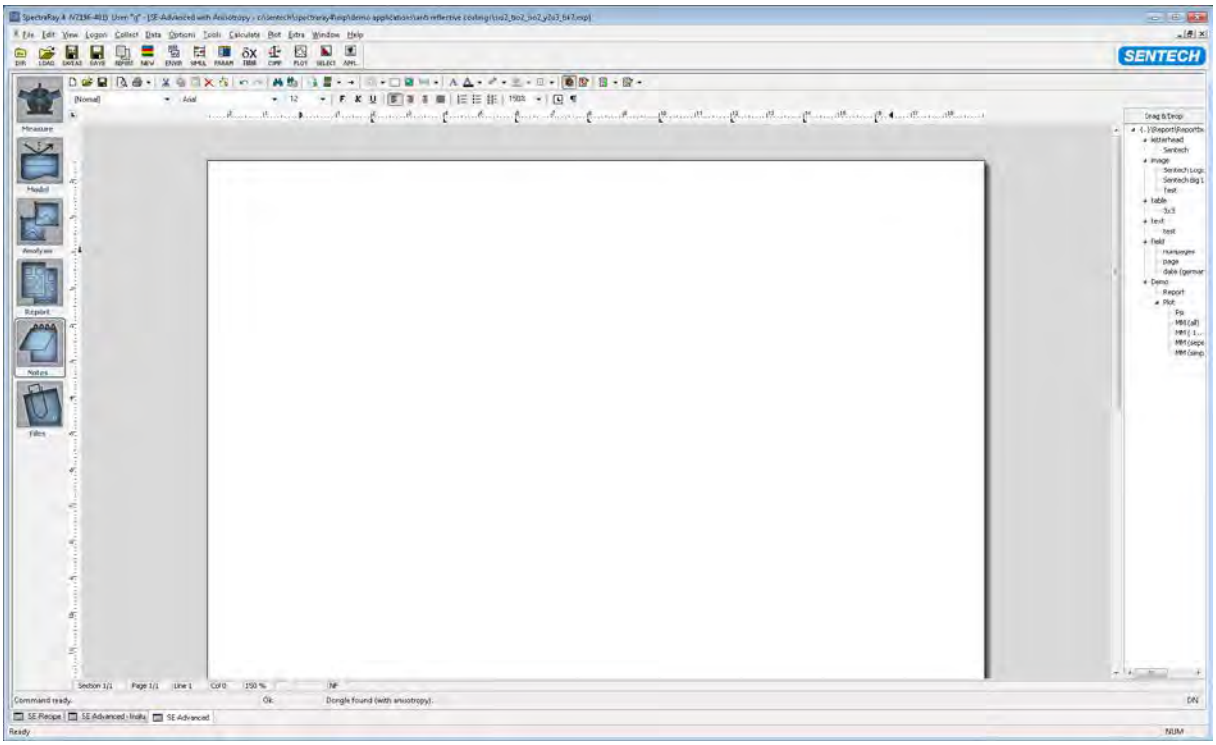


Fig. 8-6 Notes windows

Files:

It is also possible to save external files within your current experiment. You can ad files up to 260 MB.

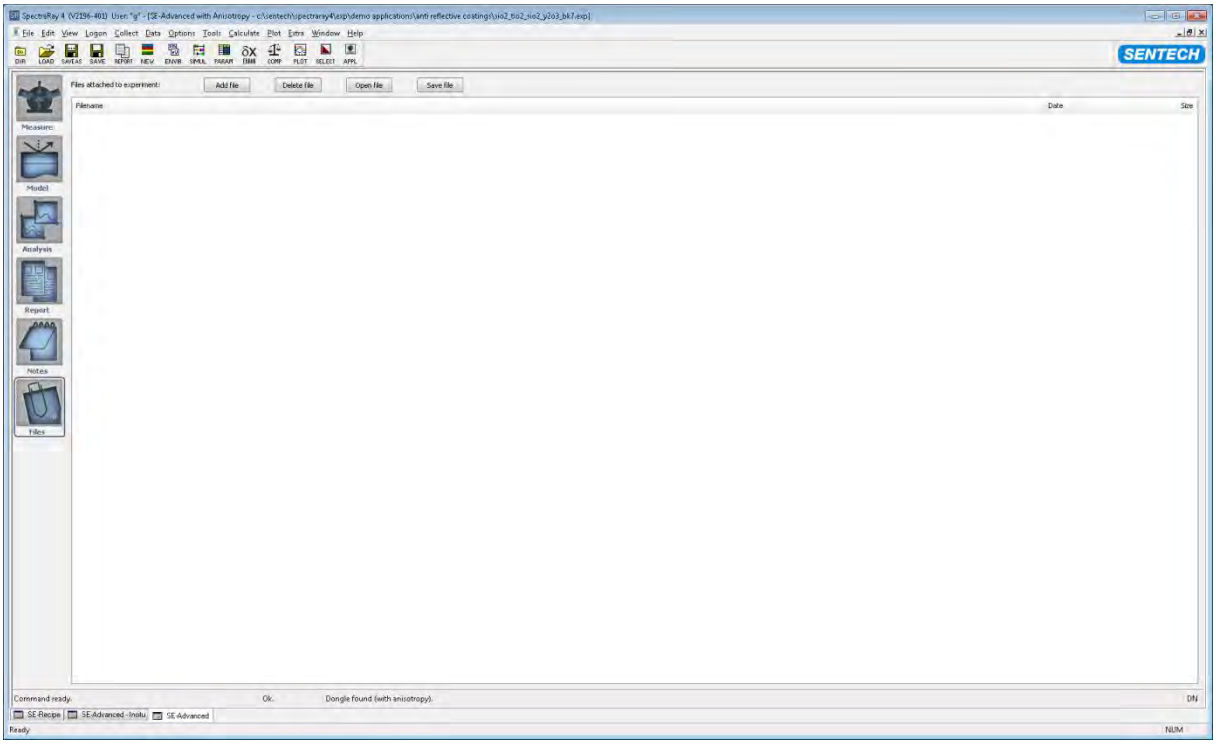


Fig. 8-7 Files window

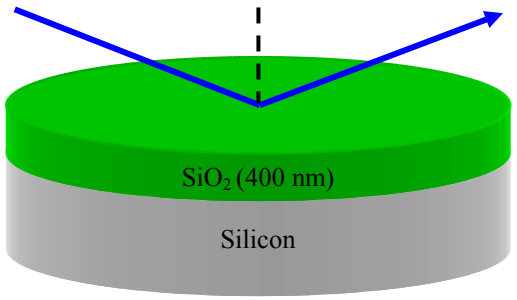
8.1.3 Five basic steps of operation

The sample measurement and analysis can be summarized in five basic steps of operation:

1. **Sample alignment**
2. **Ellipsometric measurement**
   - **2.1. Starting the measurement**
   - **2.2. Renaming the measurement**
3. **Modeling**
   - **3.1. Creating a model**
   - **3.2. Selecting fit parameters**
4. **Fitting**
5. **Reporting**
   - **5.1. No reporting**
   - **5.2. Measurement report**
   - **5.3. Creating manual report**
   - **5.4. Using "Simulation" for report**
   - **5.5. Exporting the simulation data to an ASCII file**

These five steps of sample measurement and analysis will be discussed in the following chapters.

The following standard sample will be used as an example:



8.1.3.1 Sample alignment

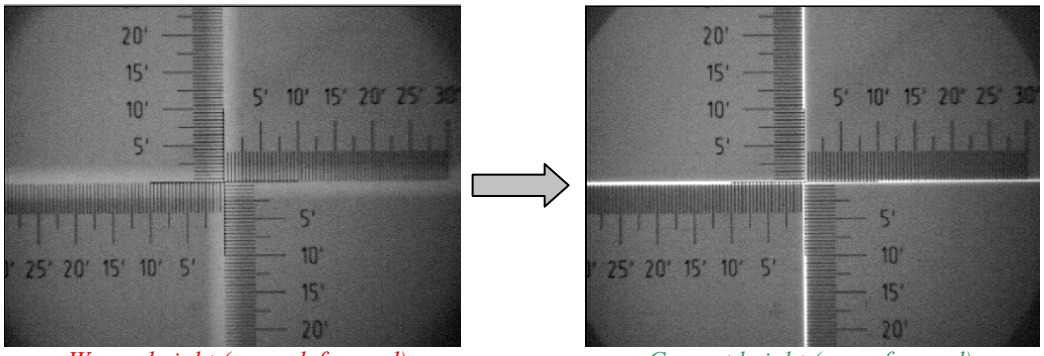
The Auto collimating telescope (ACT) in combination with the objective lens is used for the alignment.

The accurate alignment of the sample height and tilt are necessary to obtain the correct angle of incidence and (Ψ, Δ)-spectra.

Alignment of ideal samples (perfectly flat and specular)

Step a) Height alignment

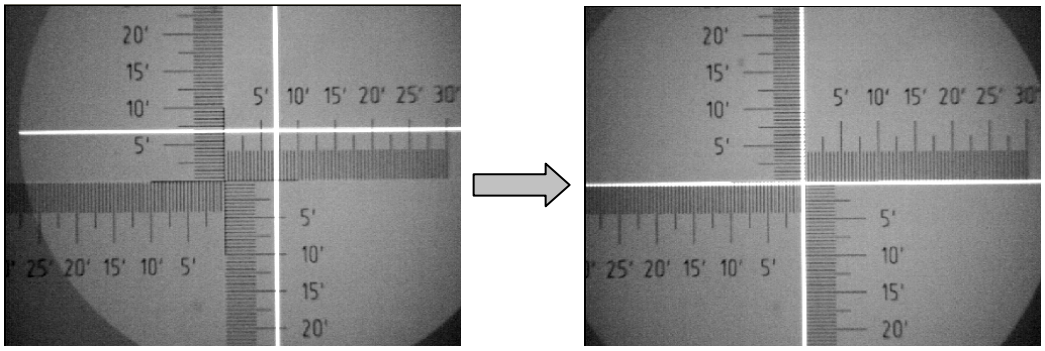
- Move objective lens into "**sample height**" position
- Use height alignment screw to focus the white cross



Wrong height (cross defocused) *Correct height (cross focused)*

Step b) Tilt alignment

- Move objective lens out to "**light tilt**" or "**dark tilt**" position
- Use the two tilt screws to align the tilt by moving the white cross towards the crosshairs.



Wrong tilt (cross not on crosshairs) *Correct tilt (cross on crosshairs)*

Step c) Height alignment (repetition)

- Move microscope back to "**sample height**" position
- Check whether the height position is still ok. If not, repeat step a).

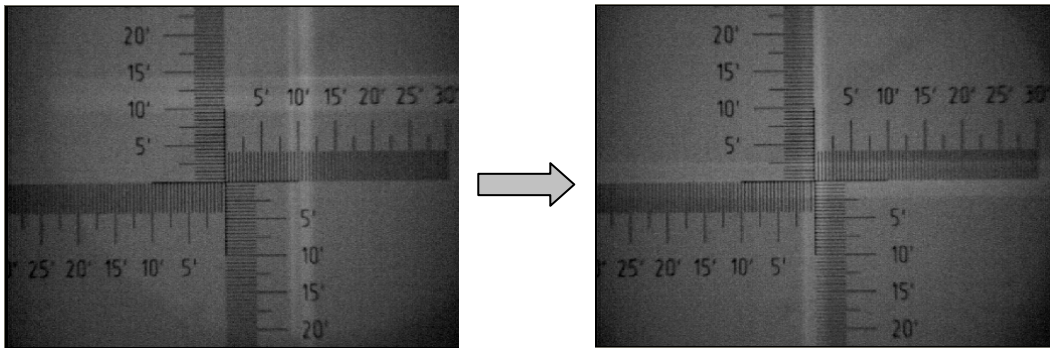
Alignment of non-ideal samples

- Alignment of non-ideal samples, specular, not flat

In case the sample is specular but not perfectly flat the cross in the tilt-mode is blurred. The "**dark-tilt**" position is recommended because it will show the sharper cross compared to the **"light tilt"** position.

Step a) Height alignment
- Move objective lens into "**sample height**" position
- Use height alignment screw to focus the white cross as it is done for ideal samples.

Step b) Tilt alignment
- Move objective lens out to "**dark tilt**" position
- Use the two tilt screws to align the tilt by aligning the white blurred cross to the crosshairs



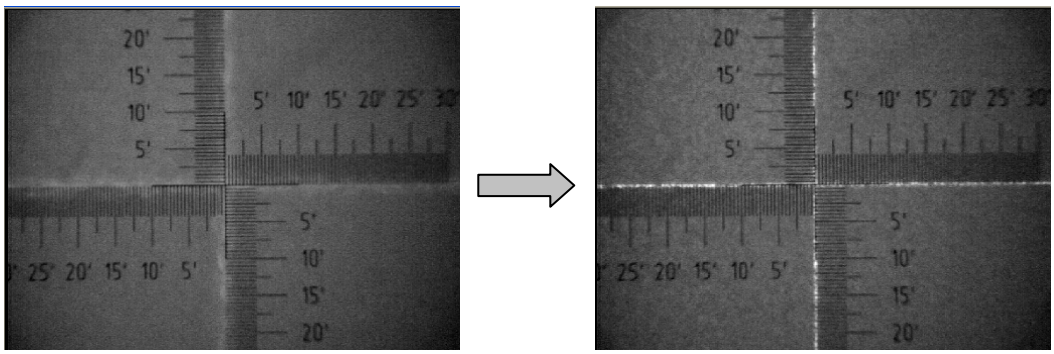
Wrong tilt (cross not on crosshairs) *Correct tilt (cross on crosshairs)*

- Alignment of non-ideal samples, not specular

In case the sample is not-specular or very rough the tilt alignment can't be done, because the white cross isn't visible anymore. Then e.g. a specular Si wafer can be used first to align the tilt of the stage which won't be changed then anymore. Then the rough sample is placed on the stage and the height is aligned. In most cases the white cross can be seen and focused and additionally the surface of the sample is visible.

Step a) Tilt alignment
- Place a Si wafer on the stage. Move objective lens out to "**light tilt**" or "**dark tilt**" position
- Use the two tilt screws to align the tilt by aligning the white cross to the crosshairs

Step b) Height alignment
- Place rough sample on the stage and move objective lens into "**sample height**" position
- Use height alignment screw to focus the white cross as it is done for ideal samples.



Wrong height (cross defocused) *Correct height (cross focused)*

8.1.3.2 Ellipsometric measurement

Performing the measurement

- Press the “Measure” icon  in the tool bar to open the “measurement window”
- Select the standard settings as shown in Fig. 8-8.
- Choose a suitable name for the sample (e.g. “400nm SiO2 on Si”)
- Press the “Measure” button

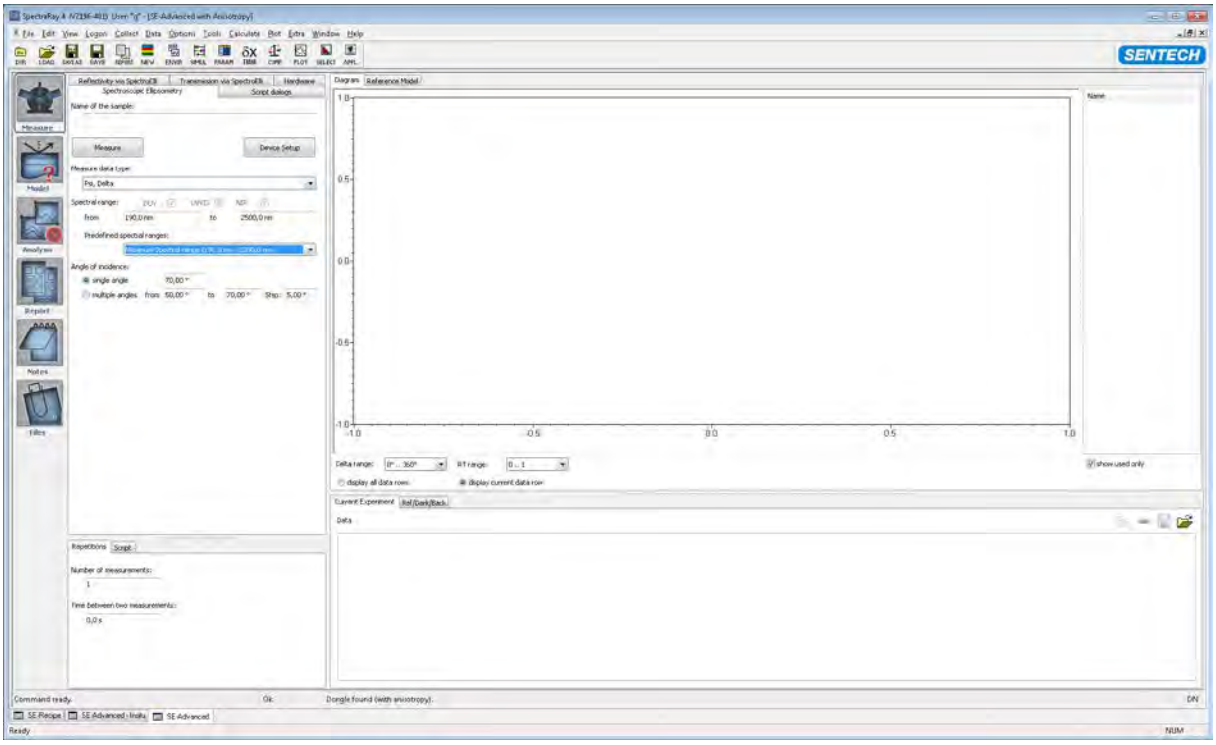


Fig. 8-8 Measurement settings

The measurement is performed now. The movements of “Analyzer”, “Polarizer”, “Shutter” and “Compensator” can be heard. When the measurement is finished the data are saved into the “Data” section.

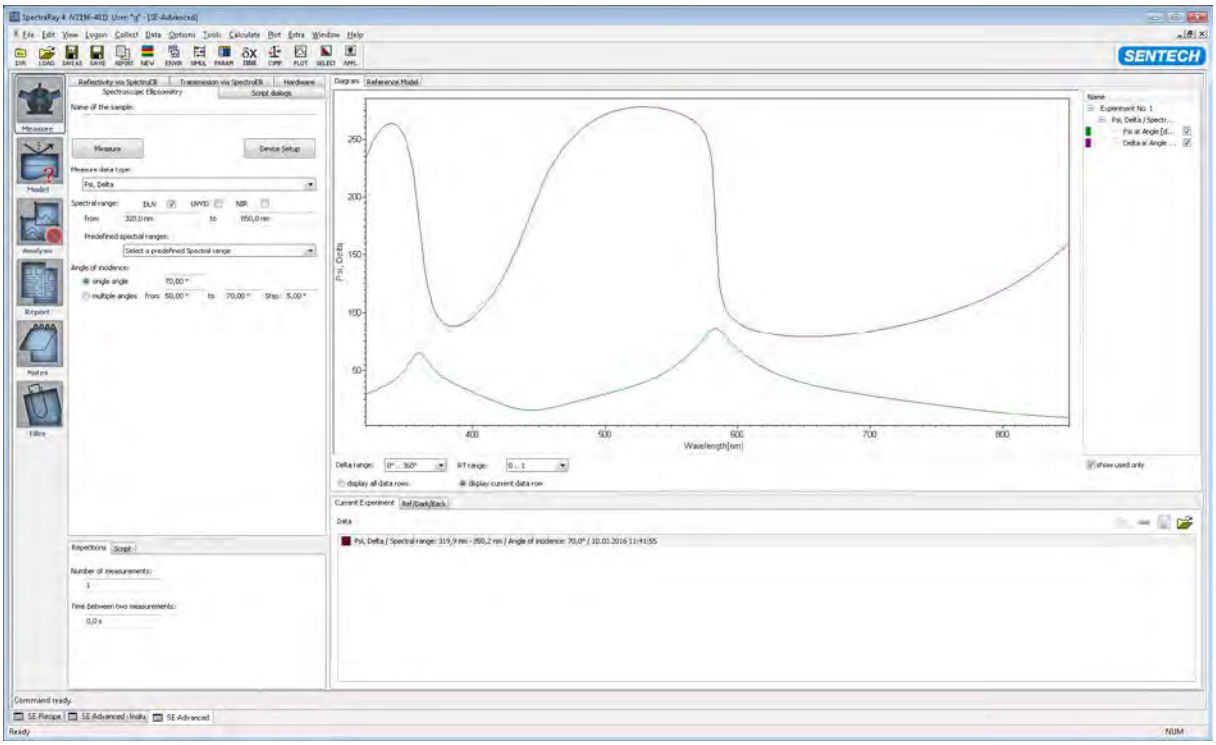


Fig. 8-9 Measurement results

The measurement name contains the information about the spectrum type, spectral range, angle of incidence, date, time and the name of the sample. The measured data are displayed in the diagram.

Renaming the measurement

You can rename the measurement by double clicking the measurement dataset and going to the “Title” tab. Enter the name in the “Name:” section.

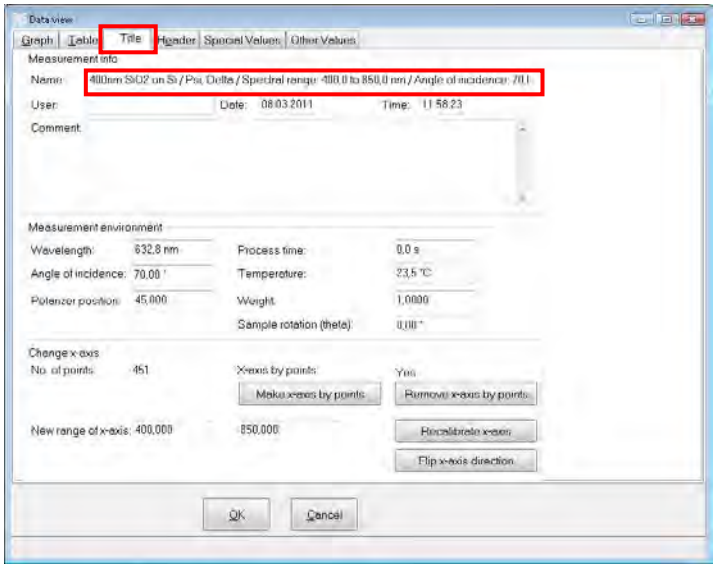
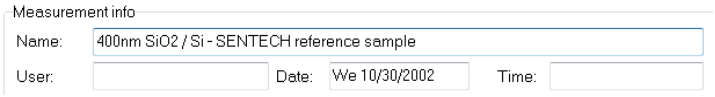


Fig. 8-10 Data view “Title”-tab

New name:



Beneath the “Title” tab, there are other tabs. Important is the “**Graph**” tab. It shows the (Ψ, Δ)-spectra versus wavelength in nm.

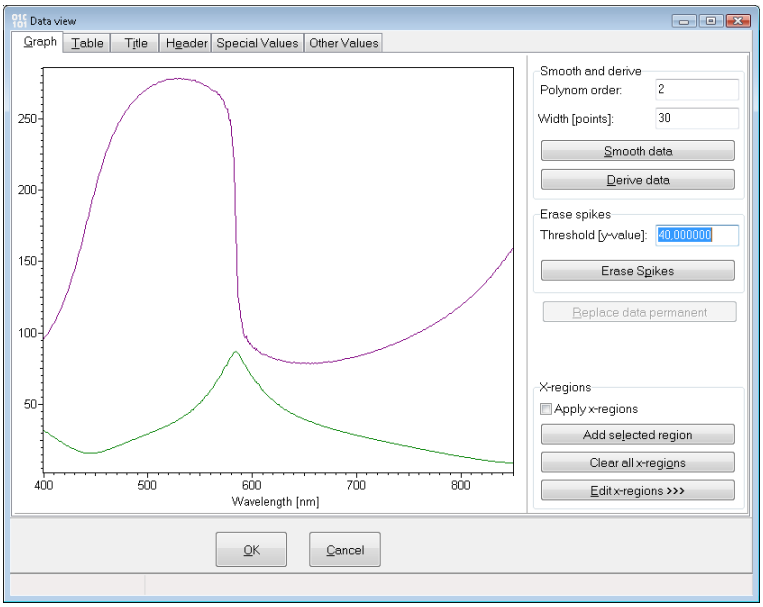


Fig. 8.-8-11 “Graph”-tab of data view

The new measurement name is shown in the “Data” section of SpectraRay.

8.1.3.3 Modeling

The optical model describes the optical and metrical properties of the sample. It consists of the substrate, the ambient (mostly air) and the layers in between. The dispersion of the optical constants n and k of ambient, layers and substrate is described by dispersion formulas. For different kinds of materials different kinds of dispersion formulas exist.

Creating a model

Click on the “Model”-button in the tool bar to open the model-window. The optical model is now built by selecting the materials from the material library. In the following example the N, K fixed layer type is used to describe the ambient air, the Cauchy dispersion is used to describe the SiO_2 layer and the File layer type is used to describe the silicon substrate.

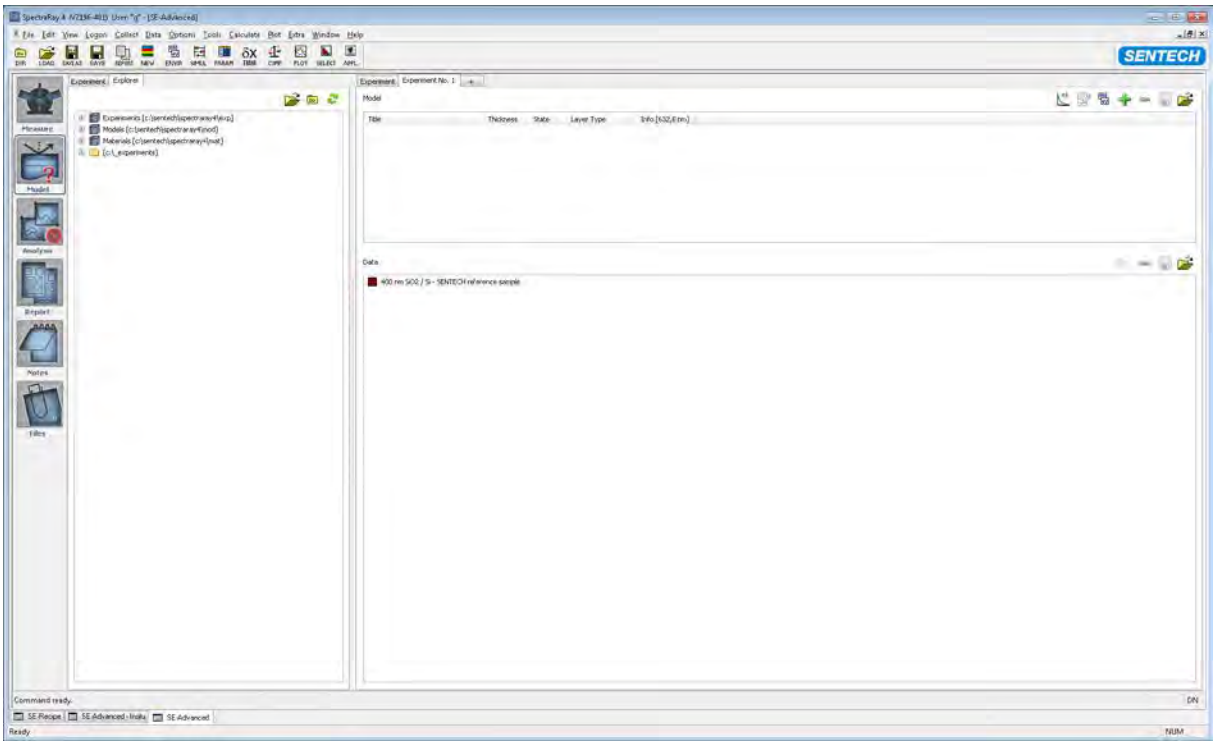


Fig. 8-12 Model window

They are moved by drag&drop from the “Explorer” window to the “Model” window in the “Experiment No. 1”-tab in the upper right. If the resulting order of the layers isn't correct it can be changed easily by drag&drop. The model for the standard sample will appear as follows:

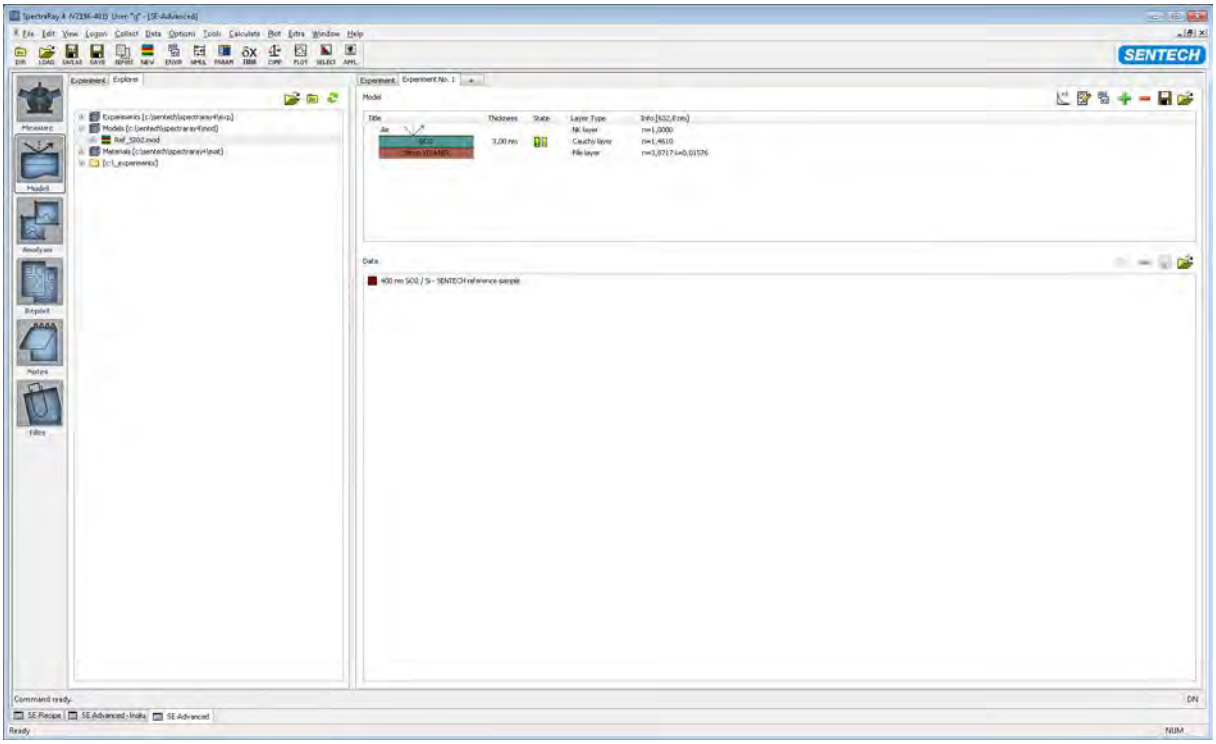


Fig. 8-13 Model for the standard sample

Selecting fit parameters

The layer “Cau-SiO2 (therm.)” (where the fitting parameters should be selected) is double clicked. The “Layer dispersion” window is opened. For “Cau-SiO2 (therm.)” the Cauchy coefficients “N0” and “N1” are selected for fitting by checking the checkboxes. The film thickness is also selected for fitting. If the approximate film thickness is known, it should be entered at “Thickness” (here: 400 nm). The window can be closed now using “OK”.

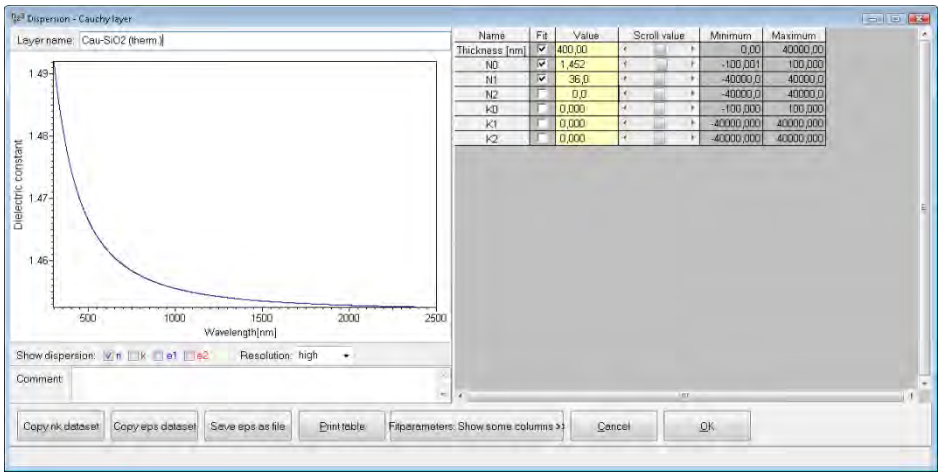
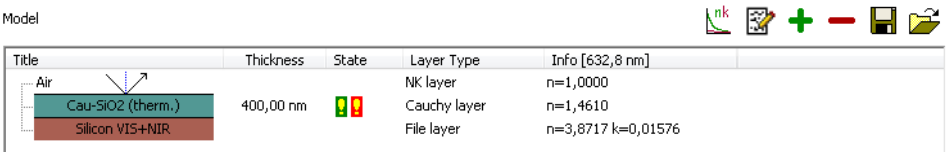


Fig. 8.-8-14 Cauchy-layer editor

The model has changed its appearance. The film thickness is 400 nm, the in the “state”-column indicates that fitting parameters are selected in this layer.



8.1.3.4 Fitting

The fitting window is opened by pressing the fitting button: 

. The “fitting” window is opened as you can see in Fig. 8-15.

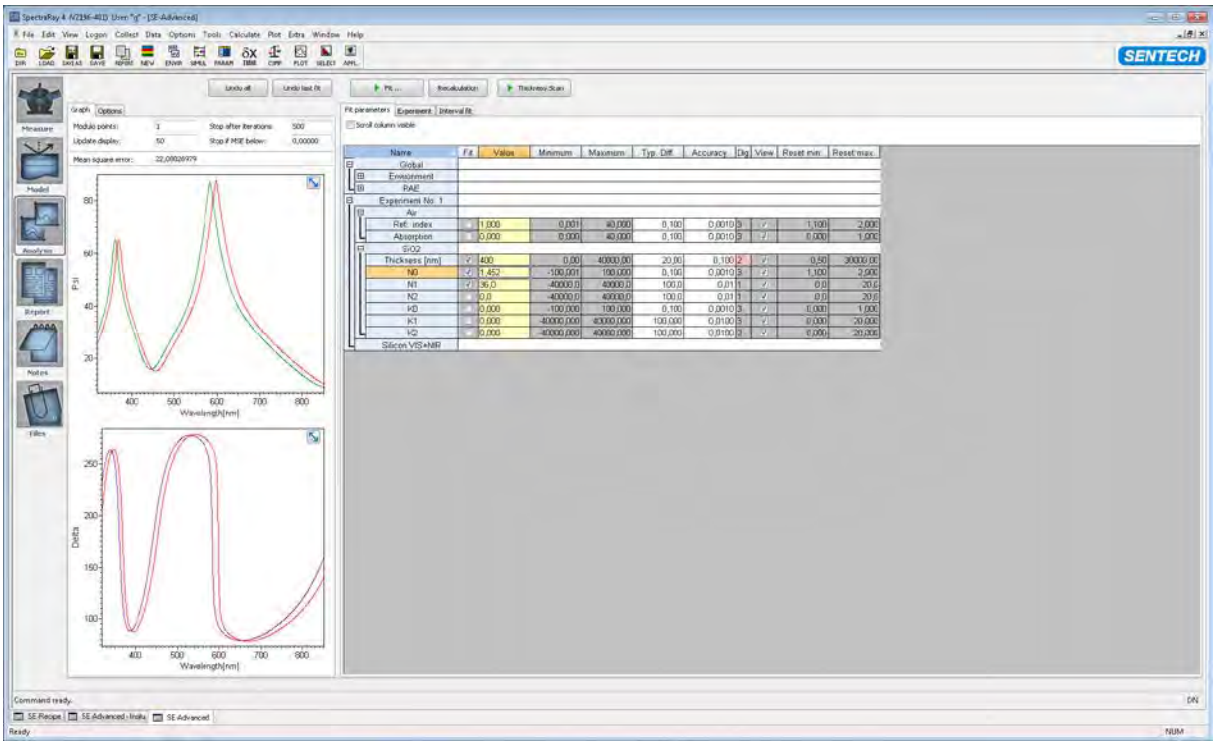
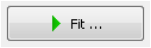


Fig. 8-15 Analysis-window

Two graphs are shown in the “graph”-tab on the left hand side, one for Ψ, the other one for Δ versus wavelength. Each screen contains two graphs. One represents the measurement the other one represents the modeled spectrum. Here the measured Ψ and Δ are displayed in green and purple colors, while the modeled Ψ and Δ spectra are displayed both in red color.

The “Modulo” value is used to increase the fitting speed. Modulo = 1 means every single point is used for fitting; slow but most exact. Modulo = 4 means every 4th point is used; faster but some points are skipped. Use Modulo = 4 in general.
Rule of thumb: the more or the sharper structures in the (Ψ, Δ) spectra appear, the lower the modulo value should be to avoid losing information.

Click on 

to initialize the fitting procedure. The software is now modifying the values of the selected fitting parameters thickness, N0, N1 in order to minimize the deviation between measurement and optical model. The goal is to achieve a perfect overlay of the measured and modeled spectra.

The deviation between the measured and modeled spectra is expressed in the MSE value (MSE: Mean square error). During the fit procedure the actual “iteration step” (No.), the MSE value and the fitting parameters are displayed in the lower left corner.

When the fitting procedure stops the results window is shown:

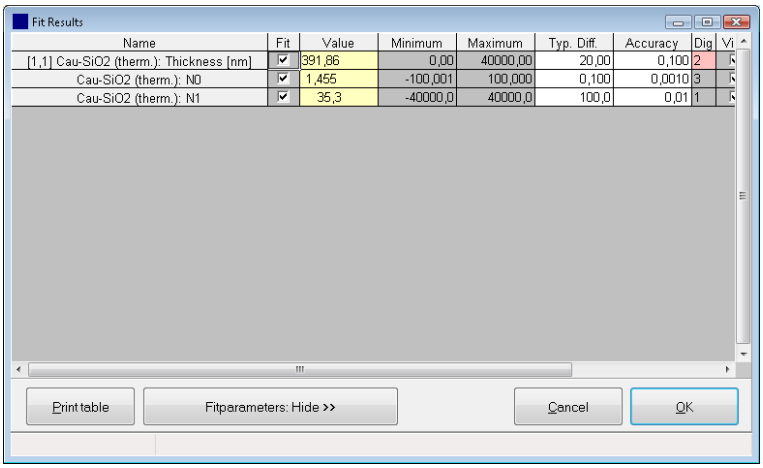


Fig. 8-16 Fit results

It can be closed with “OK” to return to the fitting screen.

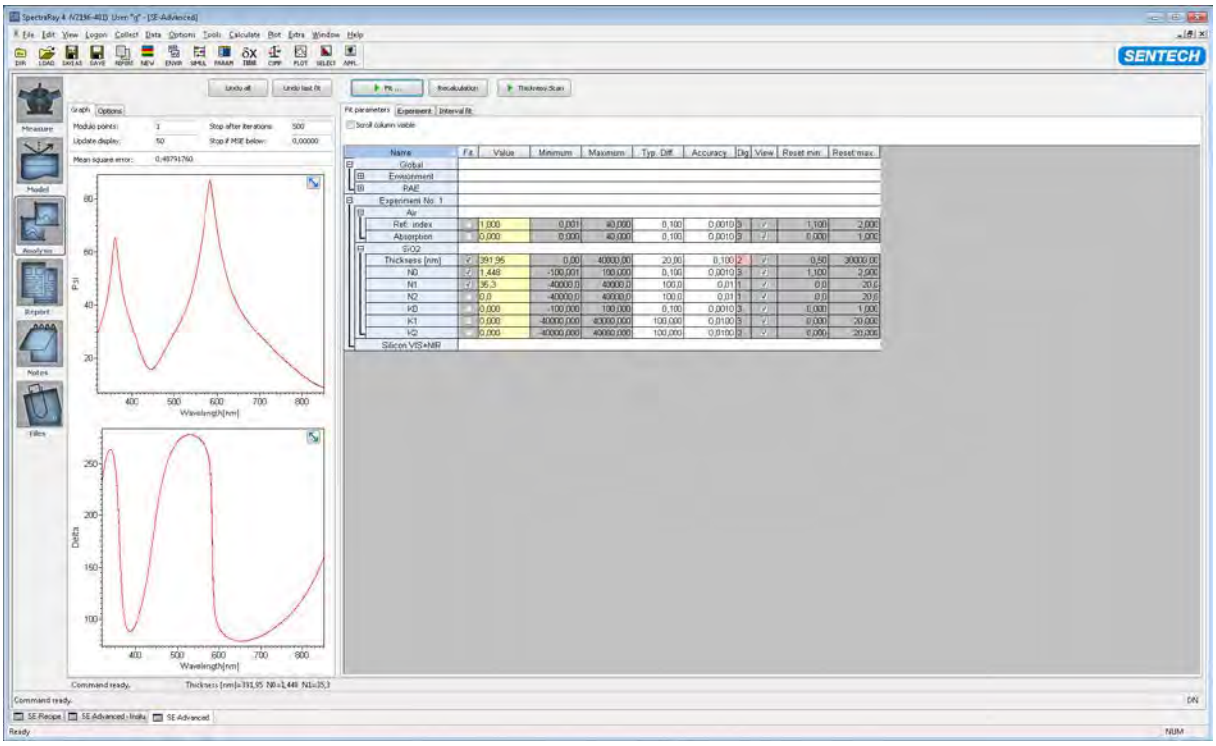


Fig. 8-17 Resulting fit parameters

Now a decision is necessary:

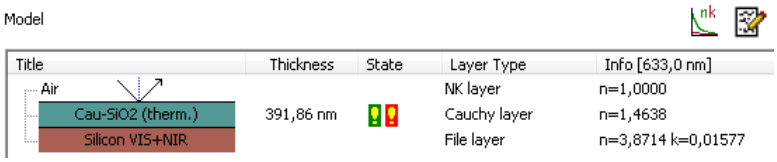
Fit quality is good → ready → proceed with “Reporting”
Fit quality is below expectations → not ready → the optical model must be improved

Here the actual fit is perfect. That means the mathematical equations of the optical model now exactly describe the measurement. We can proceed with “Reporting”.

8.1.3.5 Reporting

8.1.3.5.1 No reporting

Without any reporting the main information of the fitted optical model can be read out from the Model window. The optical model is updated with results from the fitting procedure.



The correct film thickness and the refractive index n at the observation wavelength are displayed. Because of the dispersion of the refractive index n it differs in every wavelength.

How to change the observation wavelength?

The observation wavelength is defined in the “Environmental parameters”:

Click on  in the icon bar and select the tab “Values”. Enter e.g. 632.8 nm at “Wavelength” and leave this window.

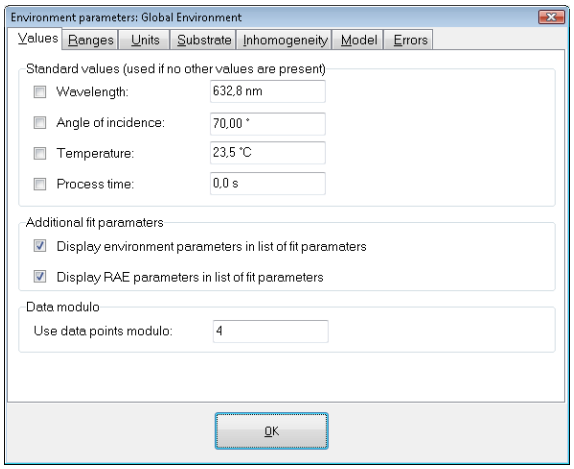


Fig. 8-18 Environment parameters – Values

8.1.3.5.2 Measurement report

An automatic report can be created and displayed as WORD™-document in the “Report”-window. After clicking on  in the tool bar the following window appears.

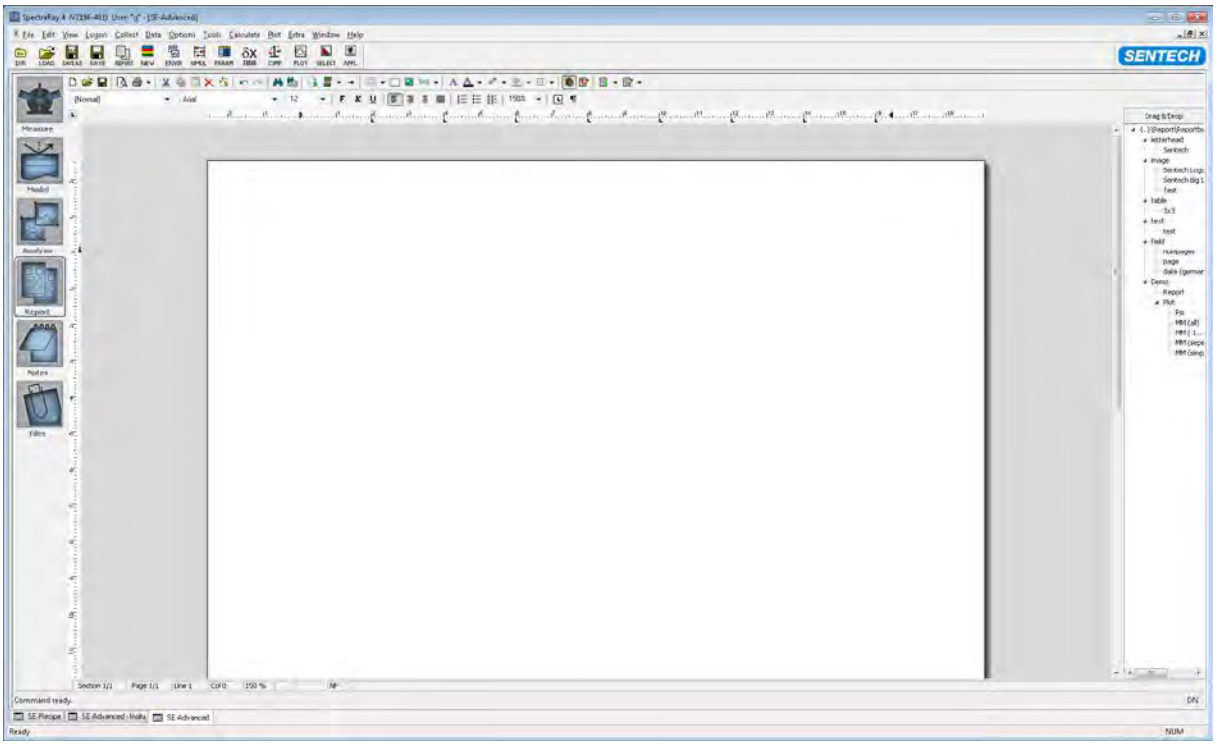
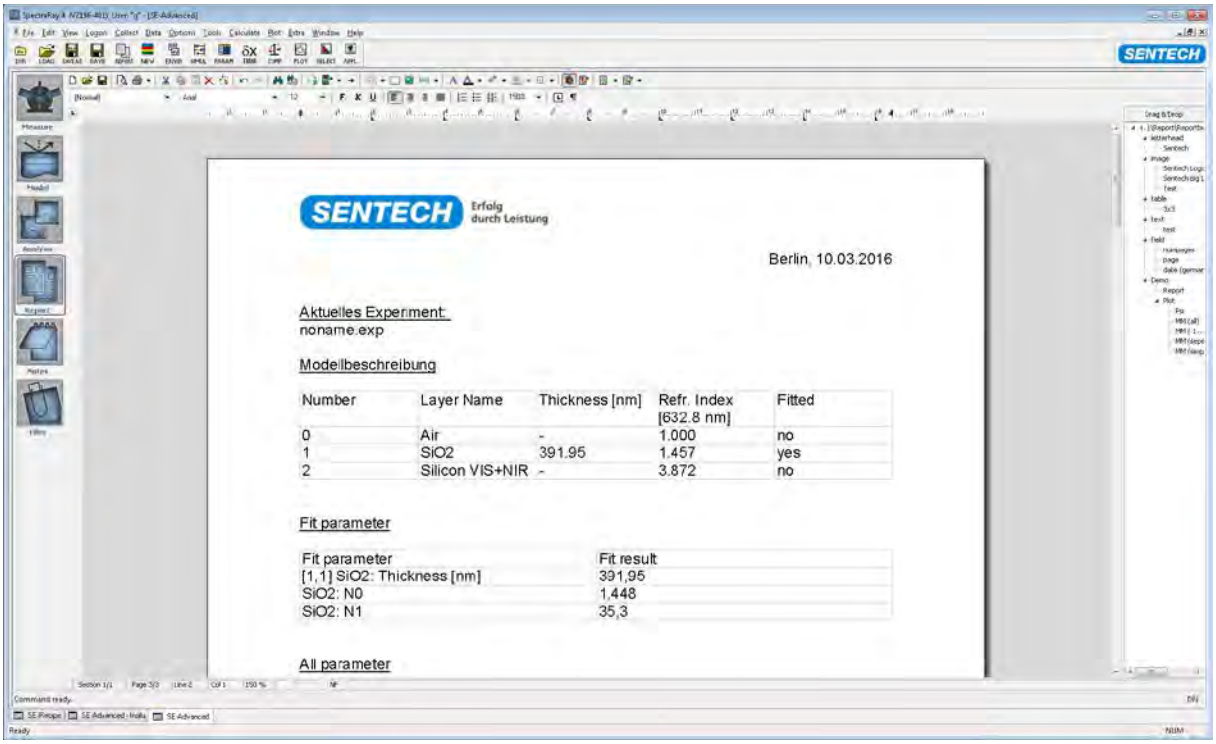


Fig. 8-19 Reporting window

Here you can create an automatic report and save it as WORD™-file. On the right hand side there is a list of elements you can insert into your report simply by drag&drop. For example dragging Demo/Report and dropping it into the WORD™-document will create a standard report of your measured data. You can simply modify your report or built your report.



SENTECH Erfolg durch Leistung

Berlin, 10.03.2016

Aktuelles Experiment:
noname.exp

Modellbeschreibung

Number	Layer Name	Thickness [nm]	Refr. Index [632.8 nm]	Fitted
0	Air	-	1.000	no
1	SiO2	391.95	1.457	yes
2	Silicon VIS+NIR	-	3.872	no

Fit parameter

Fit parameter	Fit result
[1,1] SiO2: Thickness [nm]	391,95
SiO2: N0	1,448
SiO2: N1	35,3

All parameter

Fig. 8-20 Demo report

8.1.3.5.3 Using the “Simulation” for reporting

The “Simulation” is used to calculate data on the basis of the actual optical model. In this example the dispersion of n of the “Cau-SiO_2 (therm.)” layer versus wavelength will be calculated.

The “Simulation” is started by clicking on 

. The “Curve parameter” is the x-axis → Select “[0] wavelength [nm]”. Set the wavelength range from 300nm to 850nm (step: 1). The “Calc unit” is the y-axis → Select “n layer”. Select the “Layer”: SiO2.

Press “Calc”. The data is now calculated, displayed and saved into the “Data” window.

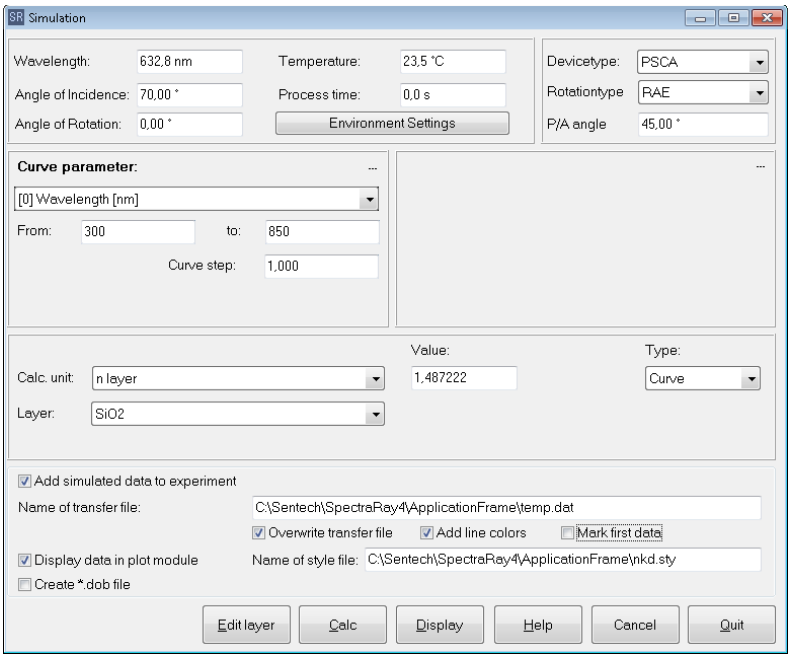
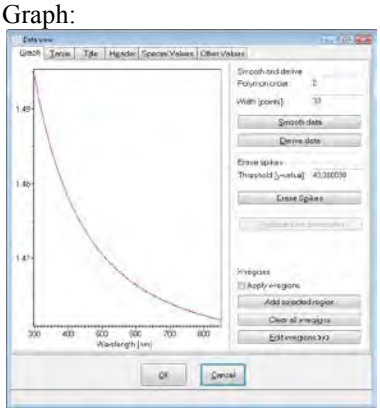


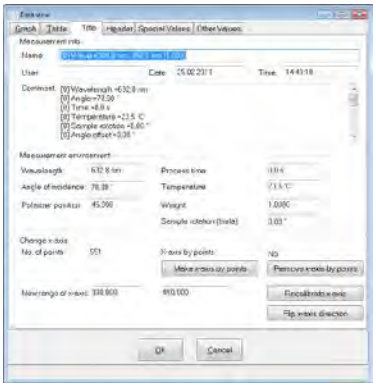
Fig. 8-21 Simulation

Leave the “Simulation” window with “Quit” to return to the SE-Advanced main window. The new dataset of the dispersion of n of “SiO2”:

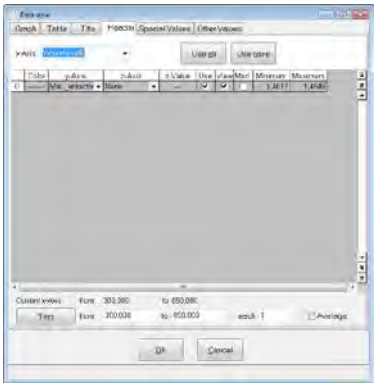
Graph:



Title:

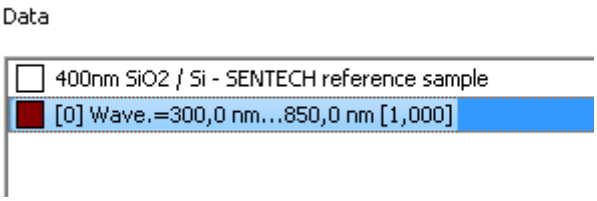


Header:



8.1.3.5.4 Exporting the dispersion data to an ASCII file:

The dataset is selected by a single mouse-click: it appears inverted.



Select from the menu: "File" → "Save as …"

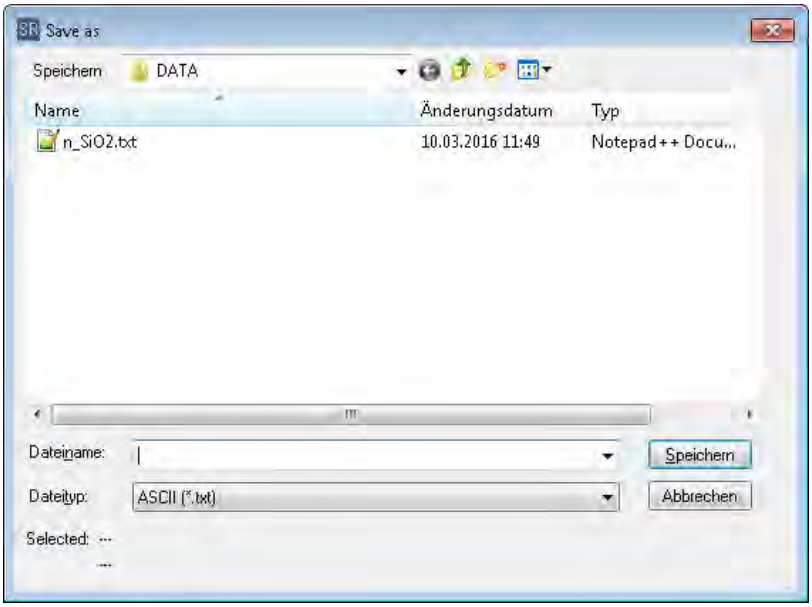


Fig. 8-22 Saving simulation data as ASCII

Select "ASCII (.txt)" as file type, the directory (free of choice) and filename (free of choice). The file is now saved as an ASCII file which can be imported to other programs like EXCEL™ or Origin™.

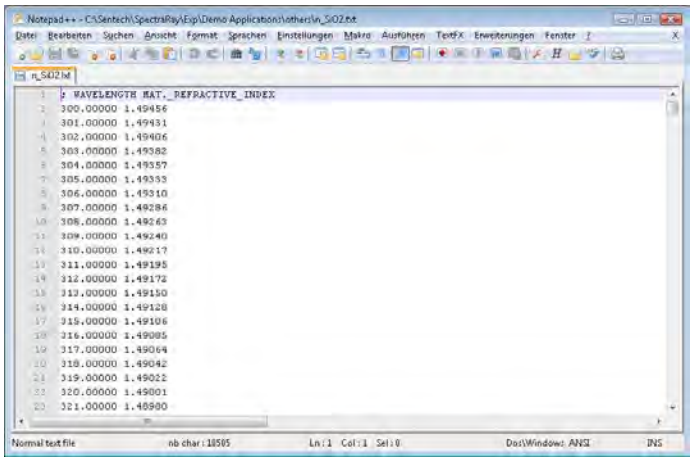


Fig. 8-23 Dispersion file of "Cau-SiO2 (therm.)"

8.2 Explanation of important SE-Advanced features

8.2.1 Parameter list

The parameter list allows the direct access to all fitting parameters of all layers in the stack and environmental parameters. It allows selecting or deselecting fitting parameters, change their actual values and influence the fitting behavior.

There are two ways to open the parameter list.

1. from the icon bar: 

2. from the analysis window

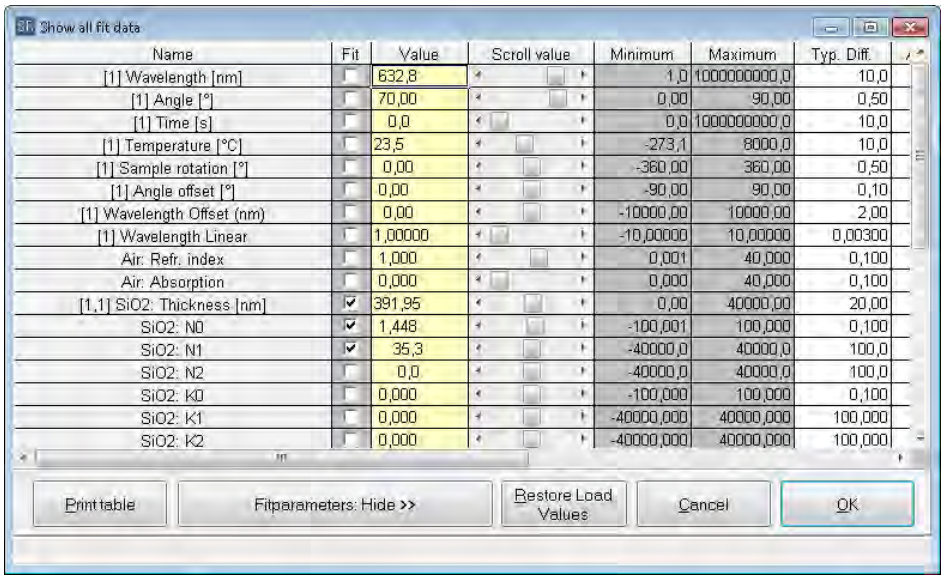


Fig. 8-24 Parameter list

In the Analysis-window the “Scroll value”-column is shown only if the “Scroll column visible” checkbox is checked. The “Scroll value” is a convenient way to find proper starting values for fitting parameters.

Column	Explanation
Name	shows the fitting parameter name
Fit	indicates whether the value will be fitted or not
Value	actual value of the fitting parameter, starting value
Scroll value	Scroll bar for quick and easy changing of "Value"
Minimum	The smallest allowed value of the parameter. The expected value of the parameter should be within the allowed range, otherwise the right value will not be found. In case of ambiguous solutions the range may help to get stable results.
Maximum	The highest allowed value of the parameter
Typical difference	This value is used in the beginning of the fitting procedure. The actual value is either plus or minus the typical difference. So the actual film thickness of 398.3 nm will be either 408.3 or 388.3 nm for the first step of iteration. The step size is adjusted automatically for further fit iteration. The typical difference value should be approximately 5% to 20% of the actual parameter value.
Accuracy	The fitting procedure will stop when the changes of all parameters are less than the defined accuracy value.
Digits	This is the amount of digits displayed for each parameter.
View	This switch decides whether the fitting parameter is displayed during the fitting procedure in the fitting window.
Reset Min.	If the minimum value is reached during fitting it is reseted to the "Reset min" value. The "Reset Min." value should be within the range between Minimum and Maximum. In case the parameter value reaches the minimum during fitting procedure the Minimum value should be decreased manually.
Reset Max	Similar to "Reset Min". In case the parameter value reaches the maximum during the fitting procedure the Maximum value should be increased manually.
Anim	Animates the value (displays sequently the dielectric function from minimum to maximum of the selected value)
Scroll Step	Steps for "Scroll value"
Sroll Min.	Minimum value for "Scroll value"
Scroll Max.	Maximum value for "Scroll value"

Tab. 8-1 Values for each parameter

8.2.2 Environmental settings

Explanation of the most important and most used environmental settings.

Tab: Values

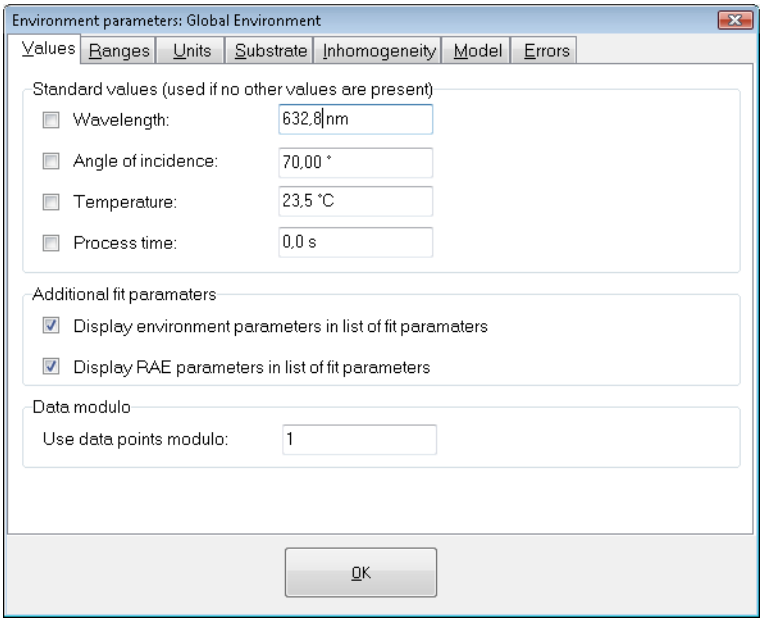


Fig. 8-25 Environment parameters: values

- **"Wavelength"** defines the observation wavelength of the display of the model
- **"Angle"** defines the angle of incidence e.g. used for the "Simulation"

Tab: Ranges

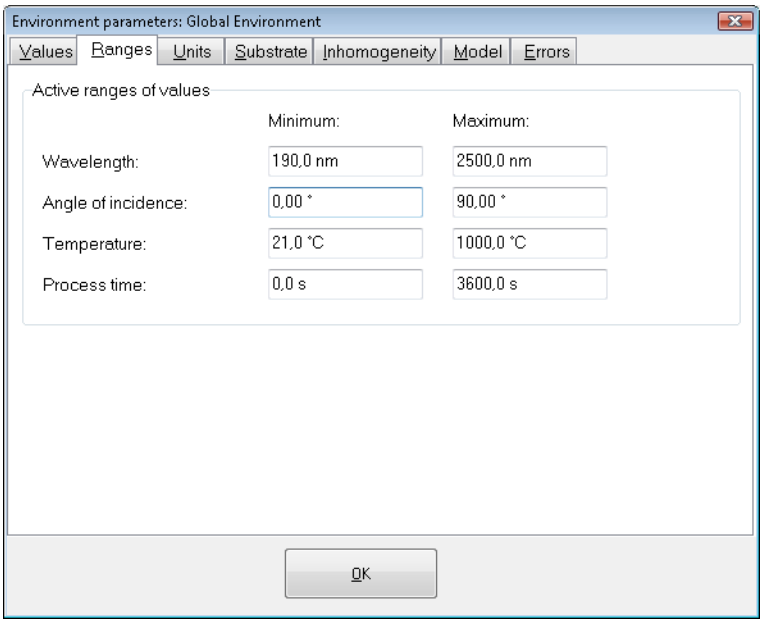


Fig. 8-26 Environment parameters: ranges

- **"Wavelength"** can be used to restrict the fitted spectral range. In case the model can't fit the measurement well below 450 nm it is possible to restrict the spectral range to 450 nm to 850 nm. The spectral range below 450 nm is neglected and not displayed.

Attention: this restriction also applies for the export of data. In case the full spectral range of the measurement should be exported, the wavelength range must be extended to the measured range.

Tab: Units

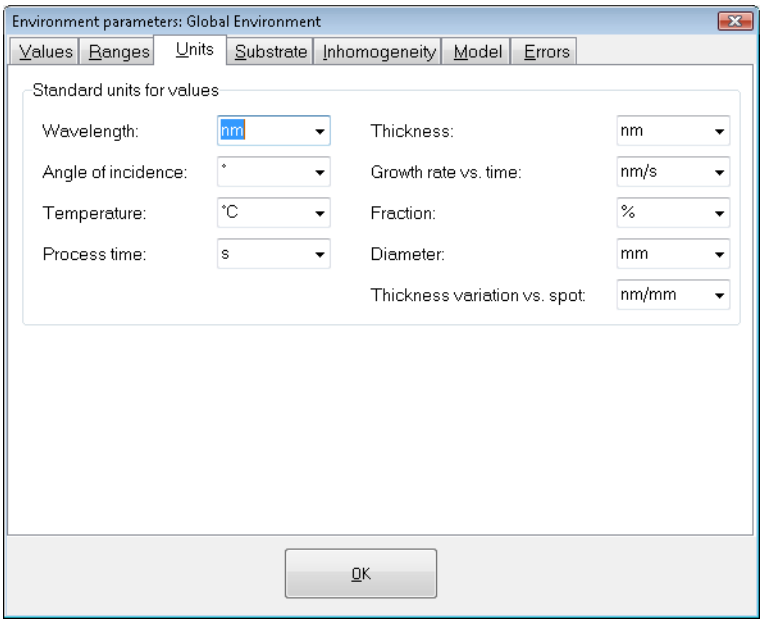


Fig. 8-27 Environment parameters: units

- **"Wavelength"** defines whether the wavelength scale is defined in "nm", photon energy "eV" or wave-number "1/cm"

Tab: Substrate

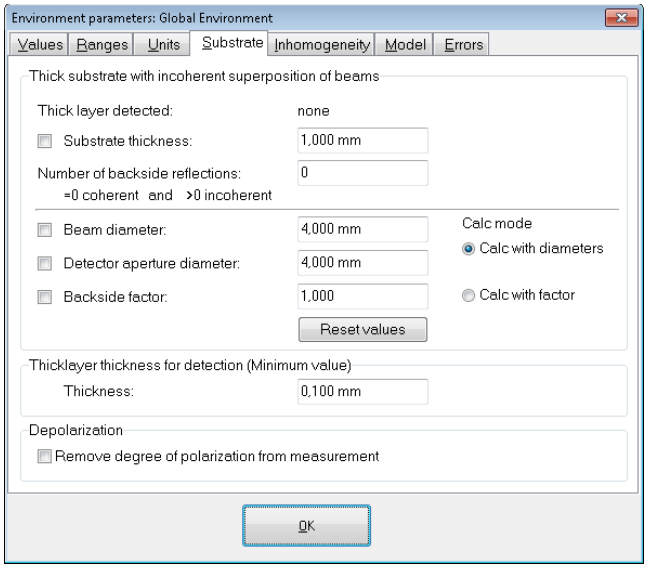


Fig. 8-28 Environment parameters: substrate

This part is used to model the influence of backside reflections in case of **transparent substrates**.

Suggestion: in order to avoid backside reflection (easier modeling) the backside of the sample can be roughened.

Tab: Inhomogeneities

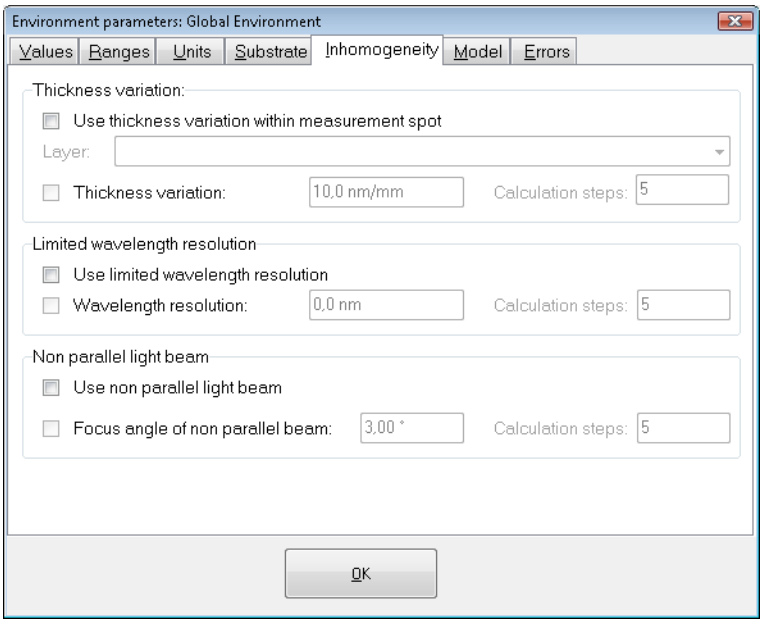


Fig. 8-29 Environment parameters: inhomogeneity

This tab is used to model imperfections of the sample or equipment. “use Thickness variation ...” describes a non uniformity of the layer (thickness variation) within the spot size of the ellipsometer.

Tab: Errors

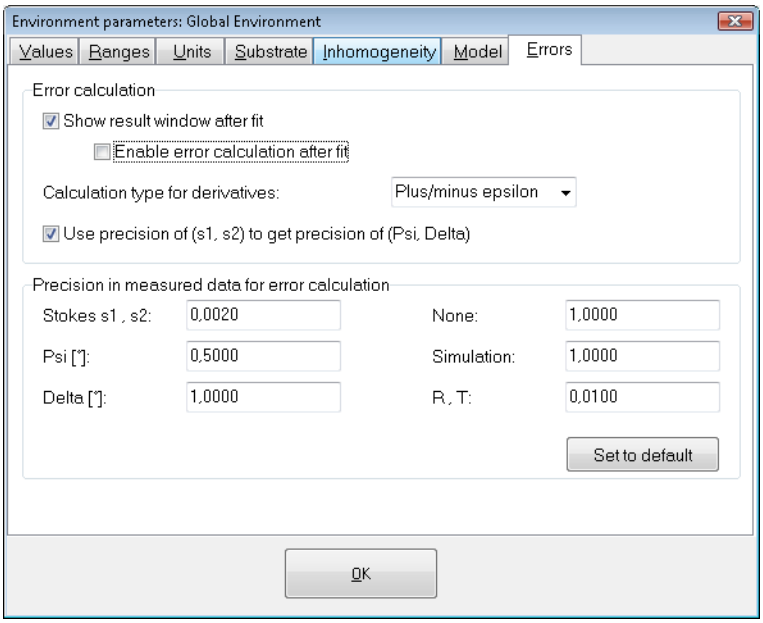


Fig. 8-30 Environment parameters: errors

This tab is used for the error calculation used for the display of the correlation matrix. There is no need to change any of these values here.

8.2.3 Simulation

The following example demonstrates the capabilities of the “Simulation”-Module of SpectraRay. The “Simulation”-module is based on the current optical model. It can e.g. calculate different values, like Ψ, Δ, R or T spectra for arbitrary angles of incidence in arbitrary spectral ranges.

Question:

How do the (Ψ, Δ)-spectra behave in the spectral range from 300 to 850 nm for SiO_2 / Si for different film thicknesses of th = 0 … 20 nm with a 5 nm step size?

Stack:

Air - n and k are fixed

SiO_2 - Cauchy

Si - File layer

Simulation:

Ψ, Δ versus wavelength and film thickness of SiO_2

Spectral range: **300 … 850** nm

Angle of incidence: **70** deg

SiO_2 film thickness: 0 … 20 nm, step 5 nm

Creating the model

Model

Title	Thickness	State	Layer Type	Info [632,8 nm]
Air			NK layer	n=1,0000
Cau-SiO2 (therm.)	0,00 nm		Cauchy layer	n=1,4610
Silicon VIS+NIR			File layer	n=3,8717 k=0,01576

The actual thickness of SiO_2 in the model is not important, because it will be changed temporarily by the simulation. Set the angle of incidence in the environment to Φ=70°.

Simulation

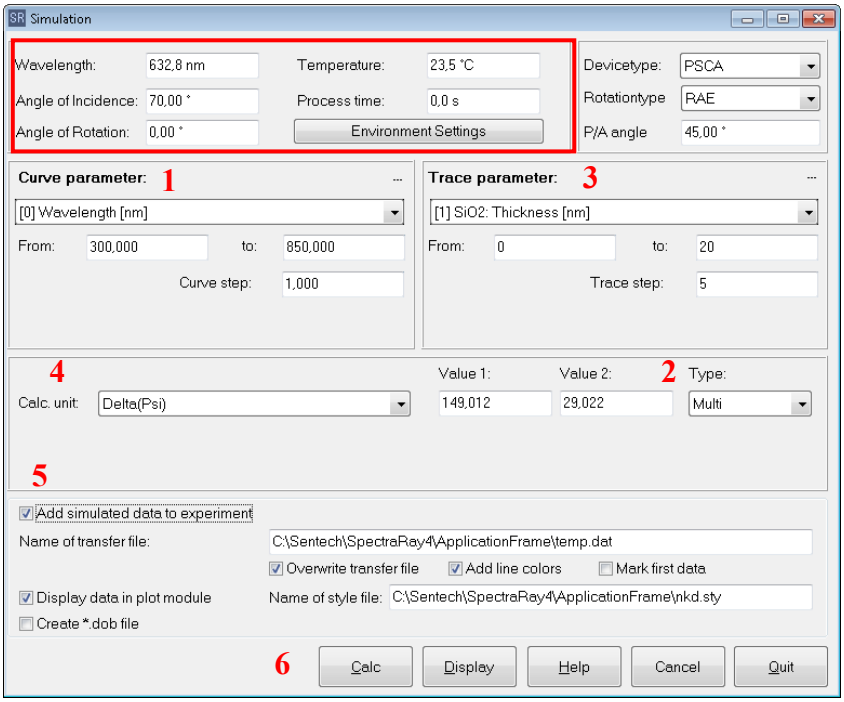


Fig. 8-31 Simulation

1) "Curve parameter" is set to "Wavelength" (defines x-axis)

spectral range: 300 – 850 nm, 1 nm step width

2) "Type" is set from "Curve" to "Multi" (enables simultaneous simulation of a second parameter)

3) "Trace parameter" is set to "SiO2 Thickness [nm]"

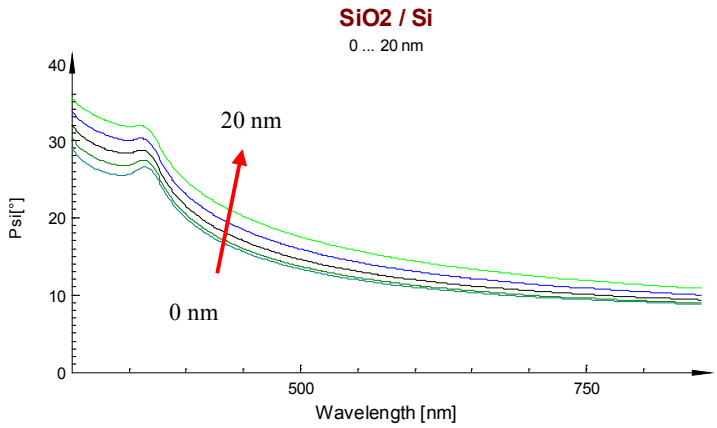
thickness range: 0 – 20 nm, 5 nm step size

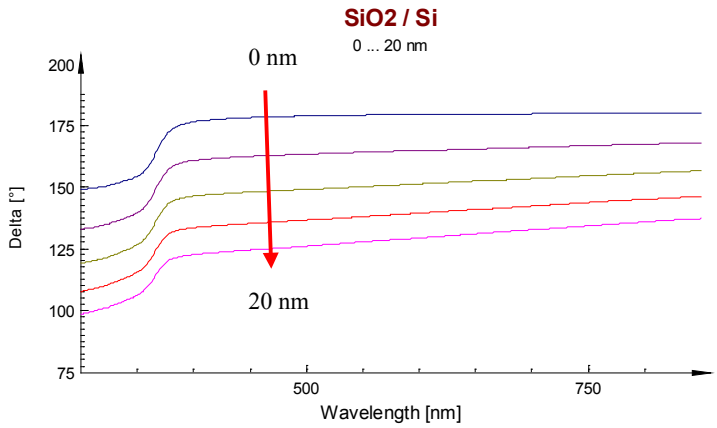
4) "Calc unit" is set to Delta(Psi) (defines y-axis)

5) "Add simulated data to experiment" is switched on to store the calculated data to the Data sub-window.

6) "Calc" is pressed to do the calculation; the results are stored in the "Data" section.

Results of the simulation





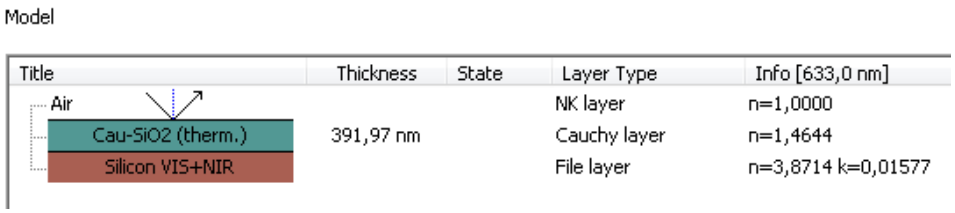
The effects in Δ are very strong. With each nm in film thickness a change of about 4° in Δ is obtained. This is the reason for the high sensitivity of ellipsometry against film thickness.

Question:

How to calculate the dispersion of n and k of a material using the "Simulation".

(This procedure is already explained in "Using Simulation for Reporting")

The dispersion of n and k of the SiO2 layer of our current model should be calculated:



The "Simulation" window is opened and the following settings are selected:

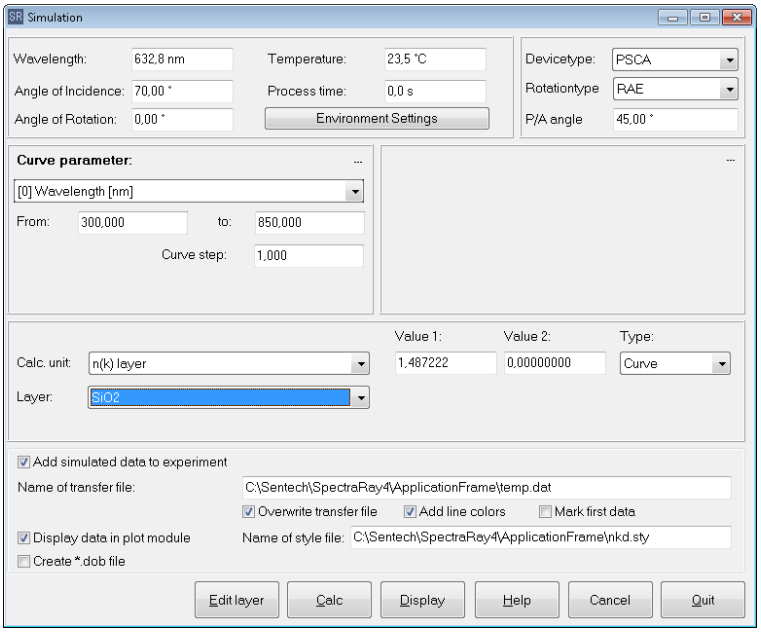


Fig. 8-32 Simulation of n and k

1) "Curve parameter" is set to "Wavelength" (defines x-axis)

spectral range: 300 – 850 nm, 2 nm step width (can be set to any values)

2) "Type" is set to "Curve" (simulation of one parameter only)

3) "Calc unit" is set to "n(k) layer" (defines y-axis)

4) "SiO2" is selected as **"Layer"**

5) "Add simulated data to experiment" is switched on to store the calculated data to the Data sub-window.

6) "Calc" is pressed to do the calculation; the results are stored in the "Data" section.

The data is saved into the Data section as a new dataset:

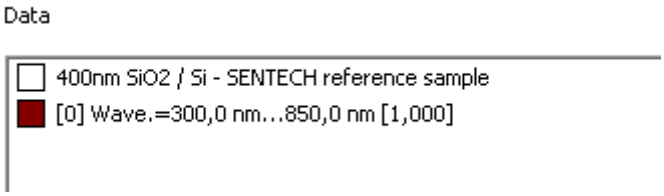


Fig. 8-33-8-34 dispersion as new dataset

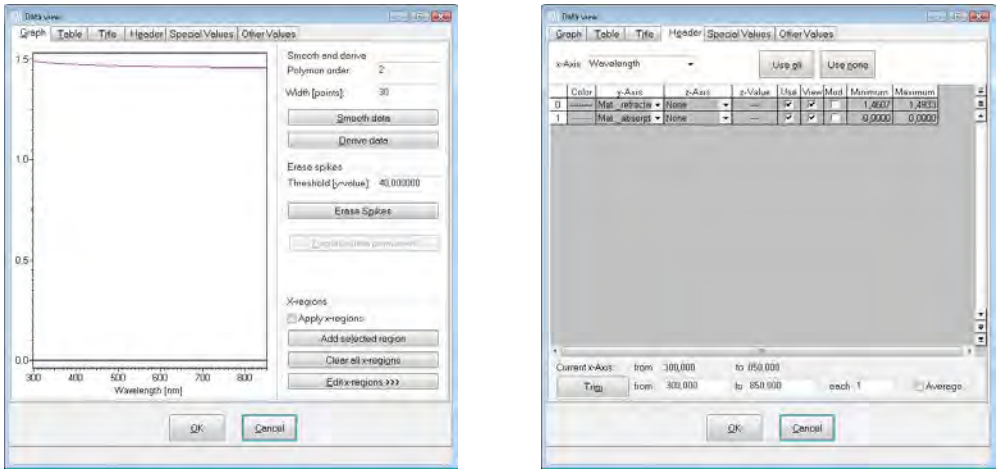


Fig. 8-35 Dispersion of n and k of SiO_2 and header tab

The dataset can be exported now as ASCII file as described in section “Import and Export of data files”.

8.3 Conversion of different wavelength or energy scale units

Conversion of wavelength ↔ photon energy (nm ↔ eV)

$$\frac{1239.85}{nm} \hat{=} eV \quad , \quad \frac{1239.85}{eV} \hat{=} nm$$

Examples:

300.0 nm = 4.13 eV

400.0 nm = 3.10 eV

632.8 nm = 1.96 eV

1239.85nm = 1.00 eV

Conversion of wavelength ↔ wavenumber (nm ↔ cm^{-1})

$$\frac{10^7}{nm} \hat{=} cm^{-1}$$

Examples:

200 nm = 50000 cm^{-1}

500 nm = 20000 cm^{-1}

1000 nm = 10000 cm^{-1}

2000 nm = 5000 cm^{-1}

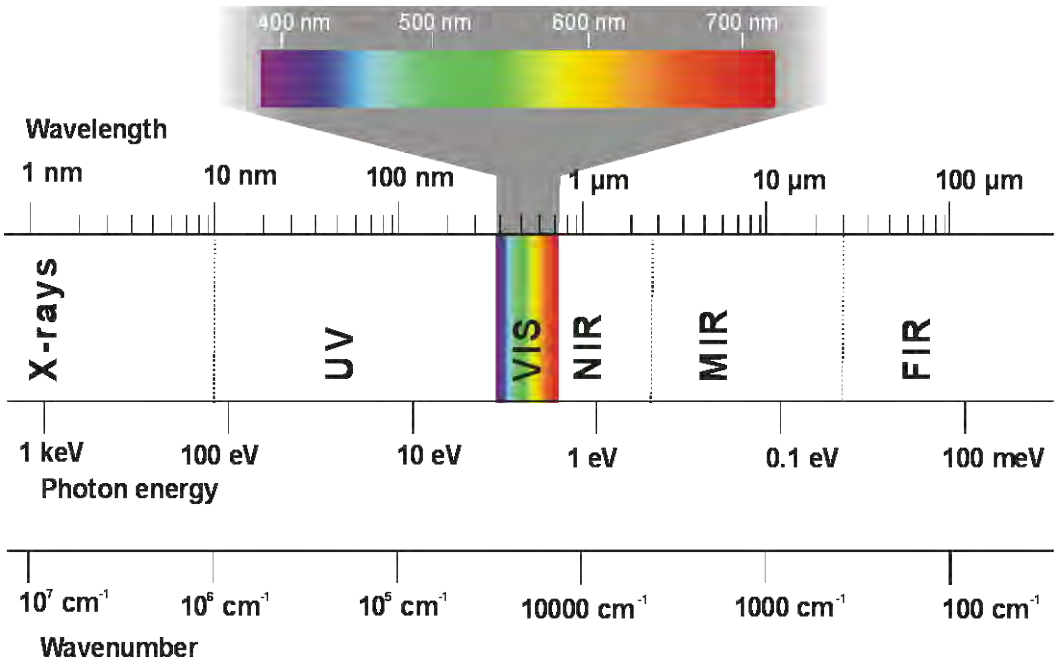


Fig. 8-36 Spectral ranges

8.4 Import and export of data

8.4.1 Import of external measured data

The results of external measurement devices like reflectance, transmission or ellipsometric measurements can be imported into the SE-Advanced client. The external data must exist as ASCII datasets. The file extension *.txt is recommended. The data must be split into different columns. The first column contains the x-axis. Usually it is the wavelength axis. The following units for x-axis are possible:

- Wavelength / nm
- Photon energy / eV
- Wavenumber / cm^{-1}

Further columns contain the y-axis data. The following units for y-axis are possible:

- Reflectance: 0 … 1 (0% to 100% is not supported)
- Transmission 0 … 1 (0% to 100% is not supported)
- (Ψ, Δ)- spectra /°
- tan Ψ, cos Δ
- Fourier coefficients s1, s2

The individual rows are separated by either spacebars or tabs. A header line is not necessary.

Example: import of a transmission measurement

The following example shows the file format for a transmission measurement from 300 to 920 nm. The first column contains the wavelength / nm. The second column contains the transmission data:

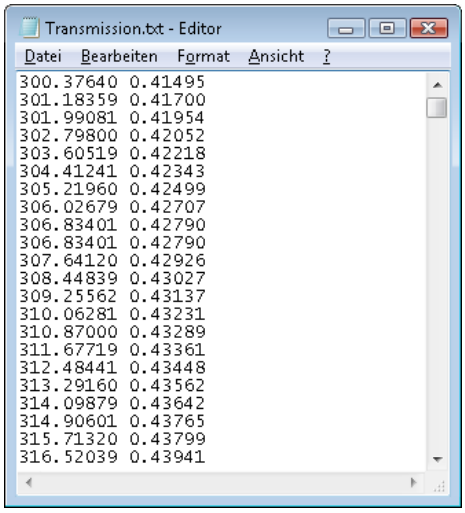


Fig. 8-37 Example for transmission data

The file is imported into the data section of the SE-Advanced client by Menu → File → Load …

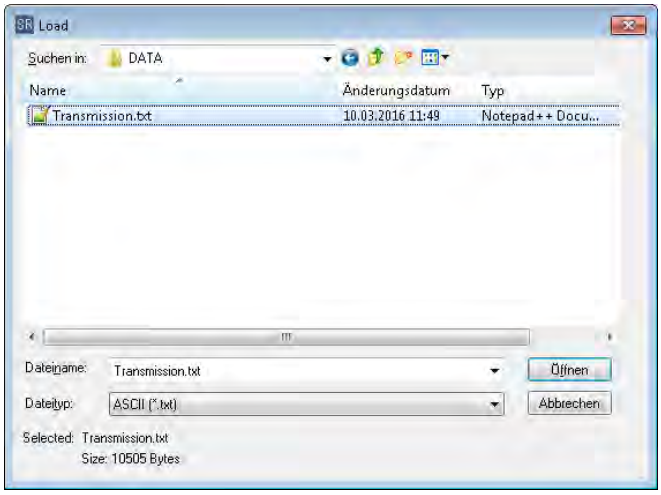
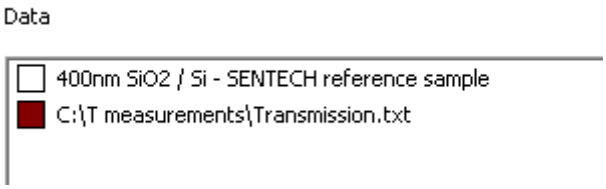


Fig. 8-38 Importing data



The units of the imported files must be set. The transmission measurement is double clicked and the “header” tab is selected.

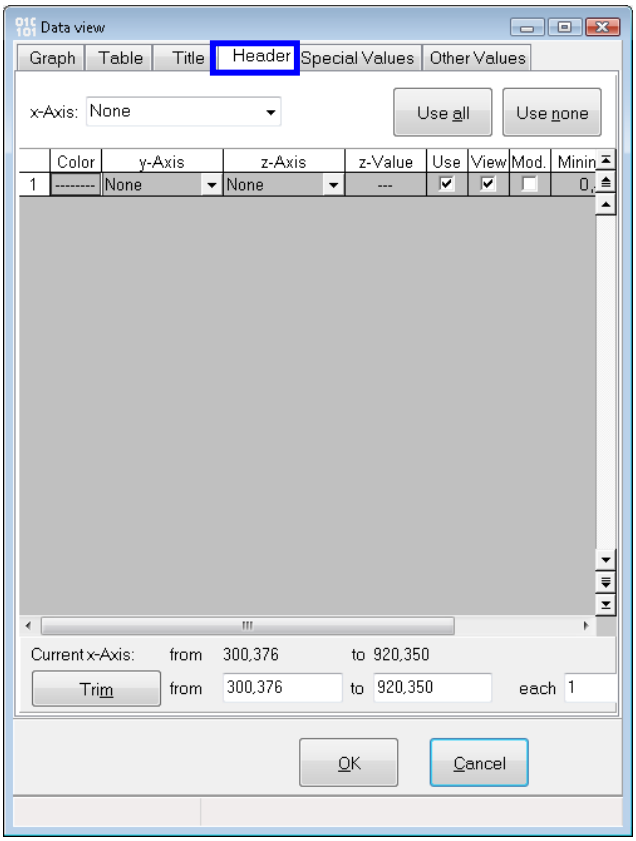


Fig. 8-39 Header tab of imported transmission data

For this Transmission file the following settings are necessary:

- x-Axis: “Wavelength”
- y-Axis: “Transmission”
- z-Axis: “Phi” (unit of the angle of incidence of T measurement)
- z-Value: “0.00” (the value of the angle of incidence)

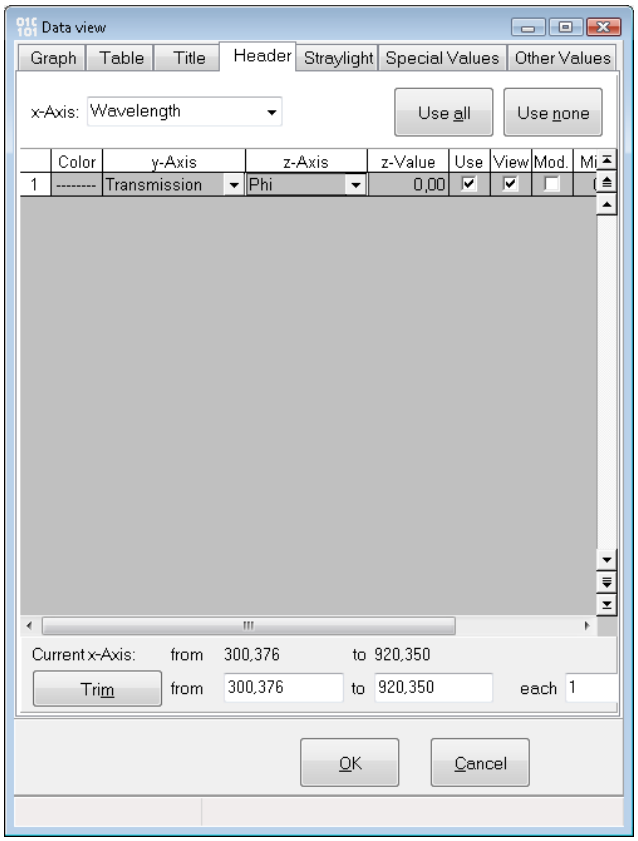


Fig. 8-40 Corrected header tab of imported transmission data

Now this dataset can be used for the modeling procedure.

8.4.2 Export of measured or simulated data

Any kind of dataset in the “Data” section can be exported as ASCII file. Here it will be shown for n, k dispersion data. The “Data” which should be exported must be selected (simply click once with left mouse button) so it appears inverted.

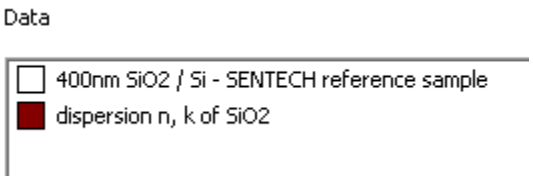


Fig. 8-41 Selected dataset

Important: Only “used” data will be exported.

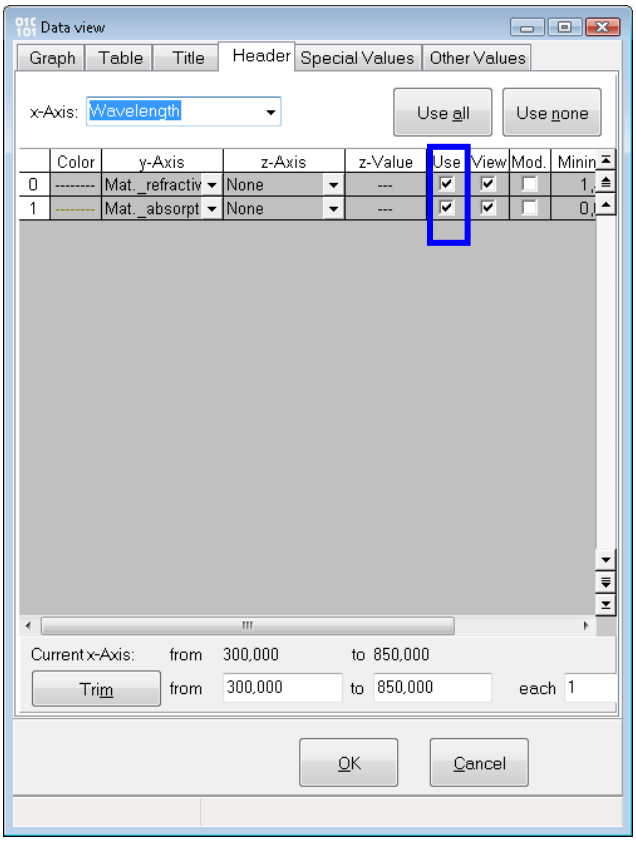


Fig. 8-42 The data with selected “Use” will be exported

The spectral range set in the Environmental settings must be equal or broader than the spectral range of the dataset. Otherwise the export will be cut to the environmental settings. Now the File → “Save As...” menu entry is selected. The file extension “ASCII (*.txt) and a filename are selected and saved.

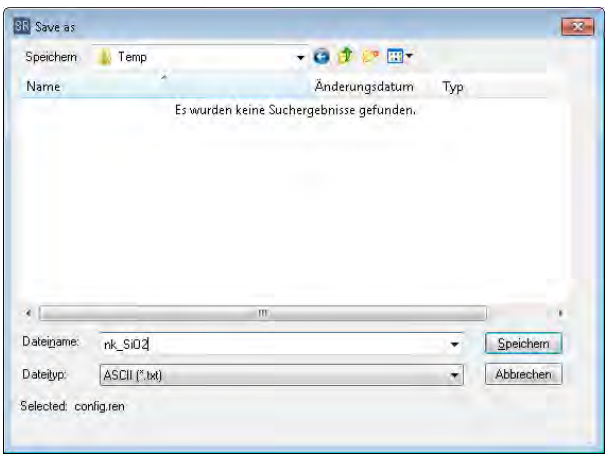


Fig. 8-43 Filename and extension ASCII (*.txt) are selected

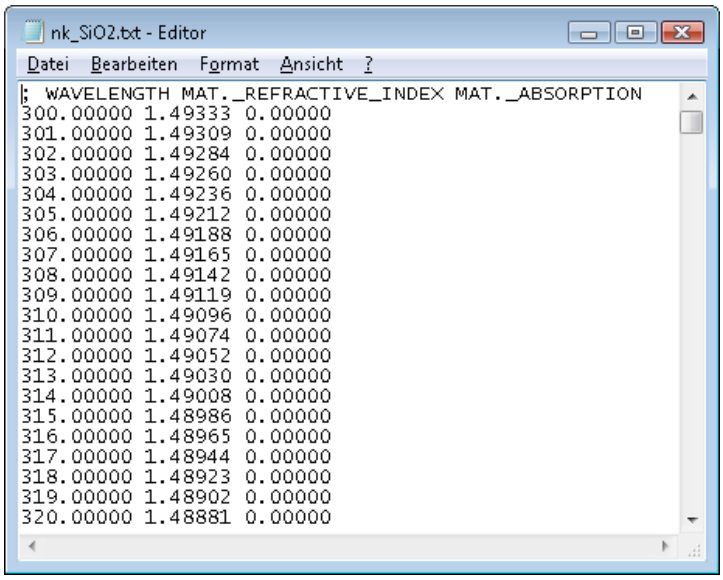


Fig. 8-44 Exported dataset in ASCII format

8.5 Dispersion formula examples

The dispersion relation (short: dispersion) describes the dependency of the refractive index n and extinction coefficient k with the wavelength: n(λ) and k(λ). Different types of materials show different types of dispersions. Four different kinds of materials illustrate the variety of different dispersion relations:

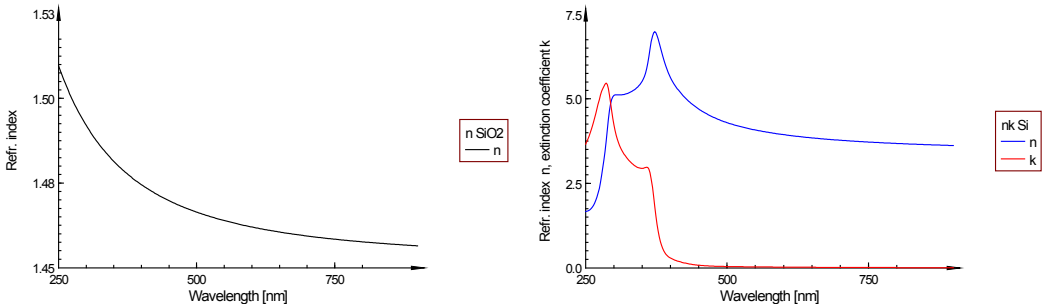


Fig. 8-45 Typical dispersions of a dielectric (SiO_2, left) and a crystalline semiconductor (Si, right)

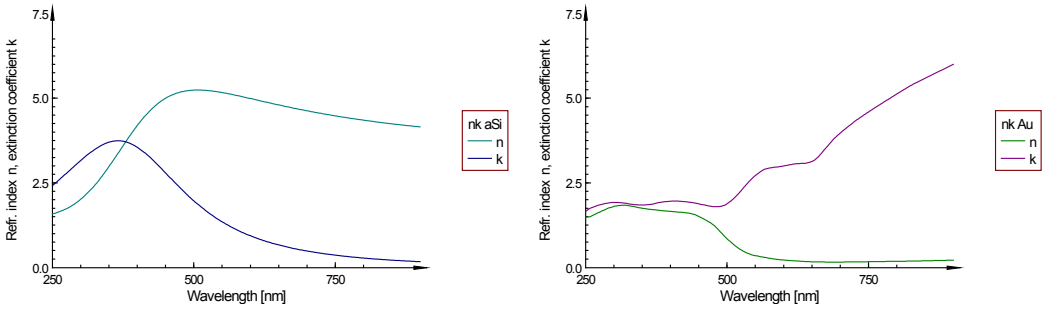


Fig. 8-46 Typical dispersions of an amorphous semiconductor (aSi, left) and a metal (Au, right)

For different kinds of material types different kinds of mathematical descriptions are necessary. The following chapter gives an overview of the dispersion relations available in SpectraRay.

8.5.1 Overview of dispersion formulas and layer types

By pressing the + icon a new material can be inserted into the model. The following table shows some of the most important dispersions:

The general description of the dispersions and their editors can be found in chapter 5.2.4.

L	Dispersion	Used for ...	Example
H	Fixed n and k	Constant dispersion	Only air
H	Cauchy	transparent dielectric materials Photoresist Glass	SiO_2, Al_2O_3, Si_3N_4, TiO_2 PMMA BK7, quartz
H	Tauc-Lorentz	Absorbing dielectric materials amorphous materials	Si_3N_4, TiO_2 a-Si, a-C
H	Drude-Lorentz	Metals TCO (transparent conductive oxide)	Au, Ag, Cu, Cr, Ni ITO, ZnO:Al
H	File-Layer	Table of wavelength, n, k, no fit parameters substrates	Good for all Si, Ge, GaAs, quartz
M	Leng-Lorentz	Crystalline indirect semiconductors polycrystalline indirect semiconduct. conjugated polymers (OLED, OFET)	c-Si, c-Ge, c-SiGe poly-Si MEH-PPV, P3HT
M	Brendel	Absorption (vibration) bands in the MIR	SiO2, SiN, CH-bonds
M	Sellmeier	Like Cauchy but for broader spectral range (VIS + NIR)	SiO_2
M	Tanguy III/V	Bandgap of direct semiconductors, also II/VI	GaAs, GaN, AlGaN ZnSe
L	Hamberg Sernelius	TCO (transparent conductive oxide)	ITO, ZnO:Al, SnO_2:F
L	Afromovitz	III/V semiconductors (specific)	GaAs, InP, InGaAsP
L	Formula	New non implemented dispersions	Good for all
L	Schott glass	Specific for glasses from Schott	AF45

L	Layer type	Used for ...	Example
H	EMA (effective medium approximation)	Mixture of two materials Roughness Interface Gradient	 mixture: Air / layer mixture: layer1 / layer2
M	Biaxial anisotropic	Direction dependent dispersion	Crystalline quartz
M	Periodical group	Bragg reflectors	20x (SiO_2 / TiO_2)
L	Table (2D)	Parameter dependent data of e.g. - Temperature - composition	 Si (0 deg C … 1000 deg) Si_xGe_{1-x}
L	Homogeneous growing layer	In-situ applications, thickness changes with time	Good for all
L	Nuclei growth	In-situ applications, island growth	Metallic film growth
L	Epitaxial Si profile	MIR, Si epitaxial layer growth	Si doping concentration and gradient

Tab. 8-2 The most important dispersions: Level of usage: High (used very often), Medium (sometimes) Low (seldom)

8.5.2 Drude-Lorentz oscillator

The Drude-Lorentz oscillator is a combination of two dispersion types: the Drude absorption of free charge carriers and a Lorentz-oscillator model. The unit of the parameters in the Drude-Lorentz oscillator dispersion is wavenumbers. Therefore it is best to change the wavelength scale to wavenumbers/cm^{-1}.

The Drude-Lorentz oscillator can be used to describe the dispersion of metals like aluminum, tantalum or silver. It is also suitable for transparent conductive oxides like ITO or ZnO:Al. The following picture shows the appearance of the Drude-Lorentz oscillator model window.

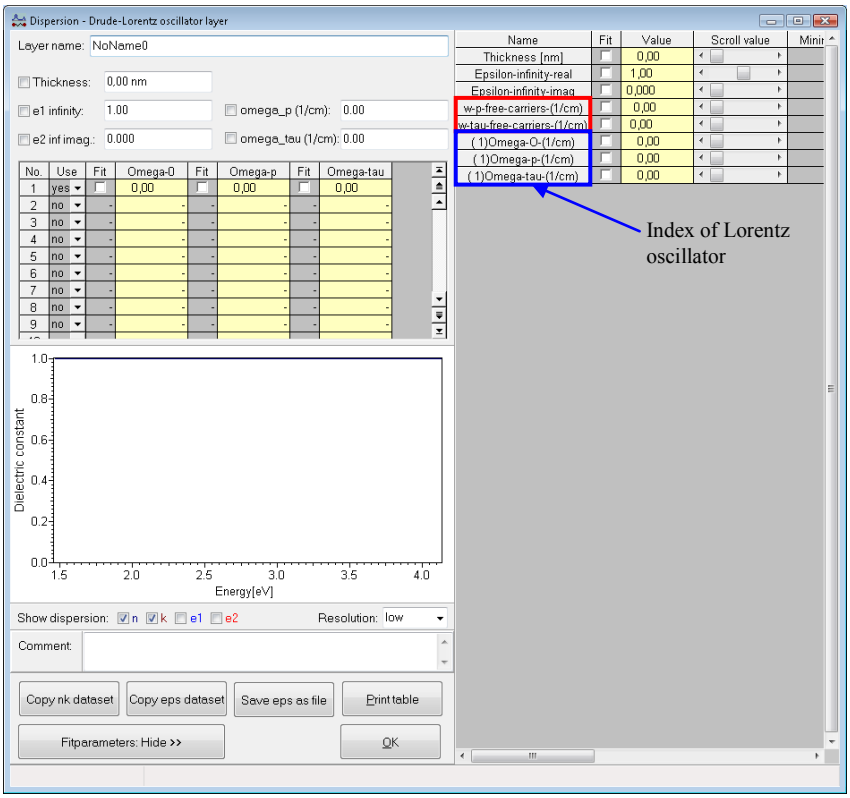


Fig. 8-47 Example for a Drude-Lorentz layer

The red box indicates the two parameters for the Drude-oscillator model. The blue box indicates the three parameters for the Lorentz-oscillator model. Up to 10 Lorentz-oscillators can be used simultaneously.

8.5.2.1 The Lorentz-oscillator

The Lorentz-oscillator consists of three parameters for the spectral position, strength and damping.
Its contribution to the dielectric function ε is:

$$\varepsilon = 1 + \frac{\Omega_P^2}{\Omega_0^2 - \nu^2 - i\Omega_\tau \nu}$$

Its parameters are summarized in the following table.

Lorentz-Oscillator	
Parameter	Description
Ω_O	Center frequency of the oscillator in cm^{-1}
Ω_P	Strength of the oscillator (amplitude)
Ω_τ	Damping of the oscillator

Tab. 8-3 Parameters of the Lorentz oscillator

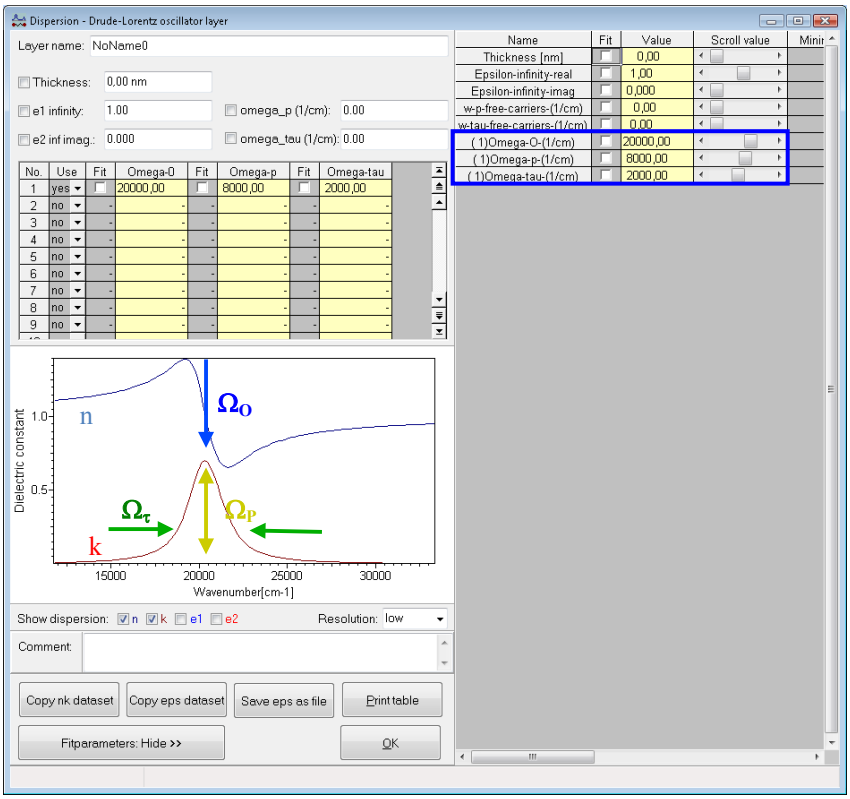


Fig. 8-48 Example for a Lorentz oscillator

8.5.2.2 The Drude-free carrier absorption

The free carrier concentration in a material leads to an oscillator with a center frequency of ω_0=0. Its contribution to the dielectric function ε is:

$$\varepsilon = 1 + \frac{\omega_P^2}{-\nu^2 - i\omega_\tau \nu}$$

Drude-oscillator	
Parameter	Description
ω_P	is dependant from the concentration N and the effective mass m* of the free carriers: $\omega_P = \sqrt{\frac{N e^2}{\varepsilon_0 m^*}}$
ω_τ	is dependant from the mobility μ and the effective mass m* of the free carriers: $\omega_\tau = \frac{e}{m^* \mu}$

Tab. 8-4 Parameters of the Drude oscillator

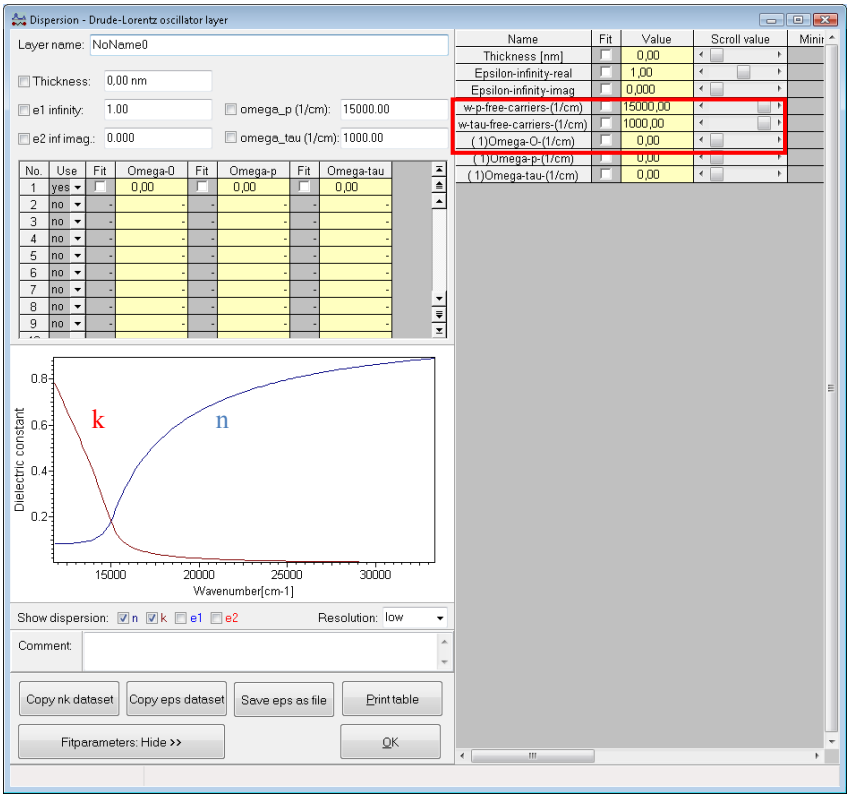


Fig. 8-49 Example for a Drude oscillator

The following two graphs show the influence of carrier concentration N and mobility μ to the dispersion of n and k for the example of a transparent conductive oxide like ITO (Indium doped TinOxide) .

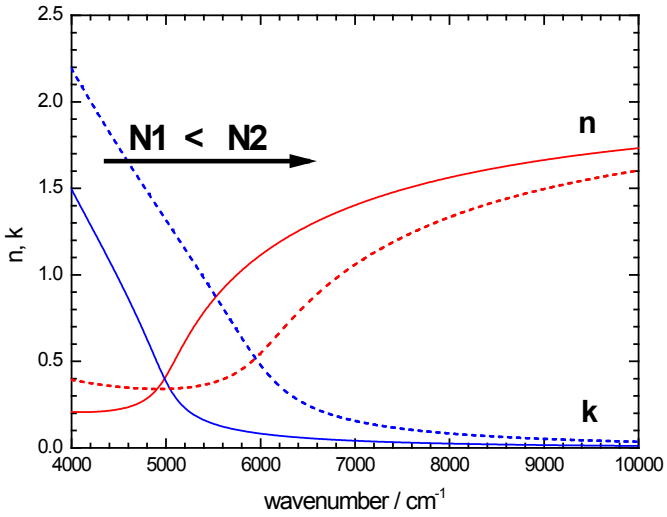


Fig. 8-50 Influence of carrier concentration N to the dispersion on n and k

→ With increasing carrier concentration the onset of the absorption is shifting to higher wavenumbers (shorter wavelength).

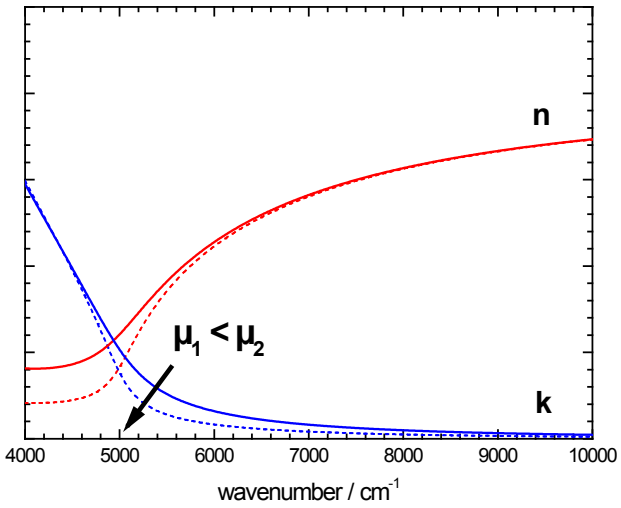


Fig. 8-51 Influence of carrier mobility μ to the dispersion on n and k

→ With increasing mobility μ of the free carriers the oscillator structure gets sharper.

8.5.3 Brendel oscillator examples

In addition to the general description of the Brendel oscillator in chapter 5.2.4.8 more examples are given here.

8.5.3.1 Dielectrics in the MIR spectral range

The following example shows the modeling of the AlO absorption band at around 700 cm^{-1}. The measurement was performed at three angles of incidence of 50°, 60° and 70°. The structure below 1000 cm^{-1} is due to the AlO band.

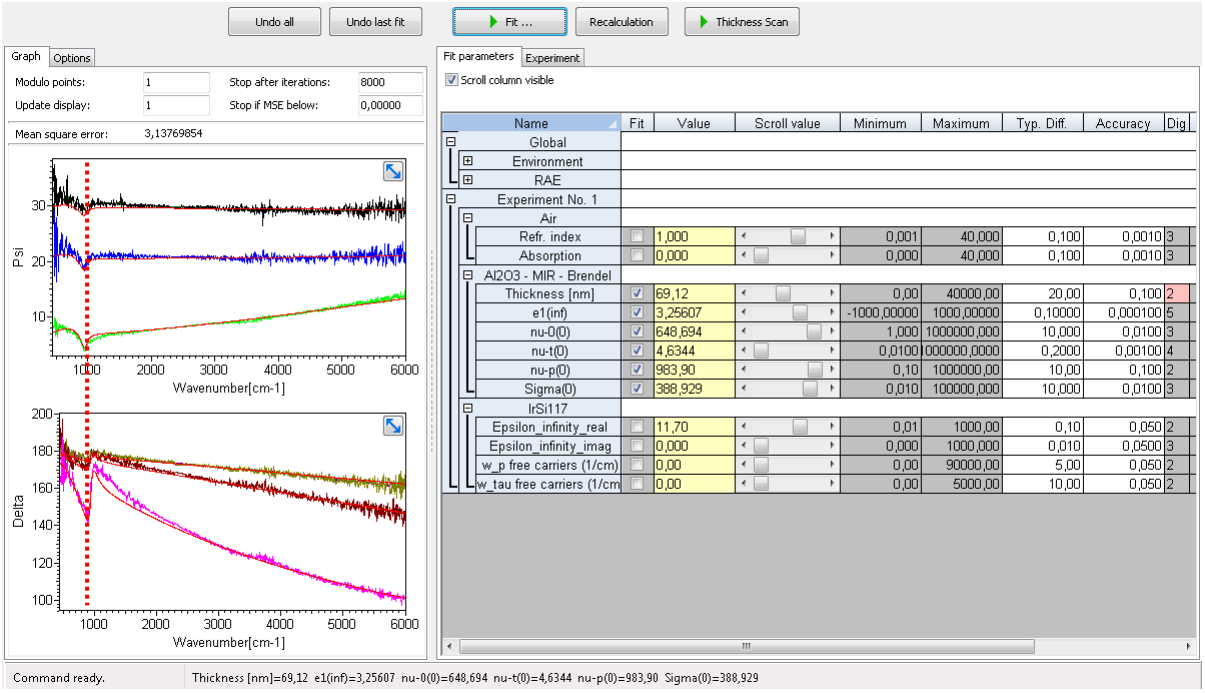


Fig. 8-52 Modeling of the AlO absorption band at around 700 cm^{-1}

The screenshot of the Brendel dispersion window for Al_2O_3 shows the dispersion of n and k using a single Brendel oscillator.

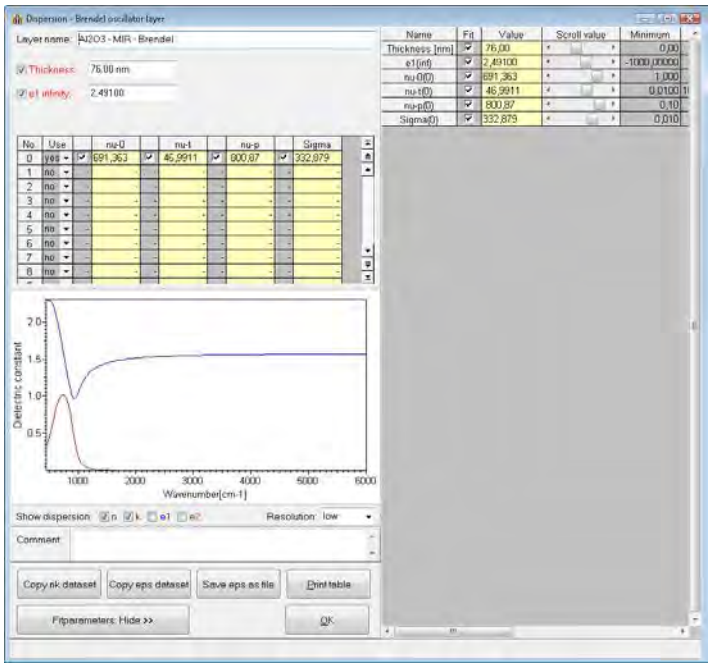


Fig. 8-53 Brendel dispersion for Al_2O_3

8.5.3.2 Metals in the UV-VIS-NIR spectral range

For the modeling of metals usually the Drude-Lorentz oscillator is used. For some metals like Au this oscillator type is not suitable because the shape of the Plasma edge can't be modeled well. Then the Brendel oscillator is mostly the better choice to model this kind of shape excellently. The following example shows an optical thick **Au film on glass**. The units of the x-axis are wavenumbers. The spectral range is 4000 – 45331 cm^{-1} which corresponds to 230 – 2500 nm. The Plasma edge at 20000 cm-1 is described excellently.

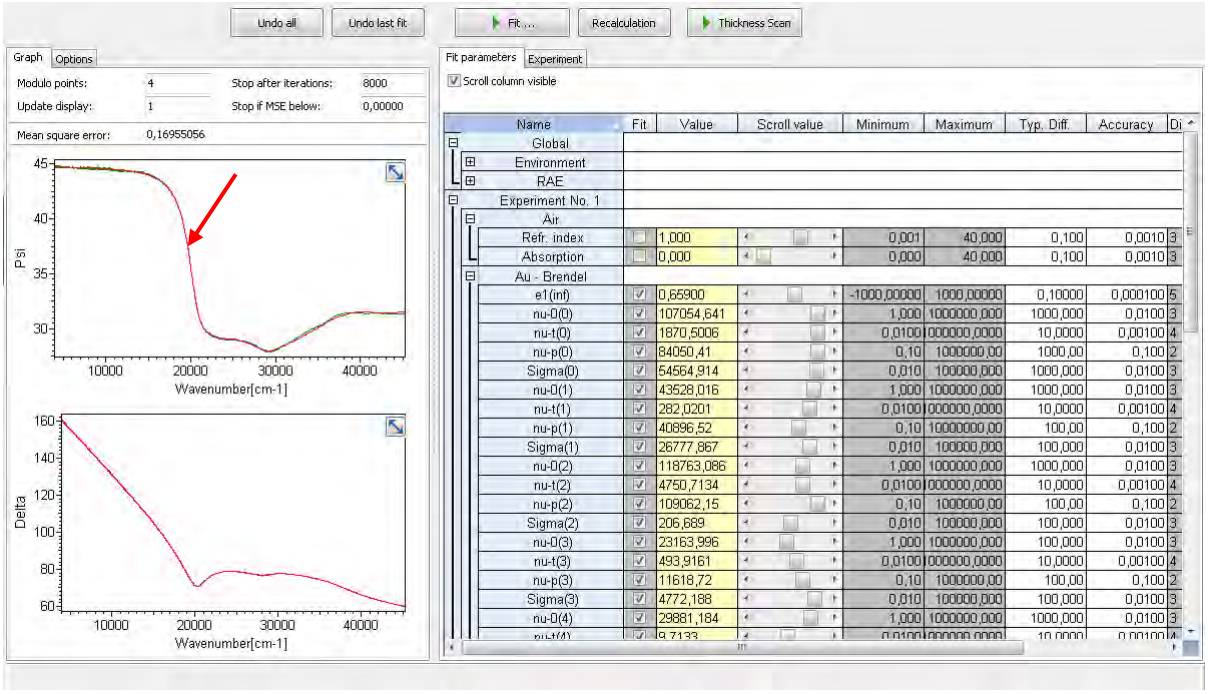


Fig. 8-54 Modeling of an Au film on glass

The following screenshot shows the dispersion of Au. A total number of 8 oscillators are used to describe the dispersion in this broad spectral range. Oscillator number 6 is placed at 0 cm^{-1} to represent the Drude oscillator.

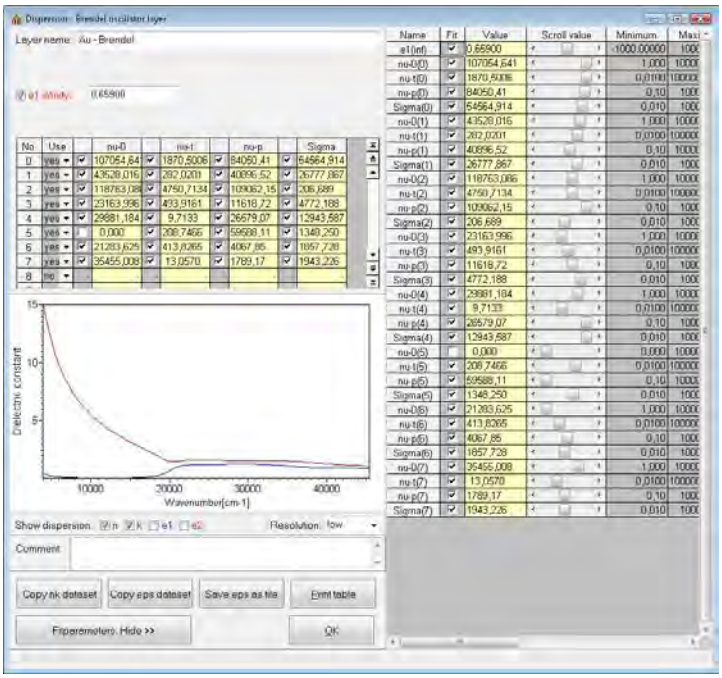


Fig. 8-55 Dispersion of Au

8.5.3.3 Glass in the VIS-MIR spectral range

Glasses like flat glass (SLG) or low iron glass show a very weak extinction coefficient. It is normally neglected in ellipsometric measurements because k is well below 0.001 and the Cauchy layer can be used well to describe the dispersion of n.

In some applications, when backside reflections occur in ellipsometric or transmission measurements, then the extinction can't be neglected anymore. In this case the dispersion can be described well using a Brendel oscillator which is shown in the following experiment where Ψ of an ellipsometric measurement and a transmission measurement are combined in one experiment.

SLG example
The upper graph of the screenshot shows the Ψ measurement the lower graph the transmission measurement. The ellipsometric measurement is performed on a rough part of the sample so no backside reflections occur. The transmission of course is with backside reflections.

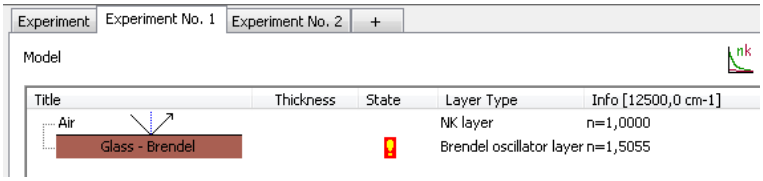


Fig. 8-56 Ellipsometric model without backside reflections

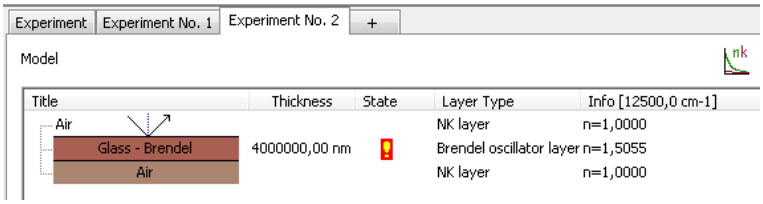


Fig. 8-57 Transmission model without backside reflections

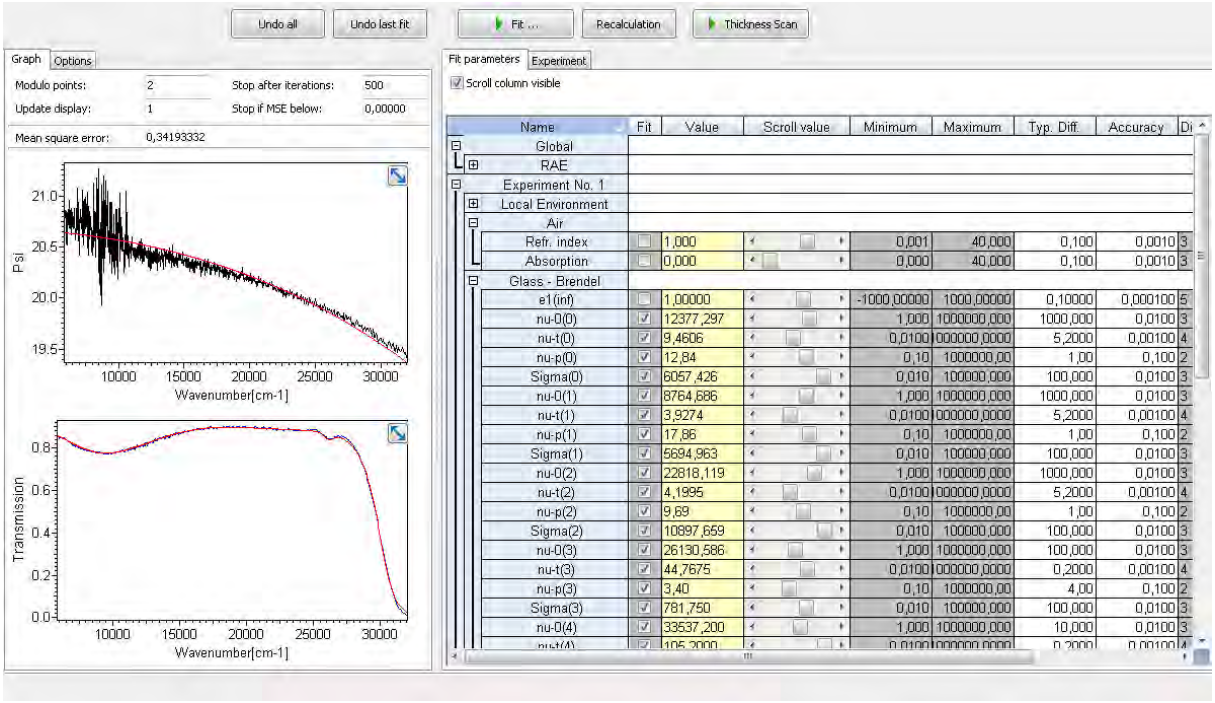


Fig. 8-58 Model and measurement of Ψ (top) and transmission (bottom)

The dispersion of n is mostly described by oscillator number 9. It is placed outside the measured spectral range. The Lorentz (nu0) damping and Gaussian (sigma) broadening are set to zero. Then no absorption will occur by this oscillator in the VIS or NIR. This is important because it will always be too large and will suppress the weak absorption structures in the VIS and NIR.

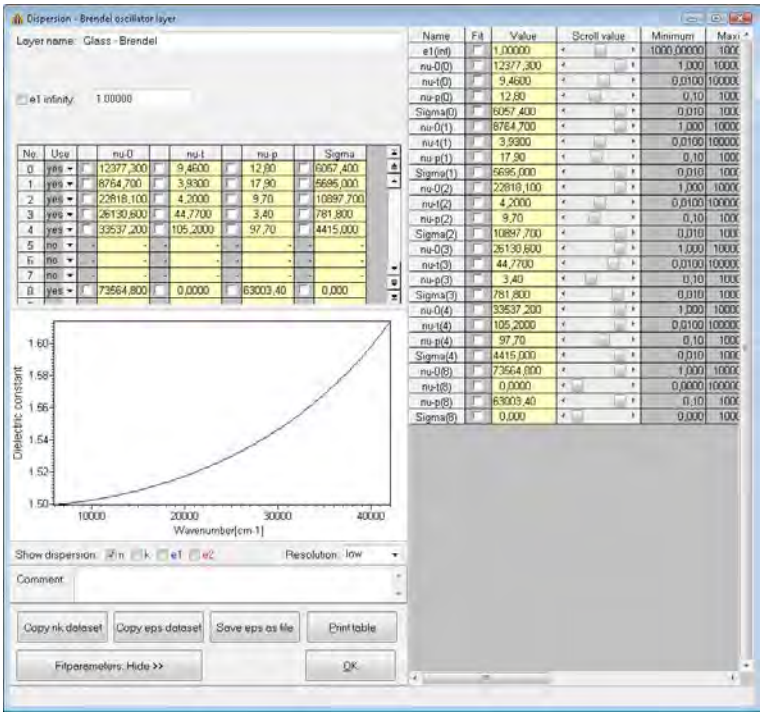


Fig. 8-59 Brendel oscillator for glass - n

The dispersion of k is described by oscillators 1 – 5. The extinction k is very weak in the range from 10^{-6} to 10^{-5}!

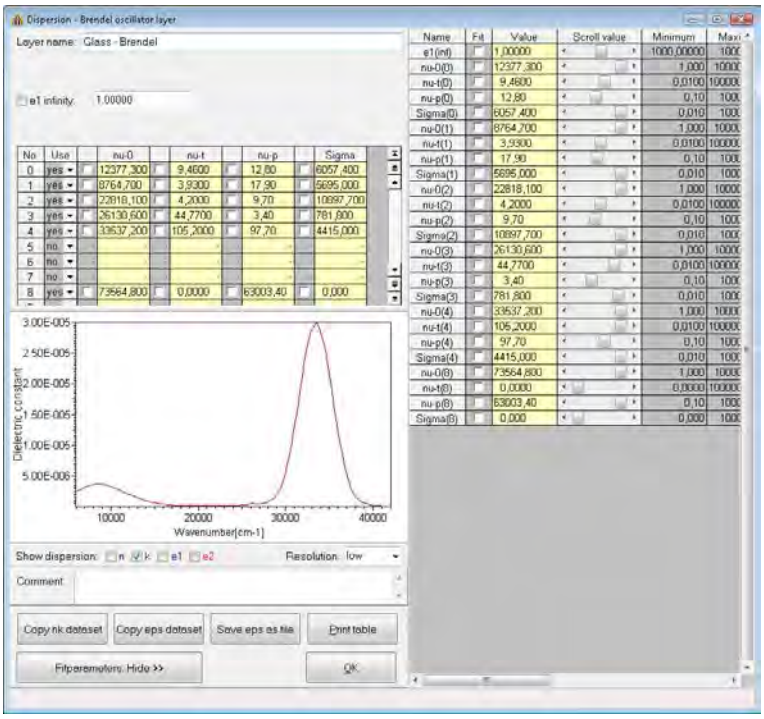


Fig. 8-60 Brendel oscillator for glass - k

8.6 Hackers guide for scripts

Scripts can be used to automate procedures in SpectraRay. They can be applied for many kinds of applications like e.g. automatic measurements, fitting, import or export of data. This chapter gives an overview how to build scripts using some useful short examples.

8.6.1 Starting the script editor to build a new script

The script editor can be opened in two different ways:

- Menu → Extra → Applications
- Single mouse click on the application icon: 

The "Application runner" is started which might already show existing scripts:

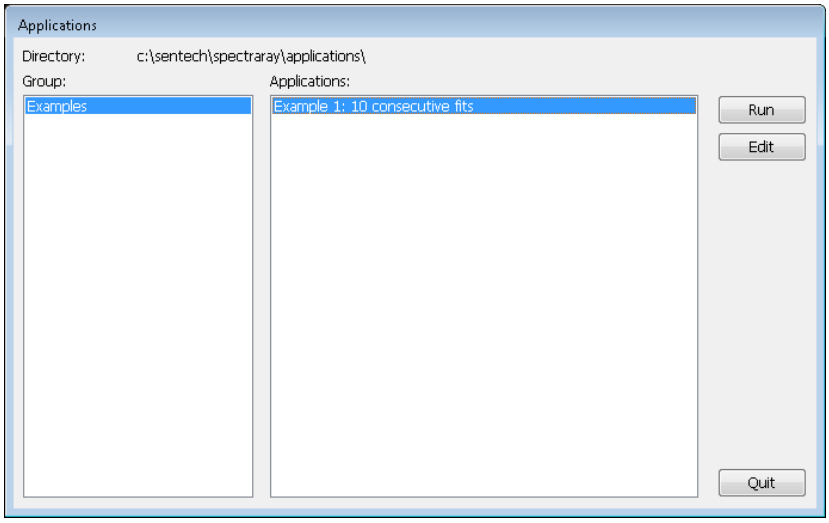


Fig. 8-61 Application runner

The existing applications are located in the folder 

. If you want to change the directory of the applications you have to click on 

in the main window:

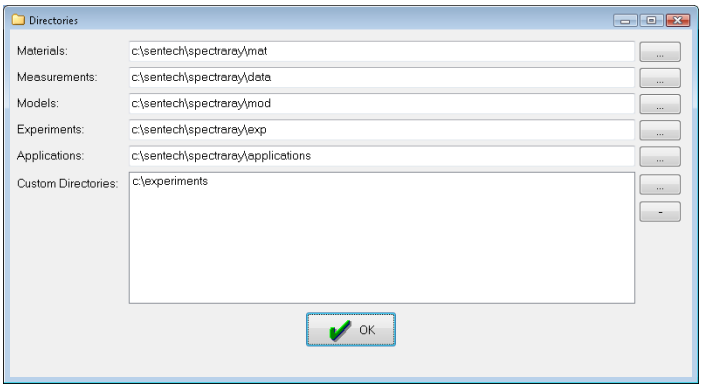


Fig. 8-62 Directories

Here you can change the default directories for materials, experiments, applications,…

If you want to create new applications you have to open the script editor by clicking “Help->Edit Script” in the main menu. The script editor allows developing, executing, loading or saving scripts.

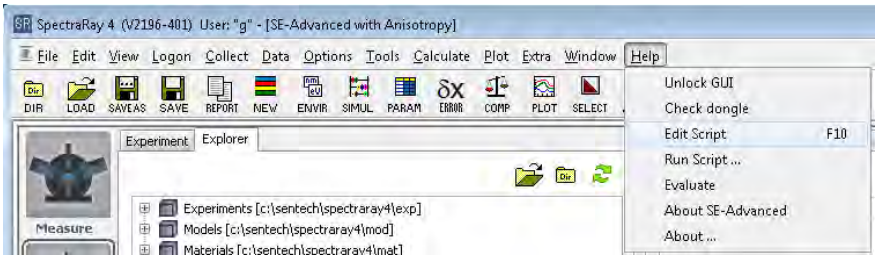


Fig. 8-63-8-64 Starting the script editor

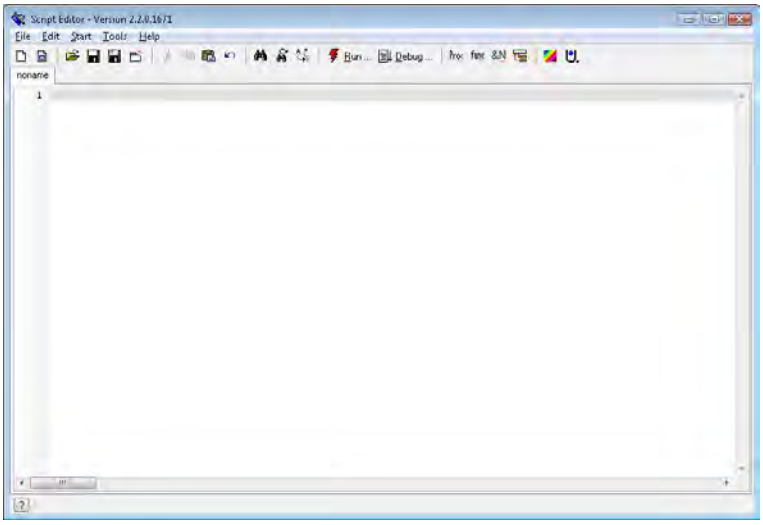


Fig. 8-65 Script editor

In the beginning a title is defined which is displayed in the “application runner” window. In order to prepare the first example the title is set to:

;title=Examples\Example 1: 10 consecutive fits

The string “Examples” before the “\” defines the group of the application, “*Example 1: 10 consecutive fits*” defines the name of the example. Then you have to save the script in the application directory and the new script appears as a new entry in the “application runner” (see Fig. 8-61).

In the “application runner” window you can modify existing scripts with Edit and start the selected application with Run.

Please obey the following scripting rules:

1. Only use one command per line
2. Don’t use underscores in Label names “Label1a” instead of “Label_1a”
3. A “Label:” ends with a colon when it is declared
4. A “Label” doesn’t end with a colon when it is addressed
5. Comments can be introduced with a semicolon “;” in the beginning of a row

8.6.2 Script examples

8.6.2.1 Script for numerous consecutive automatic fittings

In case of a high amount of fitting parameters it is often the case that the fitting procedure won't find the best fitting within a single run of the fitting procedure. Instead an arbitrary amount of consecutive fitting runs can be initiated using a script.

This example will be programmed using two different scripts. The first shows the trivial case the second uses a loop to execute the fitting procedure. The script command which is used to execute the fitting procedure is called "*SpectraRay.autofit <str FitScript> <bool WithOutProgress> [<var in TimeoutMS]"* (with two parameters and one optional parameter).

Trivial script:
The trivial script will be to simply copy the *"SpectraRay.autofit Fit 0"* command ten times into the script editor.

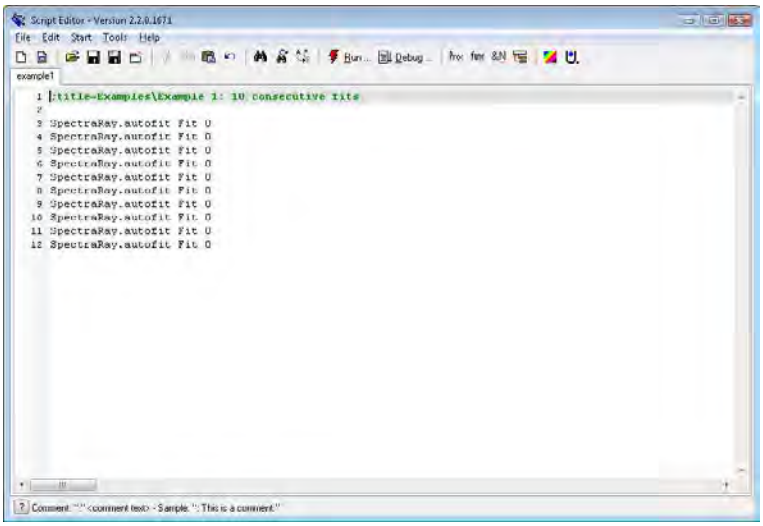


Fig. 8-66 Trivial script example

When an experiment file is loaded containing measured data, a model and fit parameters the script can be executed by pressing "Run".
The successful running script with the parameter "WithOutProgress" set to 0 now shows a small window with information about the progress of the actual fit run.

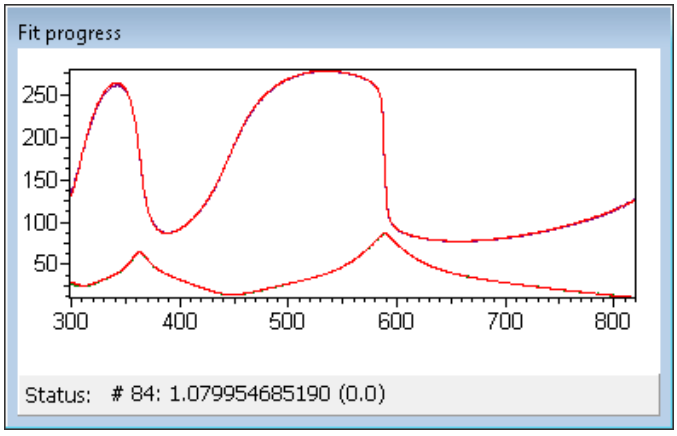


Fig. 8-67 Fit progress

The script can be cancelled before it automatically ends by holding the “CTRL” key. Then a window appears asking to confirm the cancelling.

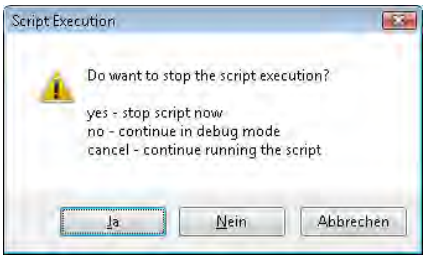


Fig. 8-68 Cancelling the script execution

Non-trivial script using a loop:

There are no loops possible known from other programming languages based on the “for ... next” structure. Therefore the loop is programmed in a different way using a “label” which can be used to jump to in the script and an “if” command. Furthermore variables are introduced and assigned in order to control the amount of fit runs and to decide when to end the script. This is the script now using the loop:

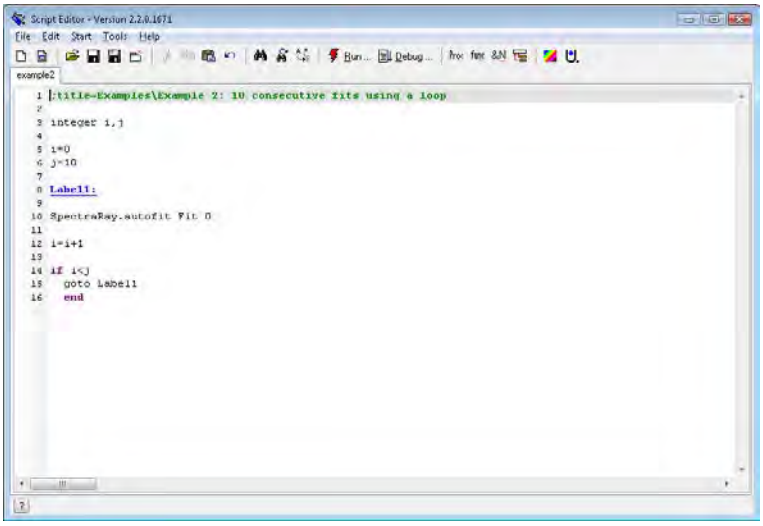


Fig. 8-69 Non-trivial script example

This is the same script but with comments:

```
;title=Examples\Example 2: 10 consecutive scripts using a loop

; declaration of the integer variables i and j
integer i,j

; assigning start values:
; number of first run
i = 0
; amount of fit runs
j = 10

; This is the beginning of the loop using the label command, the label ends with a colon ":"
Label1:

SpectraRay.autofit Fit 0
;the variable i is incremented
i = i+1

; now it is checked whether i is still lower than j, then the script jumps to Label1
; here no colon ":" is used at the end of Labe1
if i<j
  goto Label1
  end
```

This script now does exactly the same like the trivial script. The advantage is that the amount of fit runs can be easily changed by changing the value for the variable j.

8.6.2.2 Calculation of the sum of all films in a stack

Sometimes the total thickness of a stack is of interest. Then it is unhandy to use the calculator and add up all film thicknesses manually. The following script helps to automatize this procedure.

The following stack is used to add up the film thickness.

Model

Title	Thickness	State	Layer Type	Info [632,8 nm]
Air			NK layer	n=1.0000
Cau-SiO2 (therm.)	105,37 nm		Cauchy layer	n=1.4610
Cau-TiO2	136,97 nm		Cauchy layer	n=2.3864
Cau-SiO2 (therm.)	24,71 nm		Cauchy layer	n=1.4610
Y2O3 - Cauchy	50,16 nm		Cauchy layer	n=1.4600
Cau-BK7			Cauchy layer	n=1.5157

The script will read out the amount of layers in a stack, add them up and prints out the sum in a window. Additional commands are used to convert floating point variables into string variables.

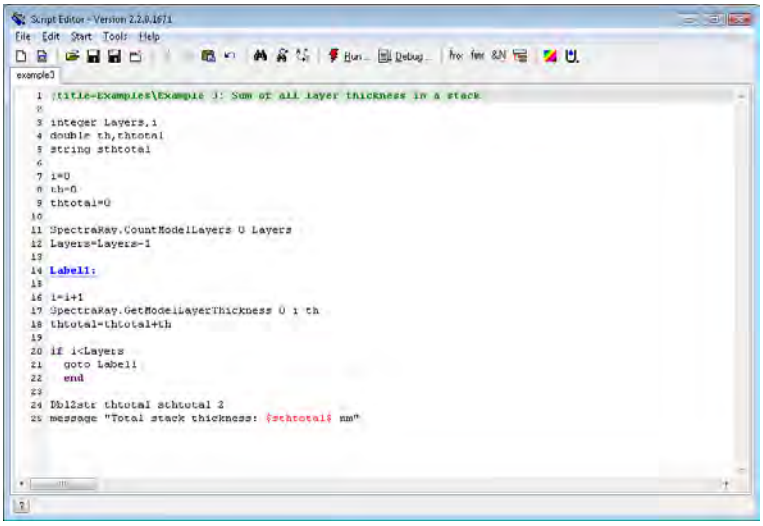


Fig. 8-70 Script example: Adding up the film thicknesses

It is important to know that the command “SpectraRay.CountModelLayers” which counts the layers will not give “4” but 5 as result. This is because it starts counting with “Air” which is layer zero and ends with the substrate layer which is layer “5”.

This result window is shown when the script is executed:

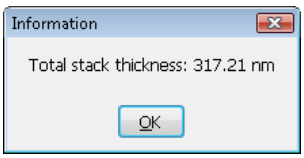


Fig. 8-71 Resulting message

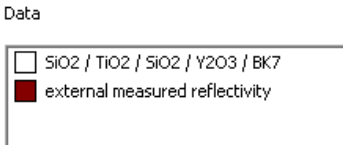
This is the script with comments:

```
;title=Examples\Example 3: Sum of all layer thickness in a stack

integer Layers,i
; floating points variables are declared using "double" command:
double th,thtotal
; a string is declared which can be printed out in a window:
string sthtotal

; the starting values are assigned
i = 0
th = 0
thtotal = 0

; the amount of layers in the first experiment (mostly there is only one) are counted
; the experiments are counted starting with "0"
; the result is stored in the variable "Layers"
SpectraRay.CountModelLayers 0 Layers;
Layers = Layers - 1

Label1:
i = i+1
SpectraRay.GetModelLayerThickness 0 i th
thtotal = thtotal + th
if i<Layers
  goto Label1
  end

; the double variable is converted into a string. The digits are cut to 2 digits
Dbl2str thtotal sthtotal 2

;message opens the result window
; the variable is put in $$ to give the content of the variable
message "Total stack thickness: $sthtotal$ nm"
```

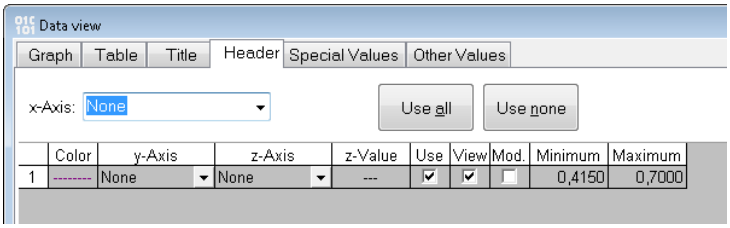
8.6.2.3 Import of external data with unit assignment

It was already explained how to import external measured data which is existent as ASCII data of e.g. two columns of wavelength and reflection data. The following script shows how to assign the units using a script.

It is assumed that the imported data is moved to the last position in the “Data” section of SPECTRARAY after manual import. The data is reflectance data measured at an angle of incidence of Φ = 8°.



The important information of the measurement are not set yet: “None”
x-Axis: None – (this will become: wavelength / nm)
y-Axis: None – (this will become: reflectivity)
z-Axis: None – (this will become: angle of incidence)
z-Value: --- – (this will become: value of the angle of incidence: 8°)



The fit script needs to count the amount of datasets to know which will be the last one in the row. Then the four parameters will be assigned to this dataset.

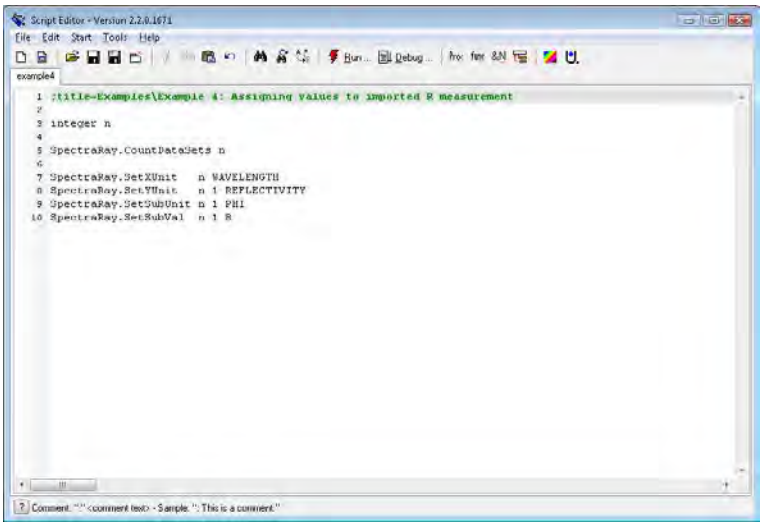
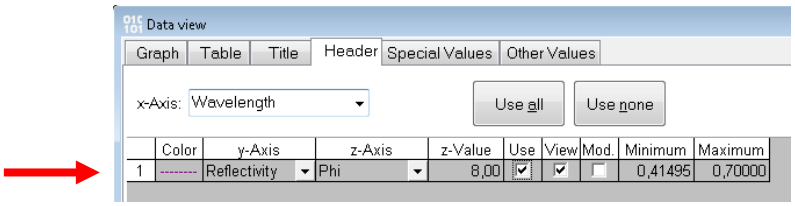


Fig. 8-72 Script example: unit assignment

Script with comments:

```
;title=Examples\Example 4: Assigning values to imported R measurement

integer n

; the amount of datasets is saved to the variable n
SpectraRay.CountDataSets n
; the x-axis is set to wavelength / nm
SpectraRay.SetXUnit   n WAVELENGTH

; the y-axis is set to wavelength / nm
; 1 stands for the first data column (see red arrow in screenshot below)
; in case of multiple column data (e.g. PSI, DELTA) additional columns appear
SpectraRay.SetYUnit   n 1 REFLECTIVITY

; the z-axis is set to the angle of incidence "PHI"
SpectraRay.SetSubUnit n 1 PHI

; the value of the angle of incidence is set to 8°
SpectraRay.SetSubVal  n 1 8
```

After executing the script all units and values are assigned as shown in the following screenshot.



8.6.2.4 Consecutive fitting of n datasets using the same optical model

The dataset holds measurements of the same sample at five different positions. The optical model should be applied to all these single measurements and the results of the film thickness and the refractive index at 400 nm and 632.8 nm are saved into a file.

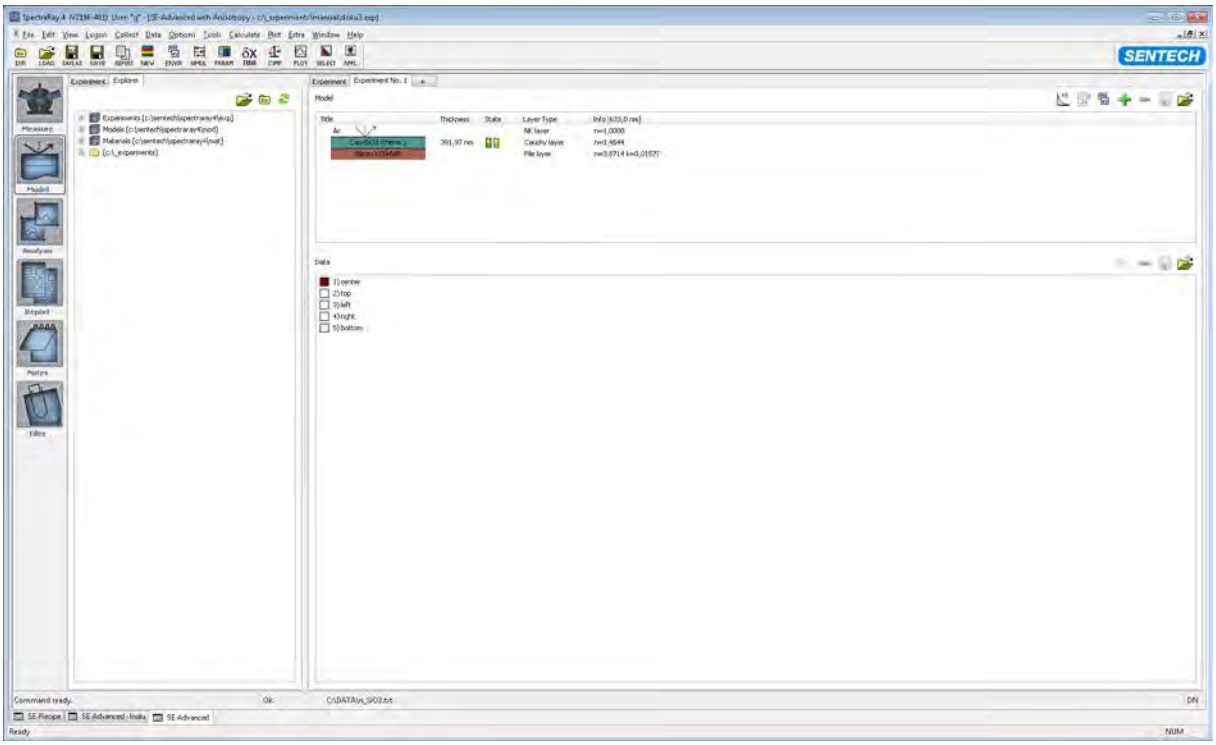


Fig. 8-73 dataset of five different positions

The following figure shows the resulting file of the script shown below.

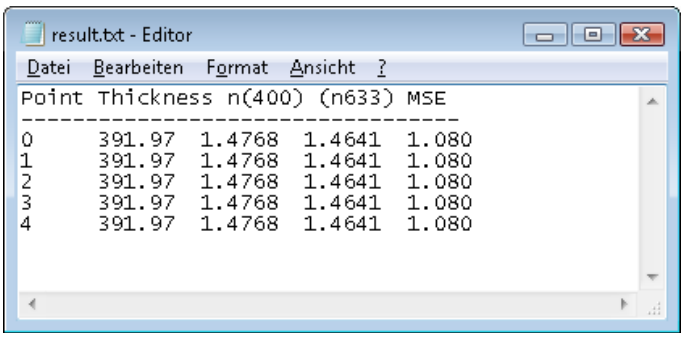


Fig. 8-74 Resulting file

This is the script file with comments:

```
;title=Examples\Example 5: Consecutive fitting of multiple measurements

integer i,n
double th,n400,n633,k,MSE
string sth,sn400,sn633,sMSE

; *************************
; Writing logfile header
; *************************

StrList.Create List
StrList.Add List "Point Thickness n(400) (n633) MSE"
StrList.Add List  ---------------------------------

; Initial settings of the variables
i = 0
SpectraRay.CountDataSets n
n = n+1

; ****************************
; Deselecting all datasets
; ****************************

; Begin of the loop1
Label1:

SpectraRay.SetDataUse i 1 0
SpectraRay.SetDataUse i 2 0
i = i+1

if i<n
  goto Label1
  end

; End of the loop1

i = 0

; ****************************
; Fit of all measurements
; ****************************

; Begin of the loop
Label2:

; Selecting the actual dataset
SpectraRay.SetDataUse i 1 1
SpectraRay.SetDataUse i 2 1
```

```
; Starting the fit
SpectraRay.AutoFit Fit 0

; Reading the film thickness of the first experiment (0) of the first layer (1)
SpectraRay.GetModelLayerThickness 0 1 th

; Reading n and k for the first experiment (0) of first layer (1) at 400 nm
; Storing the results in the variables n400 and k
SpectraRay.GetModelLayerRefrIndex 0 1 400 n400 k
SpectraRay.GetModelLayerRefrIndex 0 1 633 n633 k

;Reading the MSE value
SpectraRay.GetLSQ MSE

; Converting the double variables into strings
Dbl2str th   sth   2
Dbl2str n400 sn400 4
Dbl2str n633 sn633 4
Dbl2str MSE  sMSE  3

; The result string is written into the logfile
StrList.Add List "$i$     $sth$  $sn400$  $sn633$  $sMSE$"

; Deselecting the actual dataset
SpectraRay.SetDataUse i 1 0
SpectraRay.SetDataUse i 2 0
; incremenent of the actual dataset
i = i+1

; Jump to label 2
if i<n
  goto Label2
  end
; End of the loop

; **********************************
; End of Fit of all measurements
; **********************************

; **********************************
; Save results to file "results.txt"
; **********************************

StrList.SaveToFile List c:\\result.txt
```

8.6.2.5 Consecutive measurements

The following script shows how to run a number of consecutive measurements e.g. for in-situ applications. The number of measurements and elapsed time will appear in the SpectraRay status bar. The script can be interrupted at any time by holding the left CTRL key.

```
;title=Examples\Example 6: Consecutive measurements#

double CurrentAngle
integer i,number,ec
double tellapsed
string snumber,stellapsed


; define the current angle of incidence
CurrentAngle = 70

i = 1

; number of consecutive measurements
; the script can be interrupted by holding the left CTRL key
number = 10

; seconds since midnight
TimeDifference.Start Start

;**************************
;label, loop begins here
;**************************
jumphere:

TimeDifference.GetSec Start tellapsed
Dbl2str i snumber 0
Dbl2str tellapsed stellapsed 0

; writes status information of measurement number
; and ellapsed time into the status bar of SpectraRay
SpectraRay.Statusbar 0 "Current measurement number: $snumber$ ellapsed_time: $stellapsed$ s"

; start the ellipsometric measurement

SpectraRay.Measure.ScriptMethod.DoMeasure 1 1

; delay if necessary (waits now for 1000 ms)
Delay 1000

i = i +1
if i<number
  goto jumphere
  end

;******************
; loop ends here
;******************
```

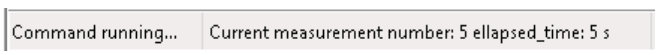


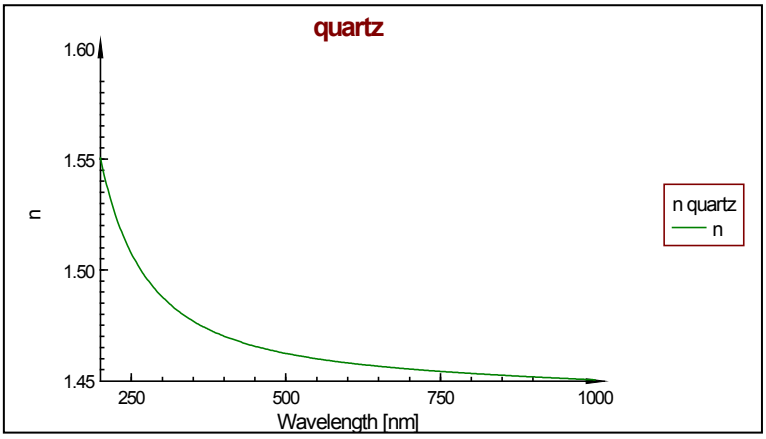
Fig. 8-75 Status bar

8.7 Application examples

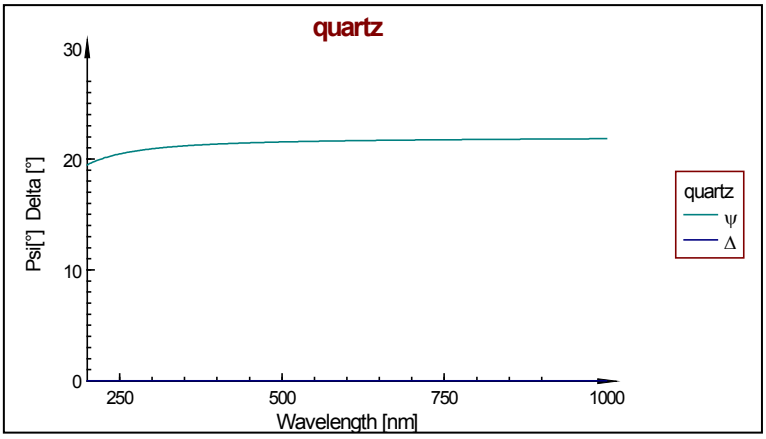
8.7.1 Measurement of substrates

8.7.1.1 Transparent substrates

The dispersion of transparent materials is strictly increasing to lower wavelength (higher photon energies). There is no additional structure in the transparent spectral range.

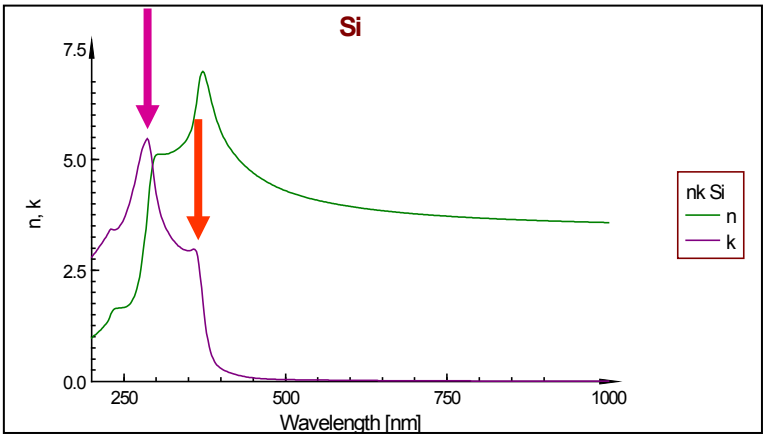


This results also in monotone spectra (here at Φ=70°). Ψ shows no particular structures. Δ is constant at 0°. It can also be constant at 180° when the angle of incidence is lower than the Brewster angle.

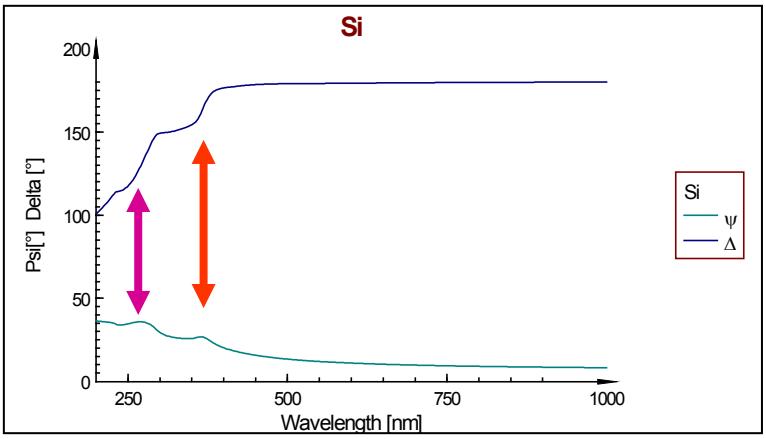


8.7.1.2 Absorbing substrates

A typical and widely used absorbing substrate is crystalline silicon. It is a semiconductor which shows characteristic absorption structures which are related to the band structure of the material.

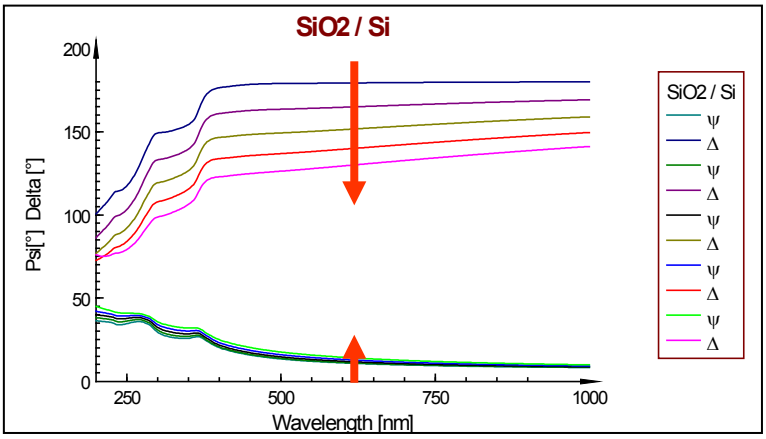


These characteristic structures appear also as structures in the ellipsometric spectra Ψ and Δ.



8.7.1.3 Transparent layers on absorbing substrates

The following graph shows the growth of SiO_2 on a silicon wafer in the range of 0 to 20 nm with steps of 5 nm. A similar graph was already shown for the explanation of the "Simulation" software module.



Δ shows a strong and almost constant shift with increasing SiO_2 film thickness. On the other hand Ψ shows only a little change, which is rather higher in the UV than in the NIR spectral range. The huge effect in Δ is the reason for the enormous sensitivity of ellipsometry to very thin films compared to reflectivity measurements. The weak effect in Ψ is the reason why for thin transplant films in the thickness range below 25 nm the optical constants are fixed and the remaining fitting parameter is just the film thickness.

8.7.2 CET procedure

CET: (**C**ombined **E**llipsometry and **T**ransmission)
Example: P2000 (polymer / C60 fullerenes blend)

8.7.2.1 Introduction

The P2000 film shows strong absorption and it is relatively thin. This leads to ambiguous results concerning the film thickness and the dispersion of n and k.

In order to overcome this ambiguity it is necessary to combine the ellipsometric measurement with a different kind of measurement. Ellipsometry is based on reflection. The light passes the layer twice. Transmission is passing only once. Therefore it is recommended to be combined with ellipsometry. It is not necessary that the transmission measurement covers the same spectral range like ellipsometric measurement. It can be shorter, equal or wider. At least both measurements should overlap partly. (A reflection measurement won't help here.)

We assume that a multiple angle ellipsometric measurement exists (50°, 60° and 70°). This measurement was performed on a roughened substrate so no backside reflections occur. The transmission measurement is done with a polished substrate of course. It is saved as an *.spc file.

Therefore the models for both measurements are identical with one important difference: the transmission measurement needs to take the backside reflection into account by introducing air below the quartz substrate. Furthermore the incoherent calculation must be activated.

This example is not an ideal example to demonstrate the power of CET because there is no ideal fitting achieved for both (Ψ, Δ) and Transmission. So it is likely not absolutely to describe the P2000 blend as a single homogeneous layer. The CET procedure can be explained anyway by this example.

8.7.2.2 Ellipsometric model

The ellipsometric model is as follows. It consists of a single film P2000 on a quartz substrate. The dispersion is described using the Brendel-oscillator model.

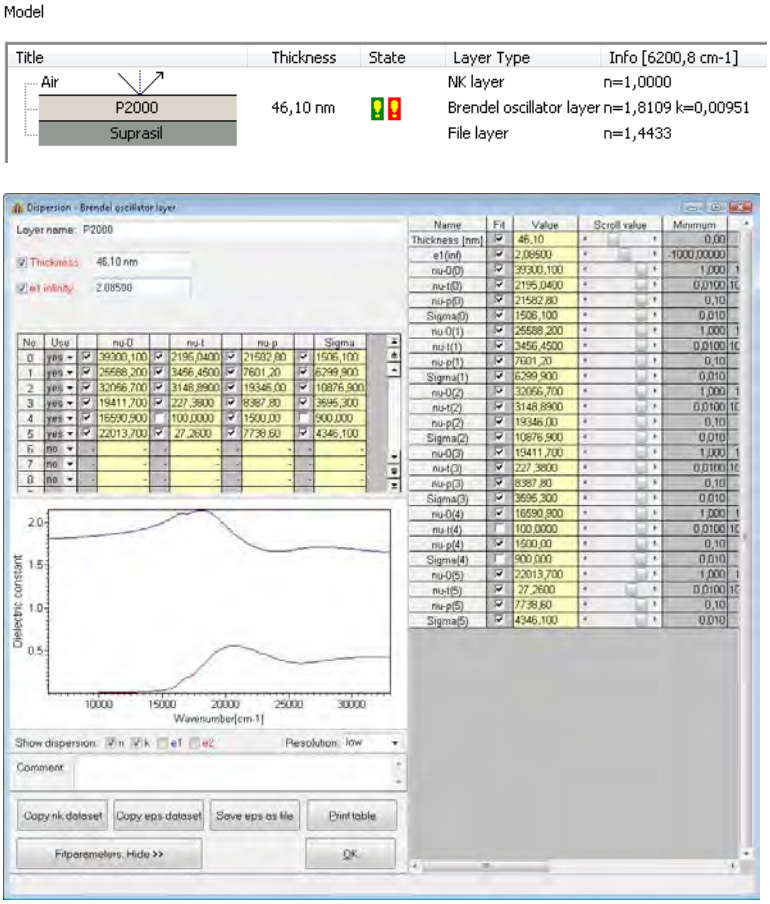


Fig. 8-76 Dispersion of P2000 describe using Brendel oscillator model

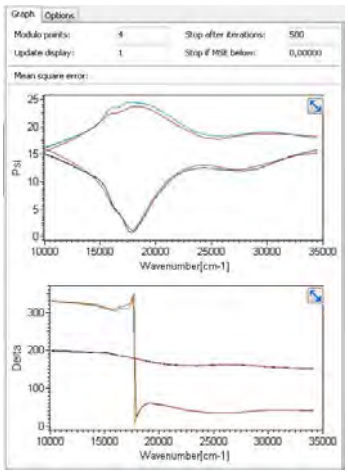


Fig. 8-77 Measurement and model at φ = 50° and 70°

8.7.2.3 Second experiment for transmission

8.7.2.3.1 Creating the second experiment

The second experiment is created by: Menu → Edit → Model + Data sets → Add

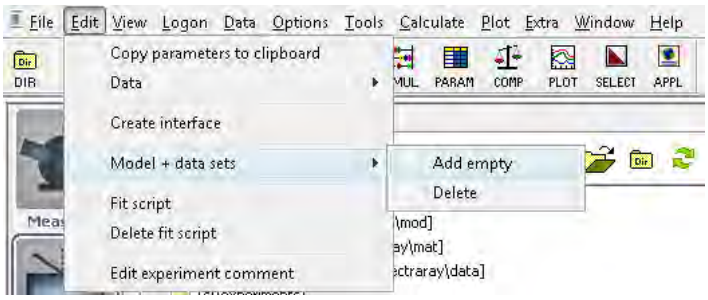


Fig. 8-78 Adding an empty experiment

On top of the model window two a second tab for the additional experiment appears. By selecting an experiment tab it can be switched between both experiments.

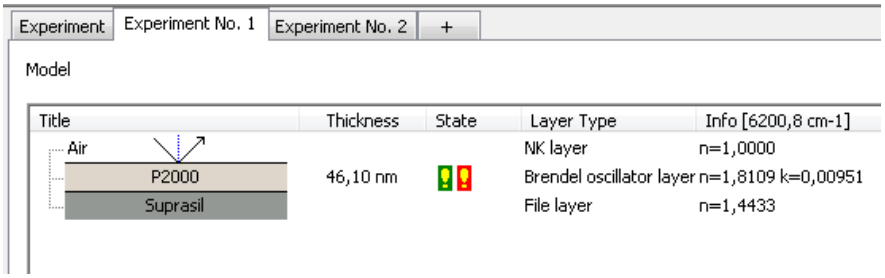


Fig. 8-79 Second experiment tab

The model for the second experiment is practically identical with some extensions. The model from the first experiment is copied to second one by:

- Selecting the first experiment
- Menu → Tools → Make equal models

Then the second experiment is selected. Air is copied below the “Suprasil” (e.g.: “CTRL” + moving Air with mouse cursor) and the correct substrate thickness is entered for suprasil.

8.7.2.4 Setting the environmental parameters for the second experiment

Then the incoherent calculation must be activated for the second experiment. Momentarily the environmental conditions are valid for all experiments. They are “global”.

This is switched off by “Menu → Options → General Options…”. The checkbox “Use global environment” has to be unchecked in the “Experiment options” tab.

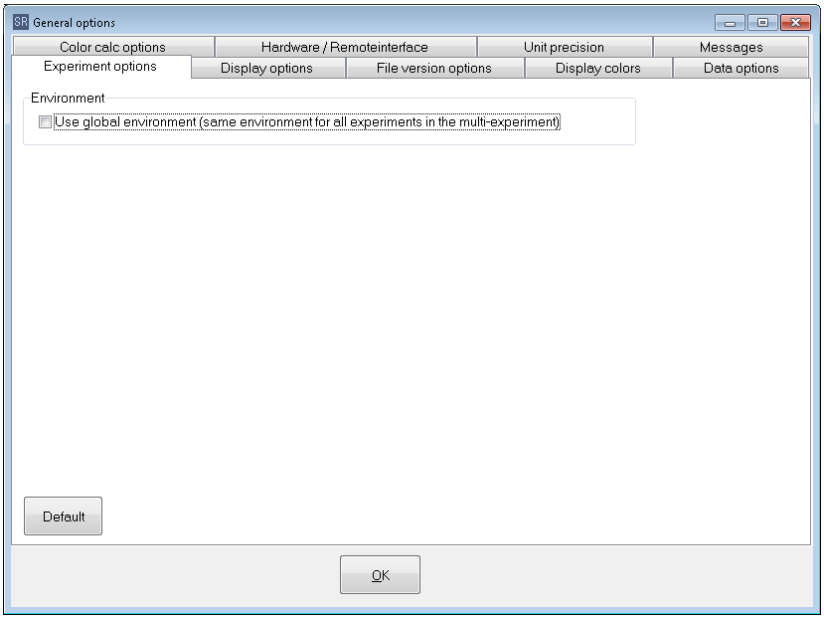


Fig. 8-80 Uncheck “Use global environment”

Now at least on backside reflection can be activated for the second experiment.

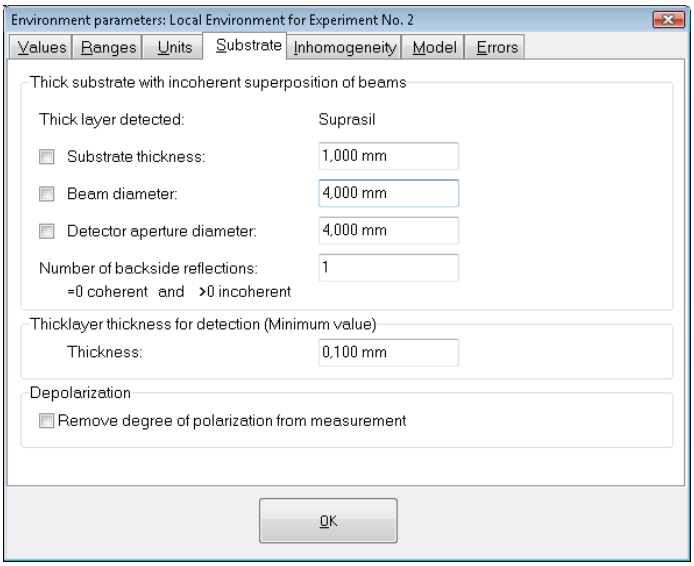
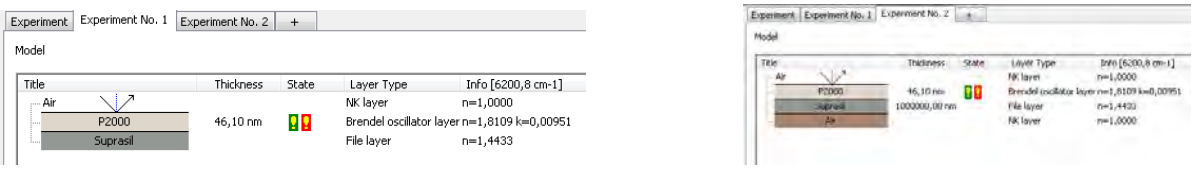


Fig. 8-81 “Substrate” settings in the environment of the second experiment

The transmission measurement is loaded into the dataset of the second experiment by Menu → File →Load (*.spc extension is selected).

The two experiments appear as shown in the screenshot:



All materials having the same name also have the same parameters with one exception: the film thickness is independent in both experiments. But the thickness also must be the same. Otherwise this combination doesn't overcome the ambiguity problems.

8.7.2.5 Creating the "fit script"

The thickness of both experiments is linked to each other using a fit script. The fit script will read out the film thickness of P2000 of the first experiment and will copy it to the second. The fit script needs to know the correct parameter name of the P2000 film thickness in both experiments. They are found in the parameter list (indicated by blue boxes:

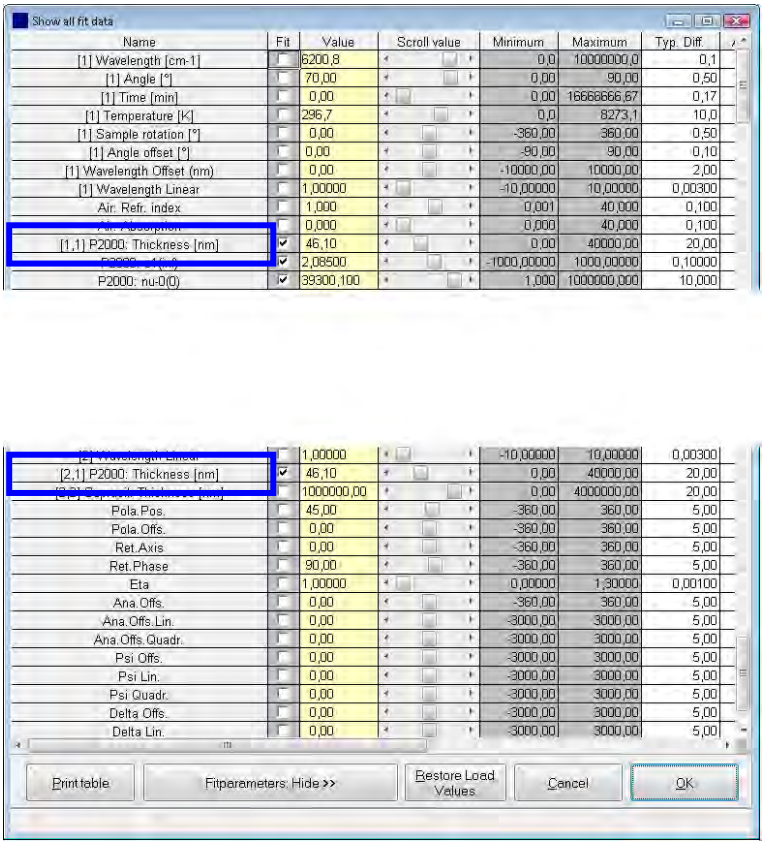


Fig. 8-82 Parameter list of both experiments

The fit script is now created by: Menu → Edit → Fit script …

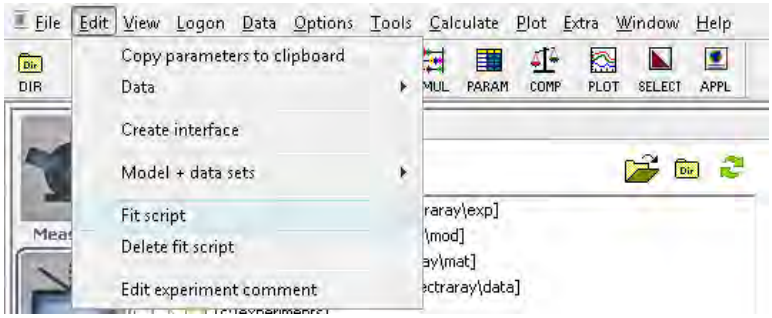


Fig. 8-83 Starting the script editor

A basic fit script is created. Momentarily this fit script has no effect. The fit script must be completed using the necessary commands inserting at the correct positions.

A variable for the thickness must be declared in the “Start:” section using the command:

```
double  dTh
string   sName,sUnit
integer iFitFlag,iDigits
```

The thickness is read out from the first experiment and copied to the second in the “BeforeCalcModel:” section:

```
SpectraRay.GetParameterAll 10 sName dTh iFitFlag iDigits sUnit
SpectraRay.SetParameter      46 dTh
```

In the parameter list below all fit parameters are listed for both experiments. Using “*SpectraRay.GetParameterAll*” you just have to add the index of parameter in the parameter list to get the values of the parameter. E.g. the thickness of the P2000 layer is at position 11, which means index 10 because the list starts with index 0.

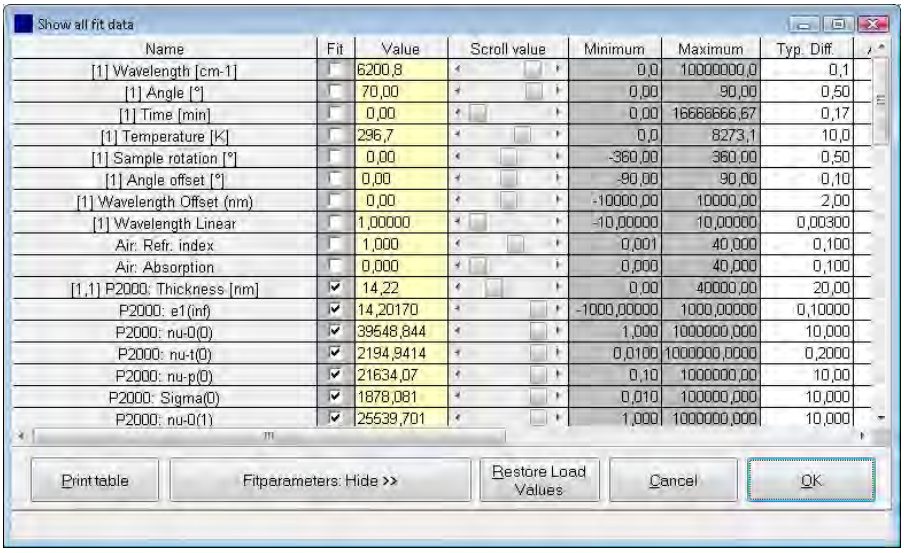


Fig. 8-84 Parameter list of the experiments

The fit script appears as follows:

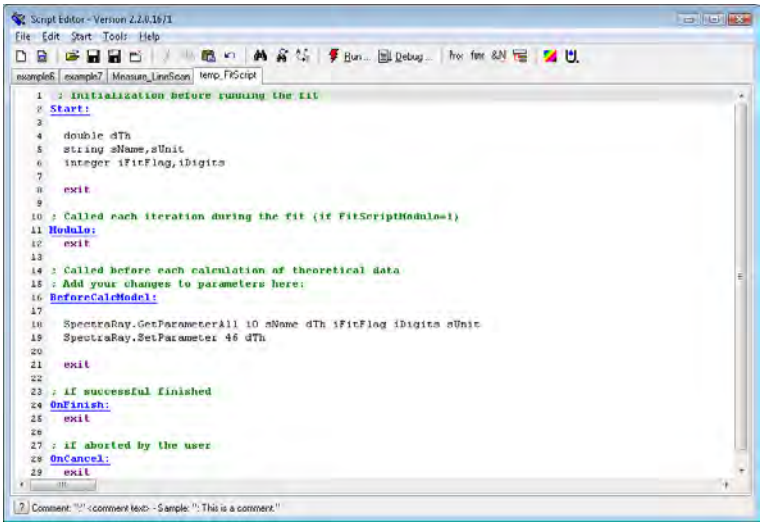


Fig. 8-85 Fit script

The fit script can be closed using “Quit”. It is not necessary to save it separately. It will be automatically saved within the actual experiment file.

8.7.2.6 Fitting the CET model

The range of values of the (Ψ, Δ)-measurement is 0 … 90° and 0 … 360° while transmission is only between 0…1. The will lead to a strong overestimation of the (Ψ, Δ)-measurement and the transmission measurement won’t have an effect.
Two ways are possible to overcome this problem:

1) The (Ψ, Δ)-measurement can be converted to the Fourier-coefficients (s1, s2). Their range is from -1…+1 and therefore very similar to the transmission range.

2) If this conversion is not wanted, then the weight of the (Ψ, Δ)-measurement for the MSE value of the fitting procedure must be reduced strongly.

This is done in the “Title” tab of the (Ψ, Δ) measurement. In this example it is reduced from 1 to 0.005.

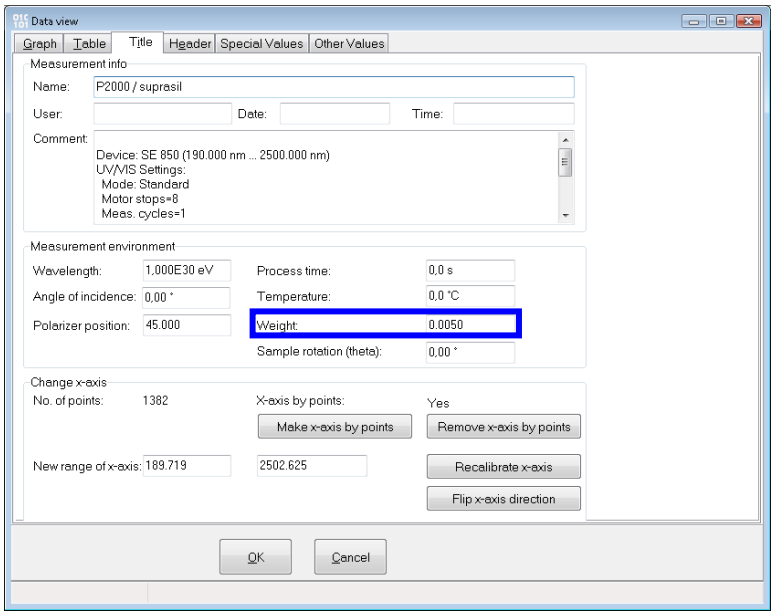


Fig. 8-86 Changing the weight of the (Ψ, Δ) measurement

When the fitting screen is opened then (Ψ, Δ) is displayed as usual. The transmission measurement is displayed in the Δ-window. It is hard to see it because it is just a straight line at zero and fitting quality can't be estimated.

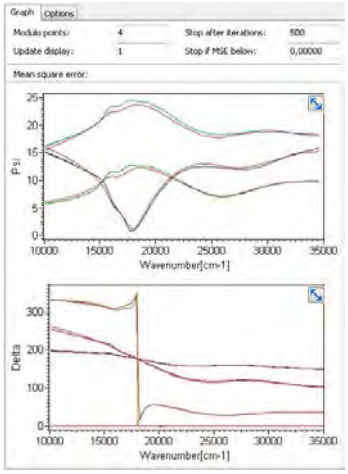


Fig. 8-87 (Ψ, Δ) and transmission measurement

In order to make Transmission visible the Δ-measurement can be hided from this display. This is done in the "Header" tab of the (Ψ, Δ)-measurement.

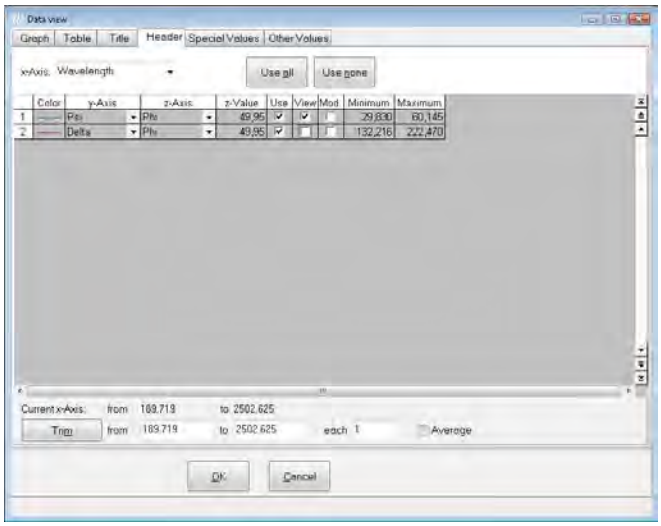


Fig. 8-88 Deselecting the “View”-column of Δ

The checkmarks in the “View” column for Δ are deselected. Now the Δ-measurement is not displayed anymore but it is still used for the fitting procedure.

The fitting procedure can be started now. The transmission measurement is now taken into account and will influence the results.

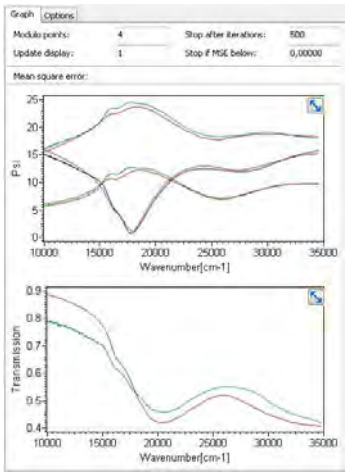


Fig. 8-89-8-90 Ψ and transmission measurement

8.7.3 Shifted Interval Fit + Parameterization with Tauc-Lorentz oscillator model

The task in this example is to measure a photoresist film on a silicon substrate. The film is transparent in the VIS spectral range. Here it can be described using a Cauchy dispersion formula. The film thickness and the dispersion of n are obtained.

In the UV it shows a complex extinction structure. Here the Tauc-Lorentz layer will be the optimal dispersion formula. Sometimes it appears difficult to find reasonable starting values to describe the extinction using the Tauc-Lorentz layer when the original (Ψ, Δ)-spectra are fitted, because interference fringes and structures due to structures in the dispersion of k are mixing up.

It is much easier to find these starting parameters, when they can be fitted to the dispersion of n and k of the film itself.

The "shifted interval fit" allows directly obtaining the dispersion of n and k of the film without applying a complex dispersion formula. Instead the spectral range is divided in small intervals. The refractive index n and extinction coefficient k are fitted separately in each interval. In the end the dispersion for the full spectral range is obtained.

The following example shows the analysis of the dispersion of n and k in the full spectral range using the "Shifted Interval fit" procedure.

This is followed by fitting the Tauc-Lorentz oscillator dispersion to the dispersion obtained from the interval fit.

8.7.3.1 Step 1) Determination of film thickness

It is necessary to know the film thickness of the photoresist accurately, because the film thickness wouldn't be a fit parameter during the "Shifted interval fit". This is necessary because in the absorbing spectral range the fit is less sensitive or even insensitive against the film thickness.

The film thickness of the photoresist film is analyzed first in the transparent part of the resist (spectral range: 450…920 nm). Multiple angle measurements are necessary. Here (Ψ, Δ)-measurements of 50, 60 and 70 deg are used.

A simple Cauchy model is applied to model the measurement.

Title	Thickness	State	Layer Type	Info [633,0 nm]
Air			NK layer	n=1,0000
Resist	112,84 nm		Cauchy layer	n=1,5882
Si DUV-UV-VIS-NIR			File layer	n=3,8736 k=0,01455

Set the used spectral range to 450 nm to 920 nm.

The fit parameters of the resist film are the film thickness and the Cauchy coefficients N0, N1, N2.

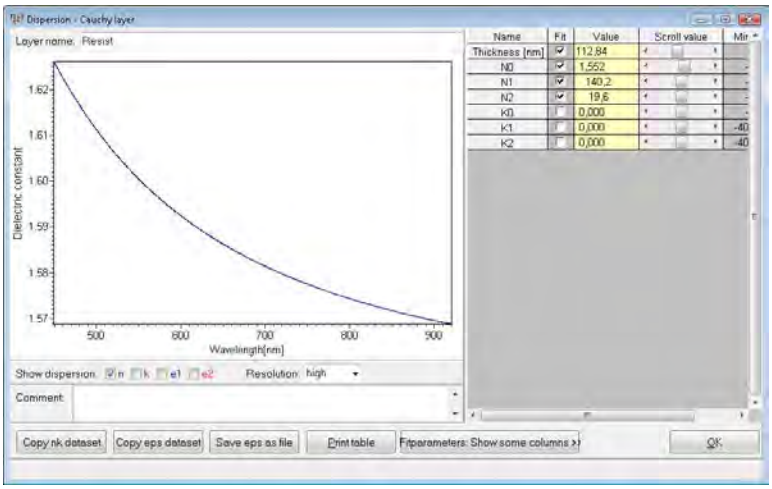


Fig. 8-91 Cauchy model of the resist film

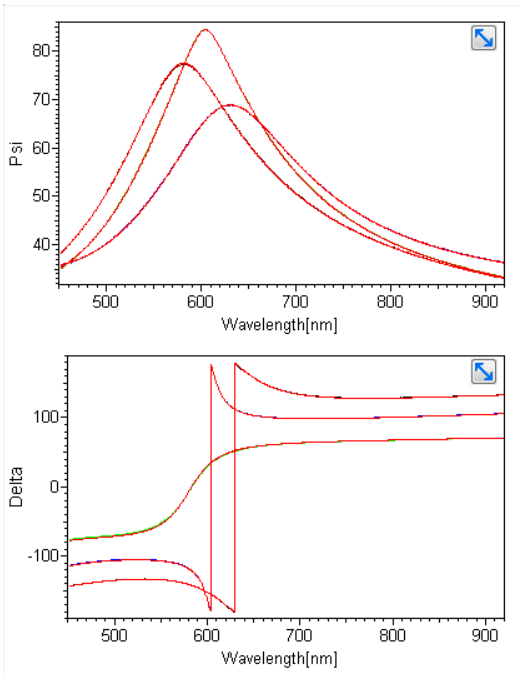


Fig. 8-92 The measurement and model after fitting

The model shows an ideal fit to the measurement. A film thickness of 112.8 nm is obtained.

8.7.3.2 Step 2) Setup of the model for the “Shifted interval fit”

The film thickness must be kept in mind. The Cauchy layer is removed. At its position a “Fixed refractive index and absorption”, also called “N,K layer” layer is inserted. Press the “New” icon from the icon bar. The “Create new material” window is opened.

Select the “NK layer” type and Press “ok”.

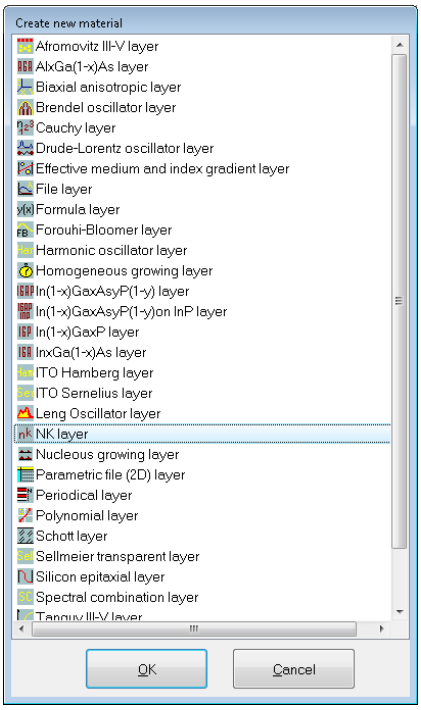


Fig. 8-93 “Create new material” window

Double click the “NK layer” layer. The “NK layer” window is opened. Enter the film thickness obtained from the former modeling (Here: th = 112.84 nm). Select n and k as fit parameter. Set a starting value for n of n=1.6.

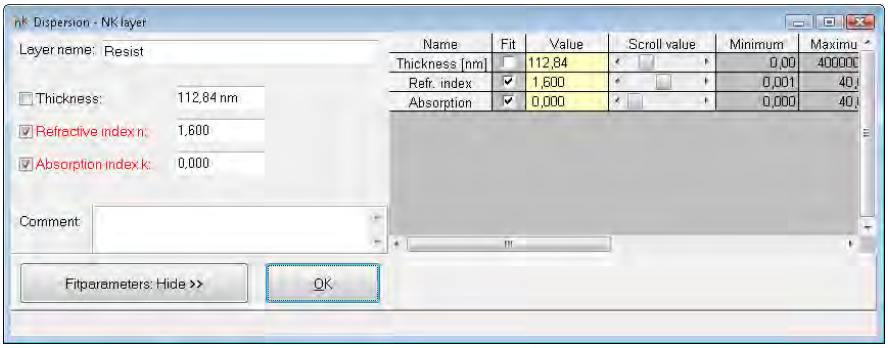
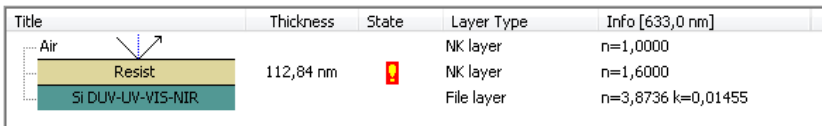


Fig. 8-94 “NK layer” window

Press “Ok”. The layer is inserted now into the model. Move it to the correct position. The model appears now as follows:



8.7.3.3 Step 3) “Shifted interval fit”

The used spectral range is set to 240 nm to 920 nm. The fitting window is opened now.

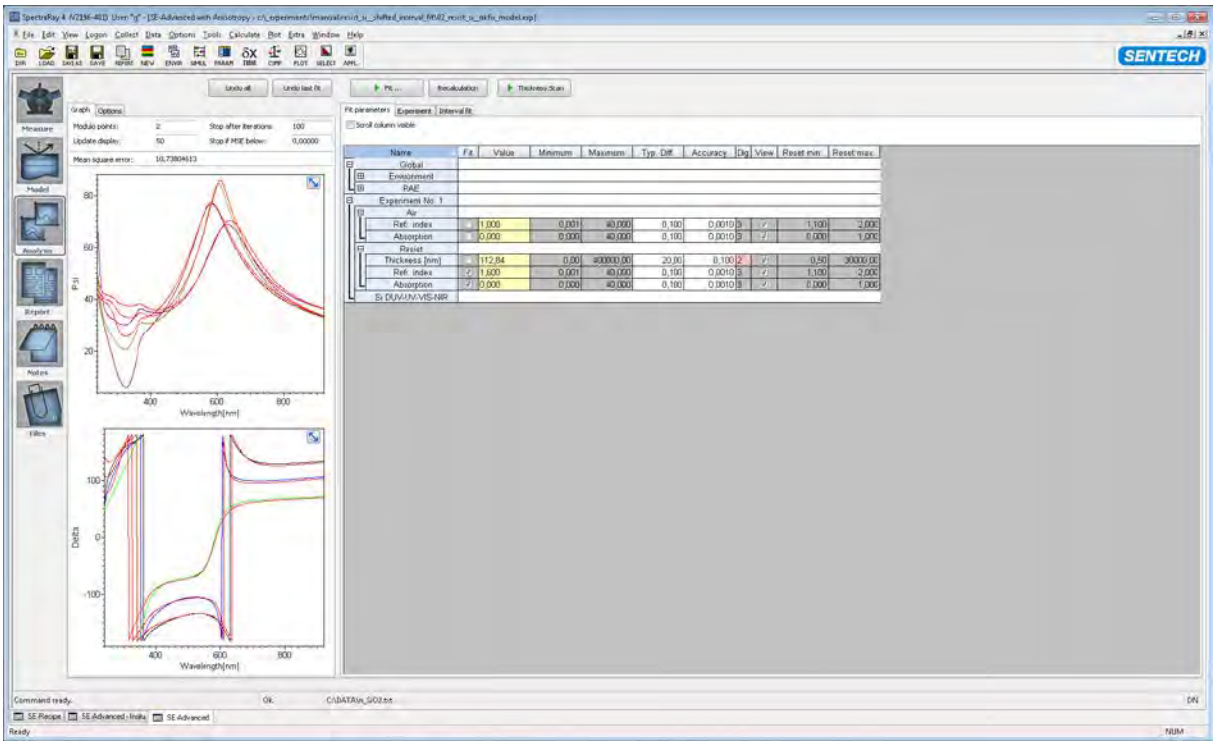


Fig. 8-95 Measurement and model with new model with “N,K layer”. The model fits well in the VIS. The UV shows deviations because the absorption of the resist is not described in the model

Select the “Interval Fit …” frame on the right side. The “Shifted Interval Fit” window is shown. Select the following settings:

x-axis: wavelength (nm)

from: 920 nm (the scan is done from the highest wavelength, because the starting values of the model are correct here, because they are known from the former modeling. In the UV they are unknown momentarily, so starting at 240 might lead to a wrong solution)

to: 240 nm

step: 5.0 nm (the step size for the intervals. It should be sufficiently narrow in order not to skip any structures in the spectrum)

width: 5 nm (width of the fitted interval. It should be sufficiently narrow in order not to average the structures in the spectrum)

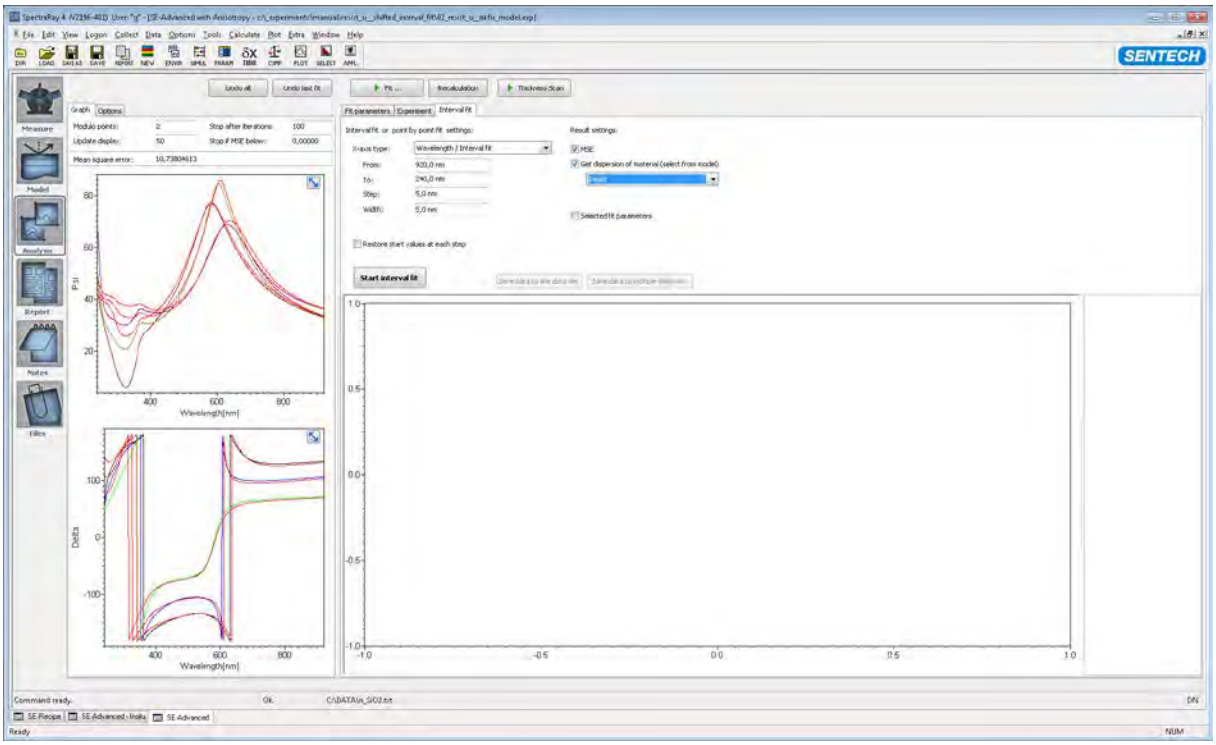


Fig. 8-96 “Shifted interval fit” window

The “Start interval fit” button is pressed to initiate the fitting procedure. The fit is now done step by step. The fitting window shows the progress for each interval. The results are stored in the results window. When the shifted interval fitting procedure is finished the results are shown in the graph. The dispersion of n and k as well as the MSE value are displayed.

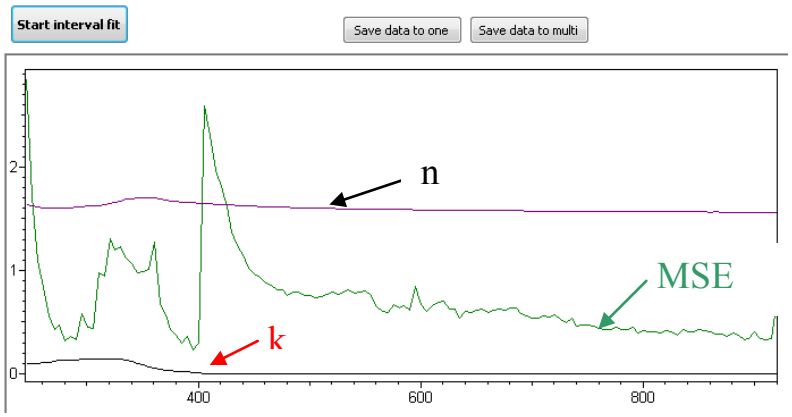
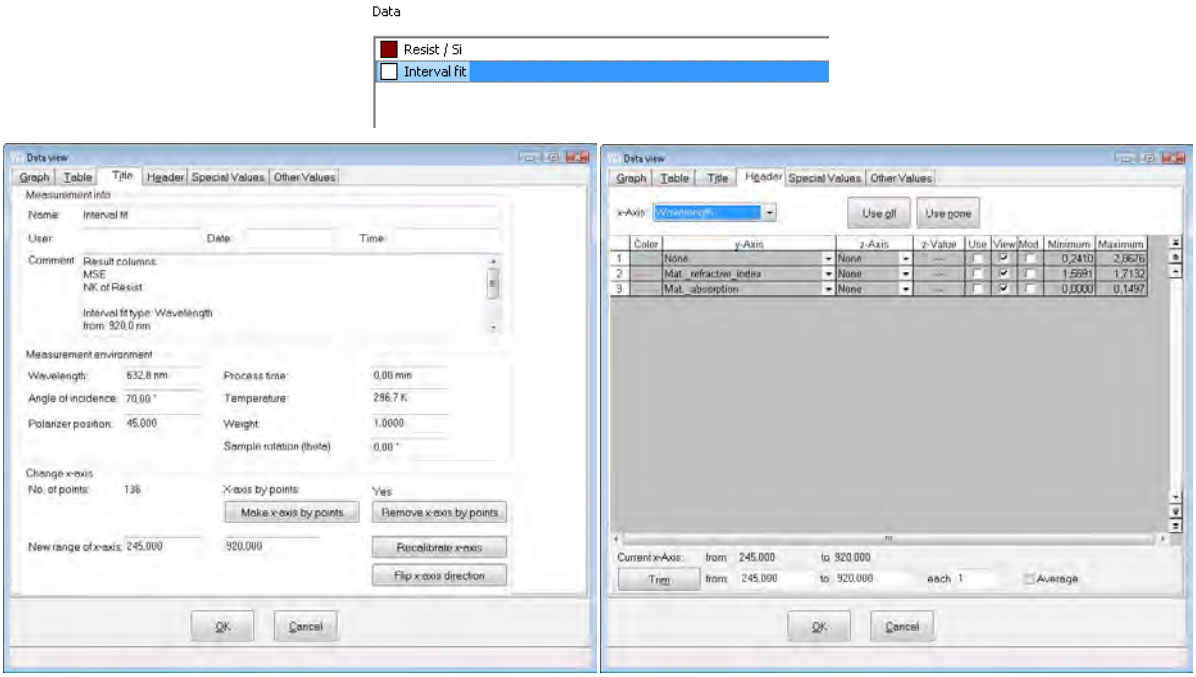
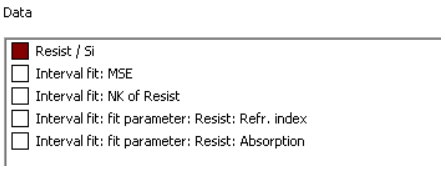


Fig. 8-97 “Shifted Interval Fit” results

The results of the fitting procedure can be saved now by pressing the “Save data to one data set” or “Save data to multiple data sets” icon. In case you click on “Save data to one data set” all fitting results are saved into one data set:

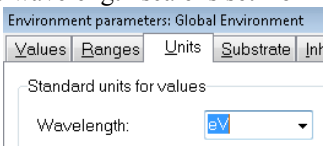


In case you click on “Save data to multiple data sets” each fitting result is saved into one data set:

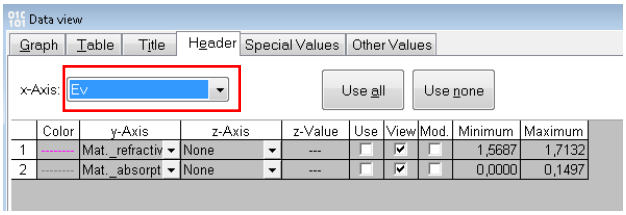


8.7.3.4 Step 4) Applying Tauc-Lorentz layer to the fitted dispersion

A new experiment is created. The wavelength scale is set from wavelength to photon energy (eV).



Select the NK data set “Interval fit: NK of Resist” and convert the x-Axis from wavelength scale to “eV” (photon energy).



8.7.3.5 Step 5) Modeling

A model with ambient “Air” and a new “Tauc-Lorentz” layer is created. The Tauc-Lorentz Layer is renamed to “Resist – TL”.

The next step is to find starting values for the Tauc-Lorentz oscillator.

The result of the “shifted interval fit” is investigated. The absorption (bandgap Eg) is located at 3.0 eV. The structure doesn’t appear like a single oscillator. Instead it seems, that one oscillator is located around 3.0 to 4.0 eV. A second one is outside the measured spectral range at higher energies than 5.0 eV.

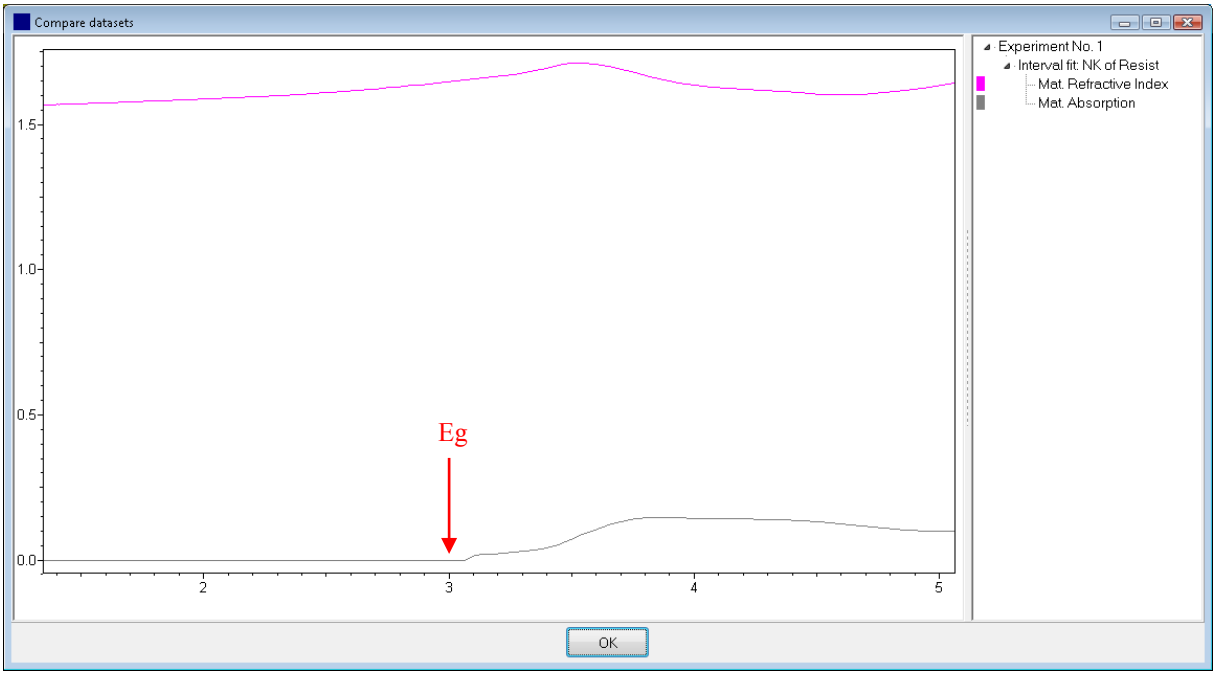


Fig. 8-98 Resulting n and k

The following two oscillators are build up using the Tauc/Lorentz oscillator model:

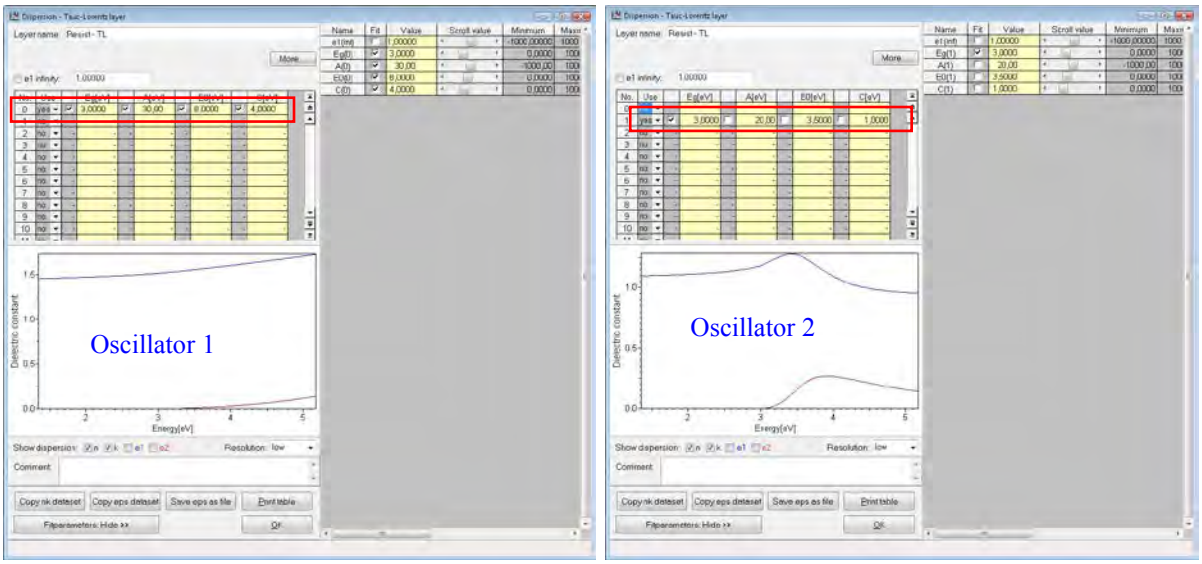


Fig. 8-99 Tauc/Lorentz Oscillators

The combination of both oscillators is already quite similar to the “shifted interval fit” results:

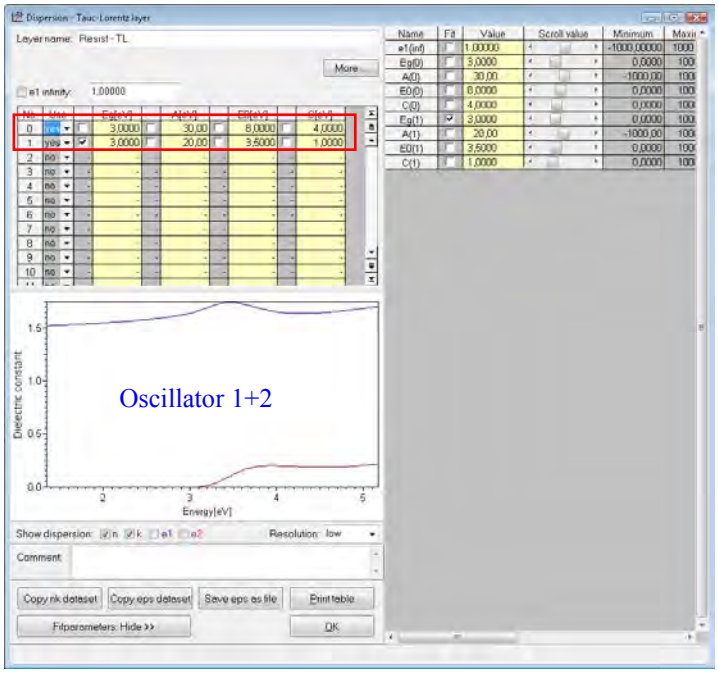


Fig. 8-100 Combination of both oscillators

8.7.3.6 Step 6) Fitting the Tauc-Lorentz layer (Oscillator 1 +2) to the “shifted interval fit” results

When the start parameters were found the “typical differences” are set to reasonable values to ensure a good fit progress. Select in the “Resist - TL” Tauc-Lorentz oscillator window the typical differences as shown in the screenshot:

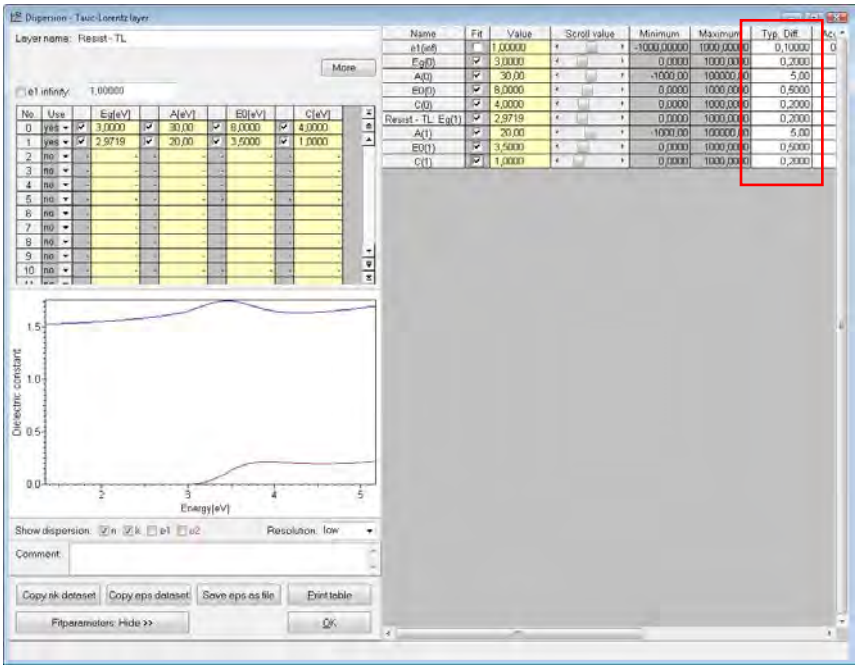


Fig. 8-101 “Typical Differences”

The window can be closed and the fitting window is opened and the fit procedure is initiated. After the fitting, there are still some deviations visible, which are indicated by the red arrows.

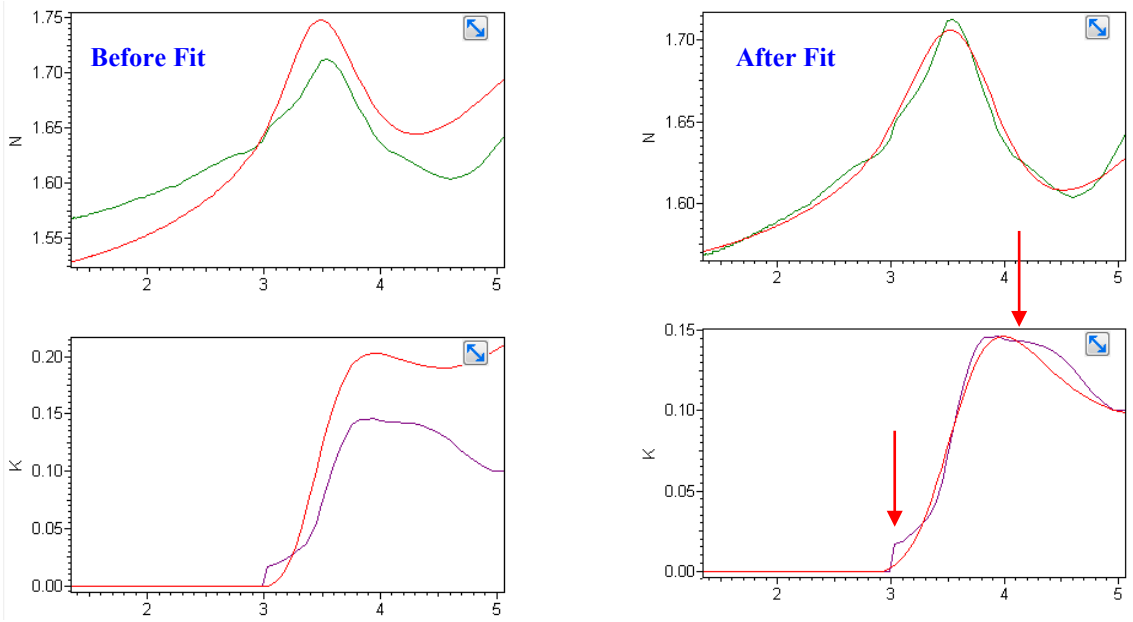


Fig. 8-102 Fit result

The deviation around 3.0 eV is likely an artifact by the “shifted interval fit procedure”. It will be neglected. The structure at 4.0 eV seems to be an additional oscillator.

8.7.3.7 Step 7) Introduction of a third oscillator into the Tauc-Lorentz layer at around 4.0 eV

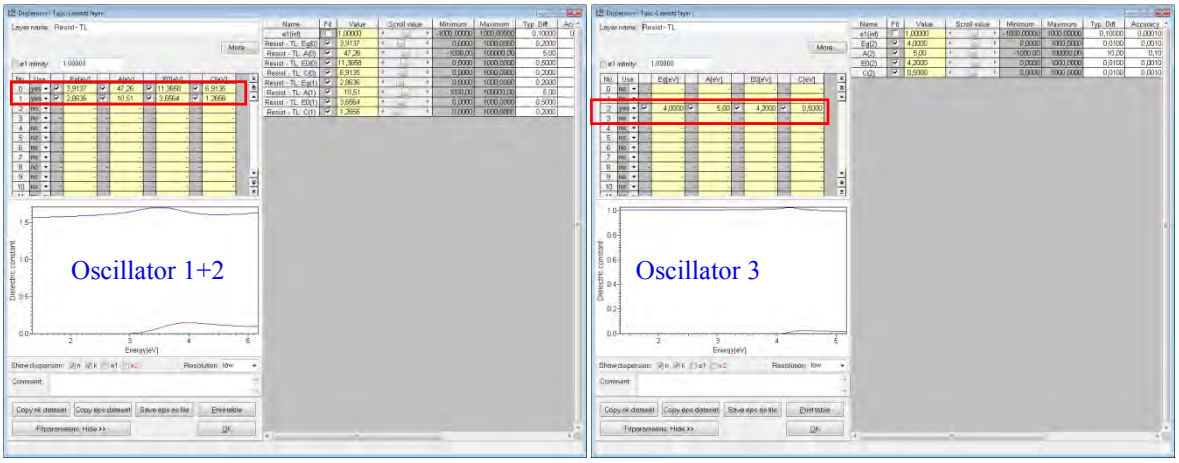


Fig. 8-103-8-104 Another Tauc/Lorentz Oscillator

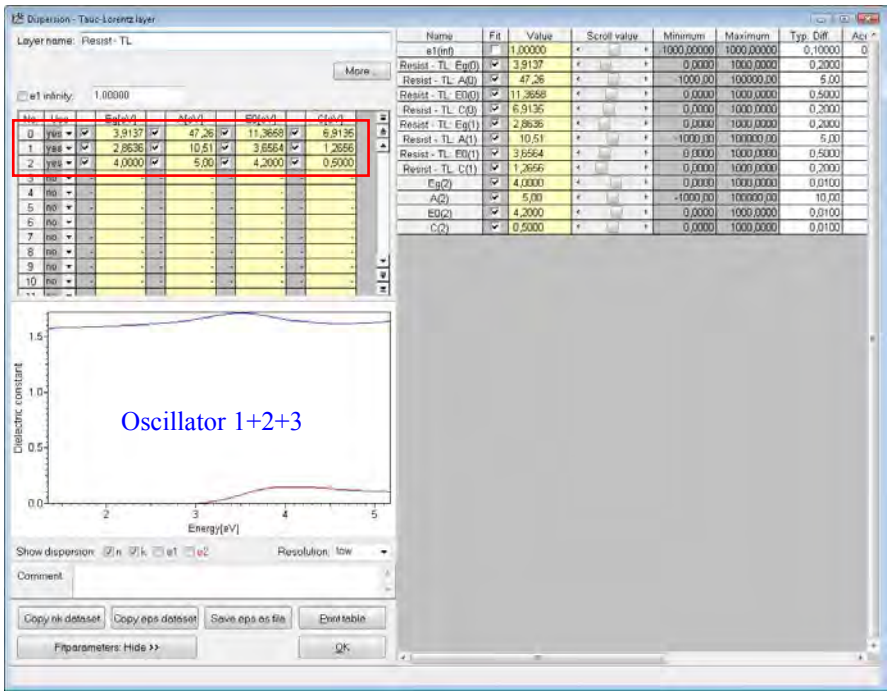


Fig. 8-105 Combination of all three oscillators

8.7.3.8 Step 8) Fitting the Tauc-Lorentz layer (Oscillator 1+2+3) to the “shifted interval fit” results

When the start parameters were found the “typical differences” for oscillator 3 are set to reasonable values to ensure a good fit progress. Select in the “Resist - TL” Tauc-Lorentz oscillator window the typical differences as shown in the screenshot:

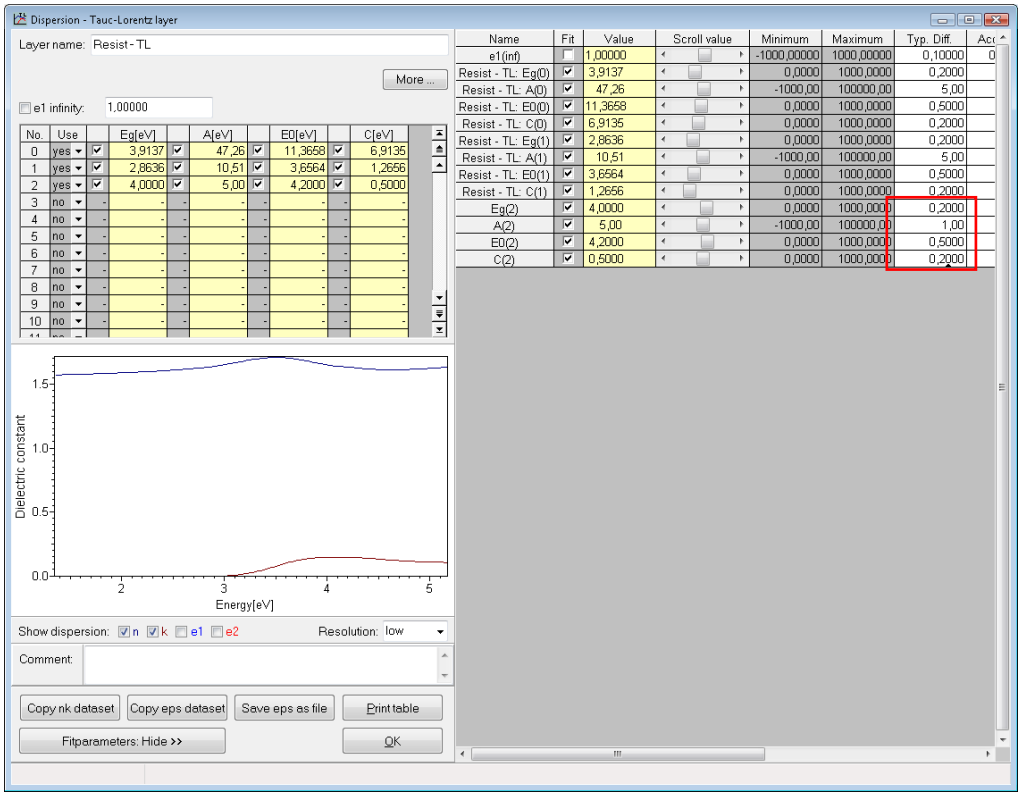


Fig. 8-106 “Typical Differences” for the third oscillator

The structure at 4.2 eV is now described well by the model.

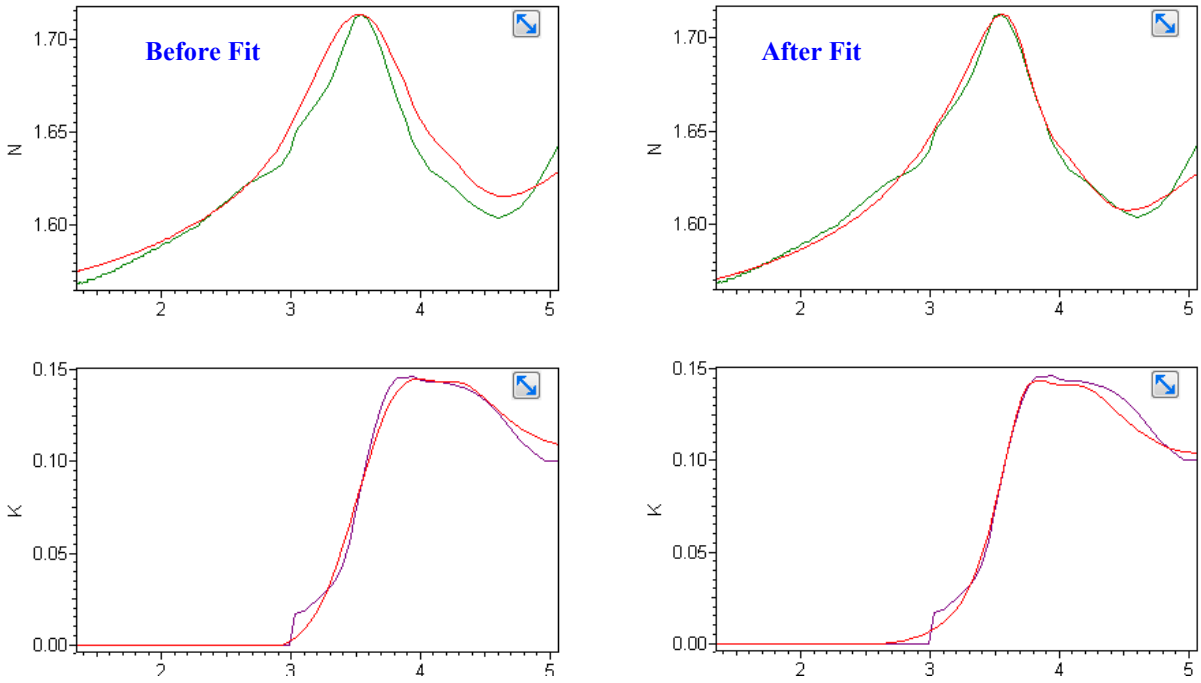
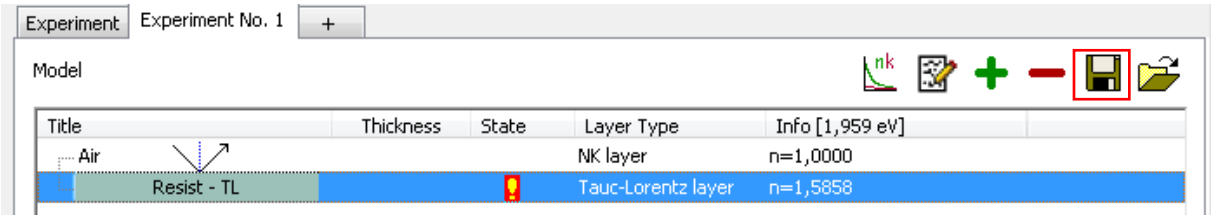
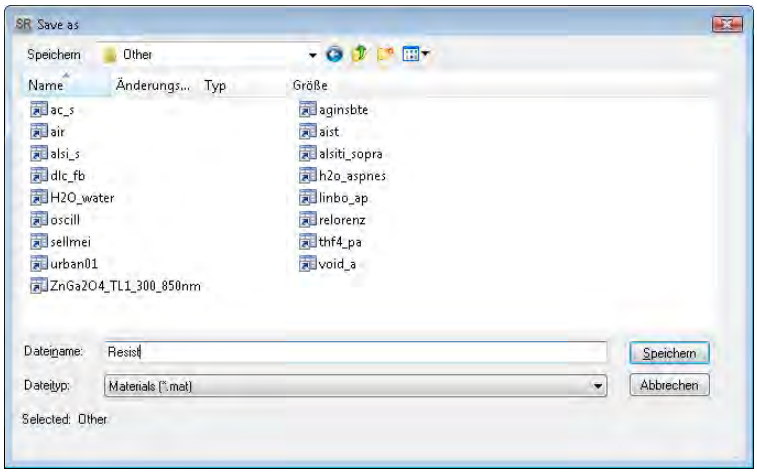


Fig. 8-107 Fitting results for three oscillators

The Tauc-Lorentz layer is now saved as a new material to the material library. Select the Tauc-Lorentz layer in the model section that it appears inverted and press the “Save” button.

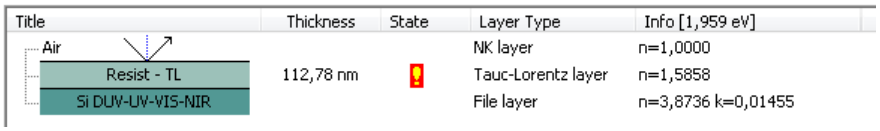




The layer is saved in “c:\Sentech\SpectraRay\Mat\Other” directory using the filename “Resist.mat”. When it is saved the material library is updated and the new material is available.

8.7.3.9 Step 9) Fitting the Tauc-Lorentz layer (Oscillator 1+2+3) to the Ψ, Δ measurement results

The initial experiment is loaded which contains the Cauchy-Model and the original (Ψ, Δ)-measurements. The Cauchy layer is replaced by the Tauc-Lorentz layer from the material library.



The spectral range is set to 240 nm to 920 nm. Then the wavelength scale is set from wavelength to photon energy (eV).

The fitting window is opened and the fit procedure is initiated.

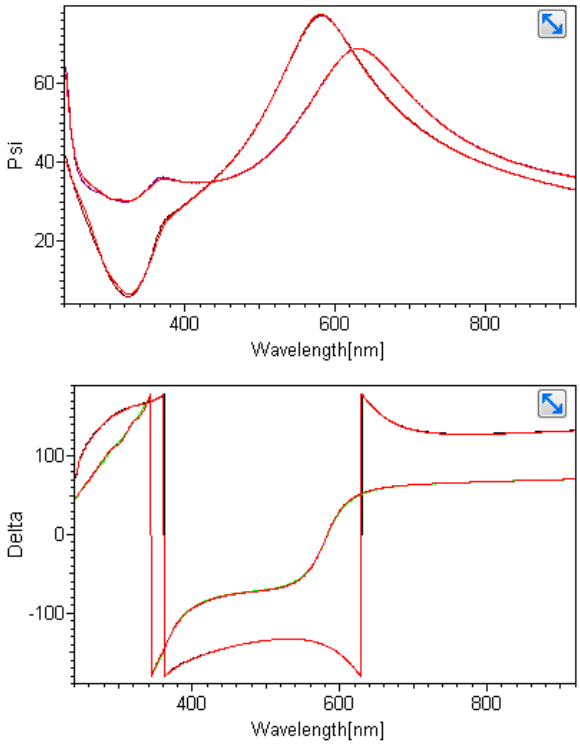


Fig. 8-108 Fitting result for the (Ψ, Δ)-spectrum

The model fits the measurement well. The final dispersion of the Resist film is shown in the following screenshot:

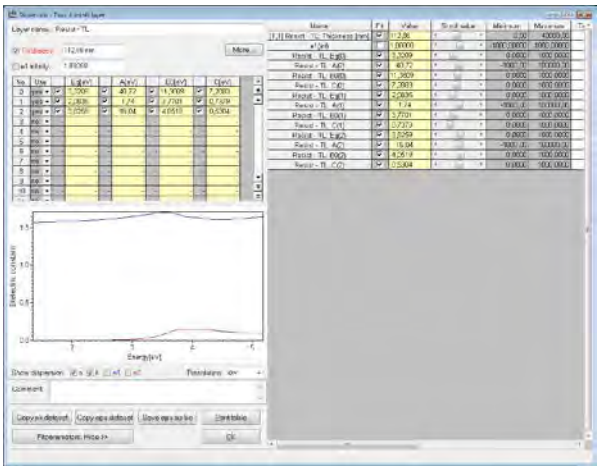


Fig. 8-109 Final dispersion

8.7.4 Anisotropic substrates

$CaCO_3$ is an uniaxial anisotropic material. A bulk $CaCO_3$ crystal is cut, so the optical axis is parallel to the sample surface plane. The measurements are performed to measure the in-plane orientation of the optical axis.

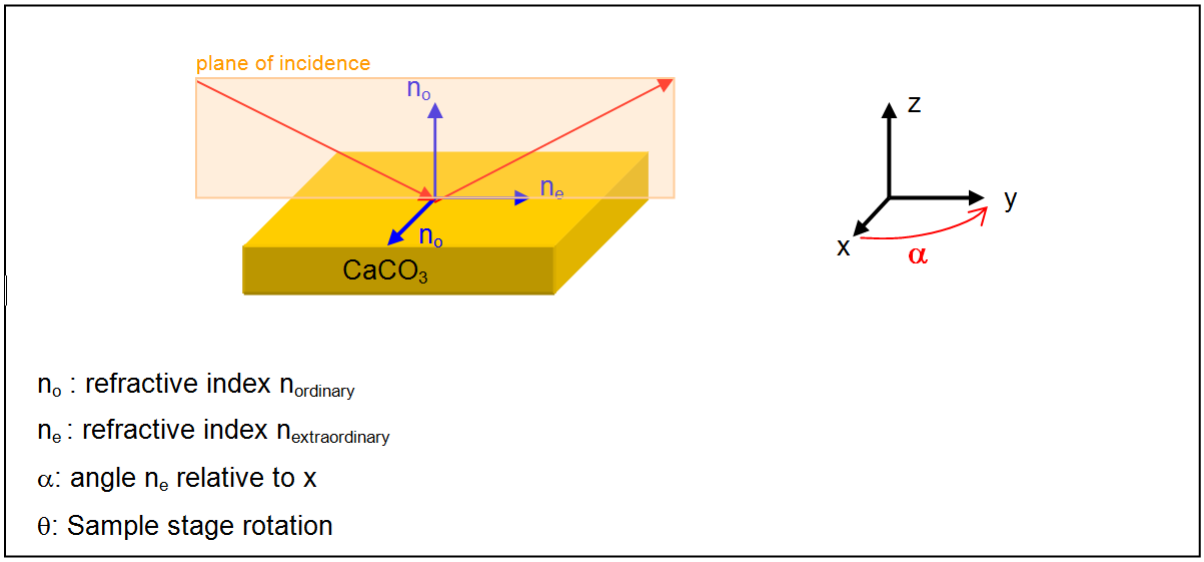


Fig. 8-110 Anisotropic sample and coordinate system

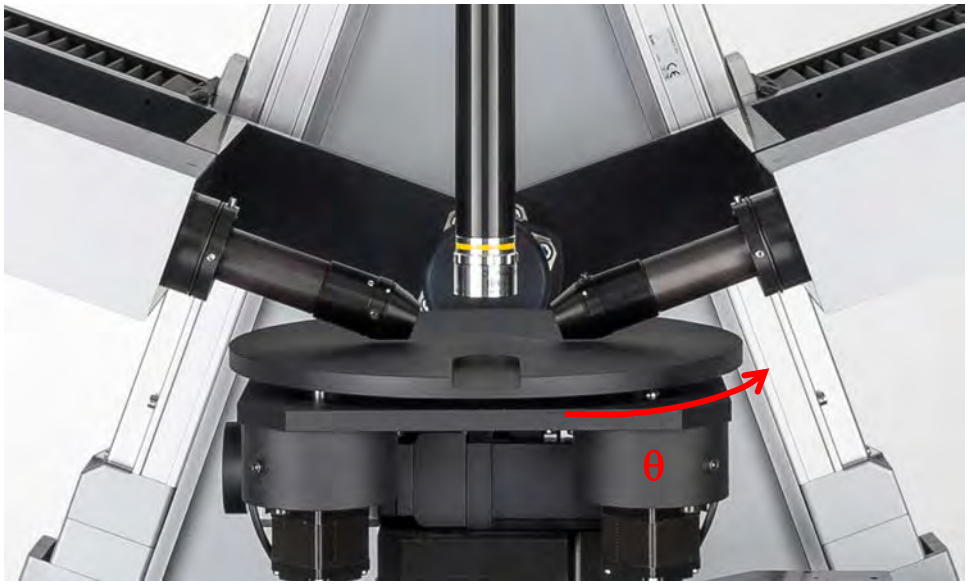
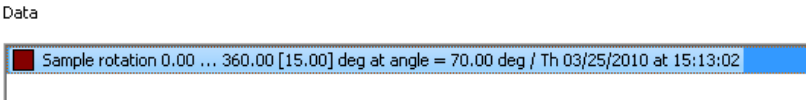


Fig. 8-111 Sample on rotatable sample stage

The rotatable sample stage is used to acquire different ellipsometric spectra for different sample rotation angles θ. The measurements were repeated for different angles of incidence φ.

The rotation conditions of the rotatable stage are added to the standard measurement dialog for spectroscopic measurements. The stage is rotated from θ = 0° to 360° every 15°. These results in a set of measurements are added as a single dataset to the data section of SpectraRay.



The tab “Header” shows the individual spectra for each angle θ.

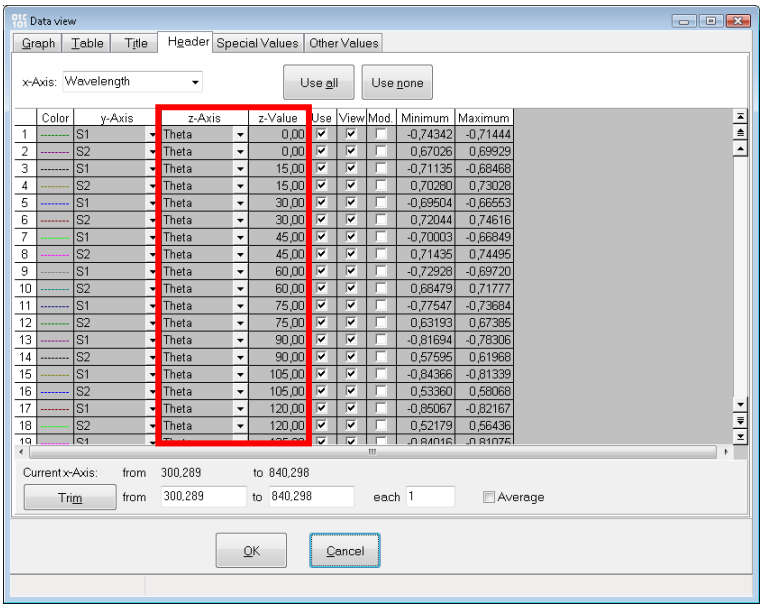


Fig. 8-112 Header-tab of the measured data

The angle of incidence is shown in the tab “Title”.

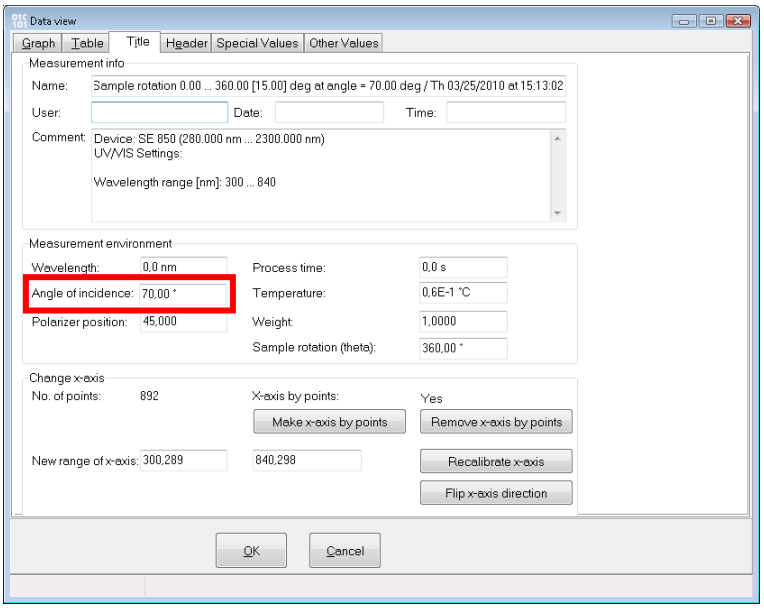


Fig. 8-113 The “Title” tab shows the angle of incidence

The Tab “Graph” section shows all measurements:

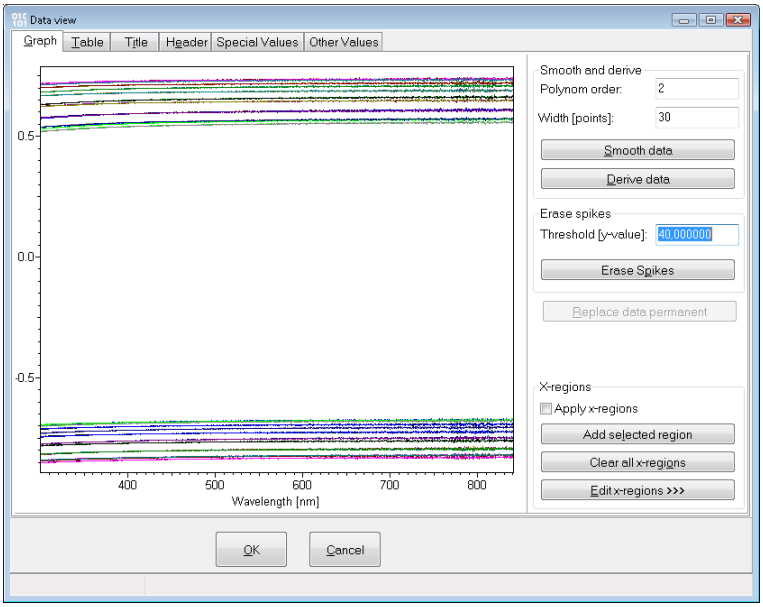


Fig. 8-114 Graph of the measured data

The different spectra taken at different sample rotation angles θ show distinct deviations as a result of the anisotropy of the $CaCO_3$ substrate. The spectra show a parallel shift to each other, so the observation at a single wavelength instead of the full spectra will be sufficient. Now the s1, s2 values for e.g. 632.8 nm (any other wavelength is possible as well) as a function of the sample rotation angle θ are extracted from these spectroscopic measurements.

This is done by using the “Trim” function which can be found in the Tab “Header” section. The same wavelength value 632.8 is selected for both “min.” and “max.” numerical entry boxes.

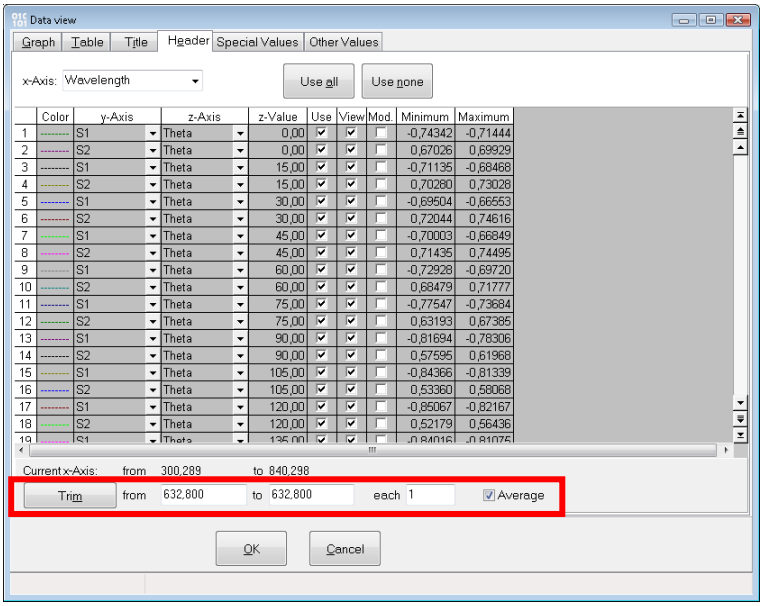


Fig. 8-115 Trimming the measured data

The results will be given for the wavelength which is closest to the selected value which will be rounded to 632.9 nm in this example.

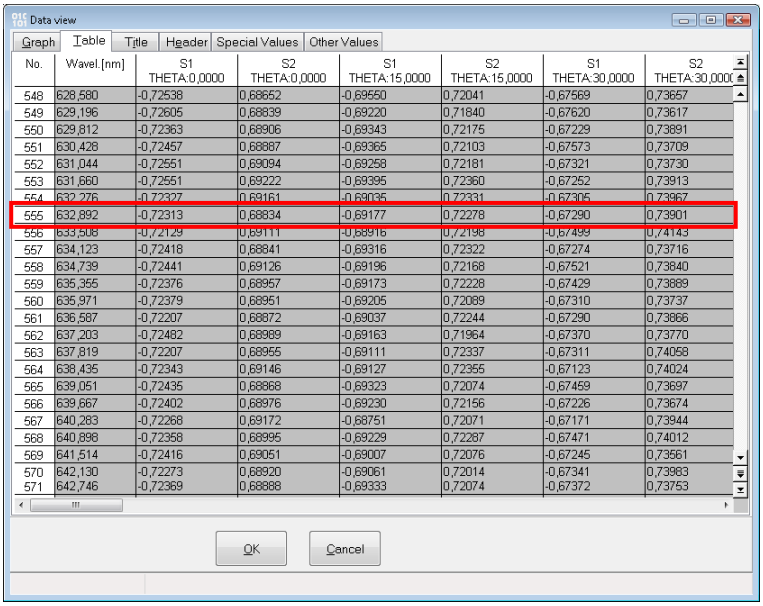
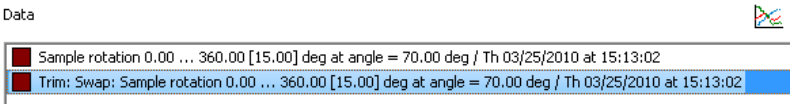


Fig. 8-116 Wavelength closest to the selected value

When “Trim” is pressed a new dataset is created containing s1, s2 at 632.9 nm as a function of the rotation angle θ indicated by “Swap” in the name of the dataset.



The units were changed now. The x-axis is changed to “theta” and the “z-axis” becomes the wavelength in nm.

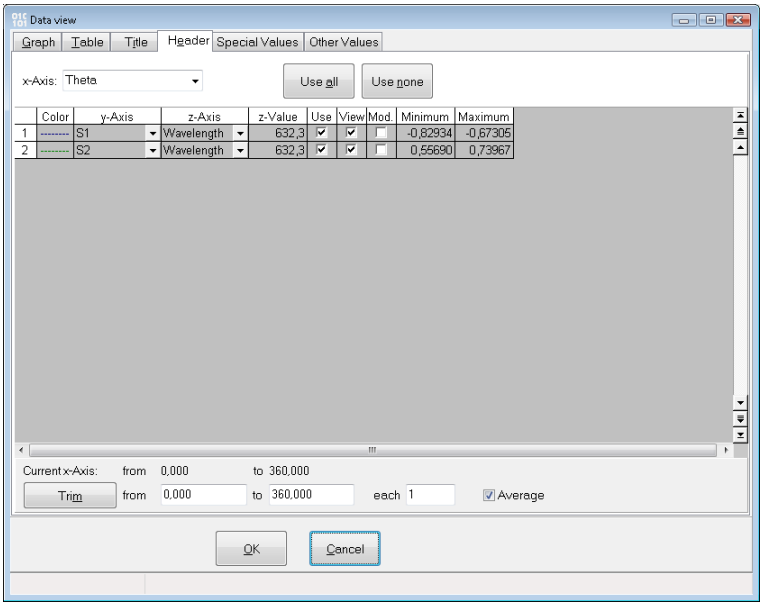
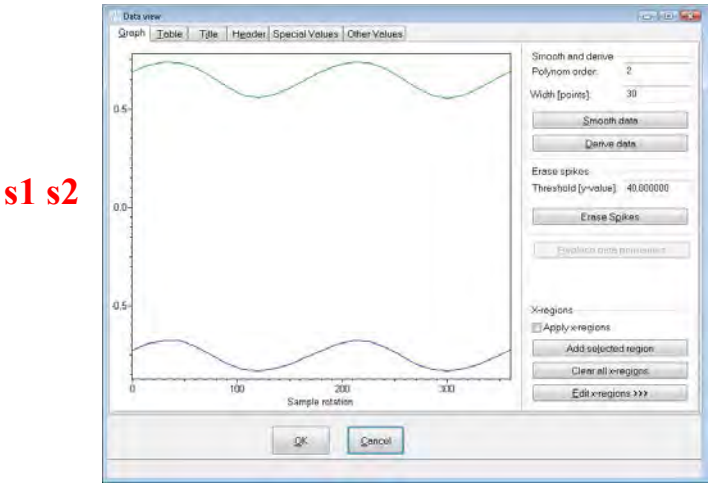
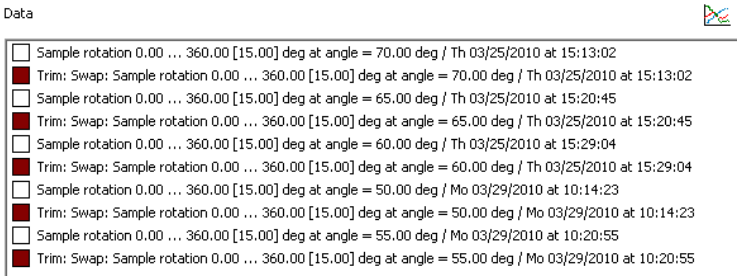


Fig. 8-117 New axis for the trimmed data



These measurements are now performed between φ=50° and 70° (steps: 5°) angle of incidence.



The spectra are shown in the following plot.

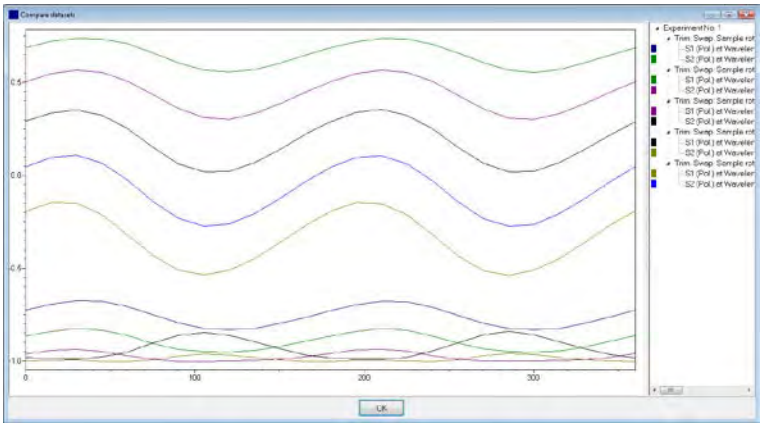


Fig. 8-118 (s1, s2) in dependence of θ for different angles of incidence

Modeling of $CaCO_3$:

The anisotropic sample is described using the biaxial anisotropic layer. Due to the fact that $CaCO_3$ is uniaxial anisotropic two of the three axes must have the same dispersion.

$CaCO_3$ is transparent and has no dispersion when a single wavelength is observed only like in this case. Then its dispersion for each crystallographic direction can be described using n, k fix (n fit only) or a Cauchy dispersion using "N0" as the only fitting parameter. The final model appears as follows (Cauchy is used here):

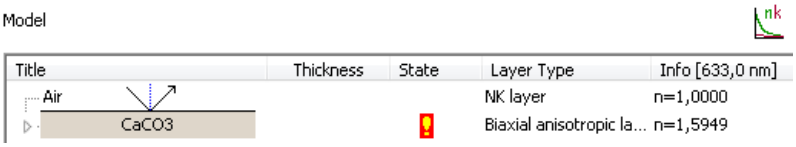


Fig. 8-119-8-120 Model for $CaCO_3$

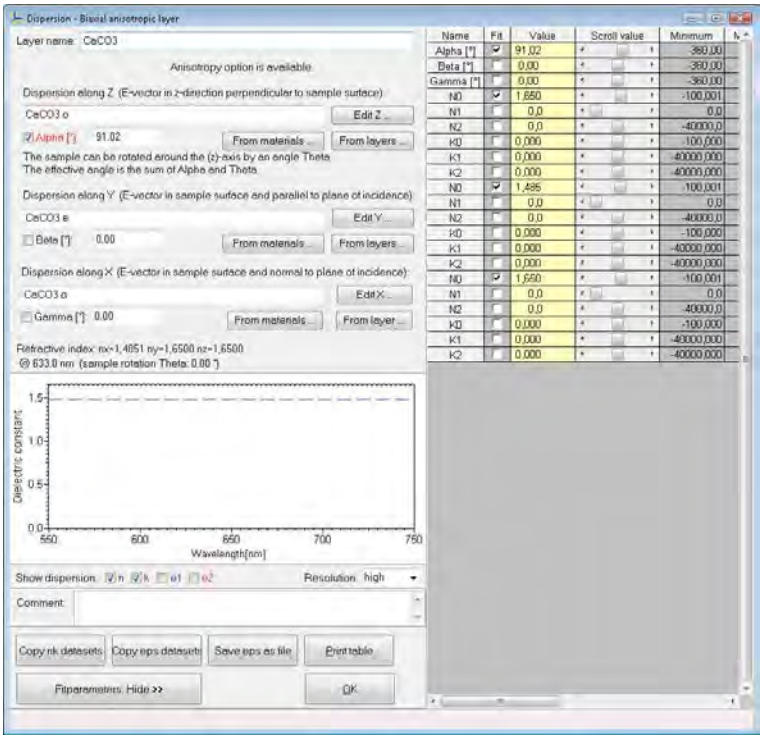


Fig. 8-121 Biaxial anisotropic layer for a uniaxial $CaCO_3$ with c-axis in surface plane. The rotation angle α is the used as fit parameter. (Here the result is already shown)

Fig. 8-122 $CaCO_3$ optical constants described by Cauchy layer with no dispersion.
"N1", "N2" and all k parameter are equal to zero.

The following graph shows the fit window of the SE-Advanced client for the correct rotation angle of the sample of α=91°.

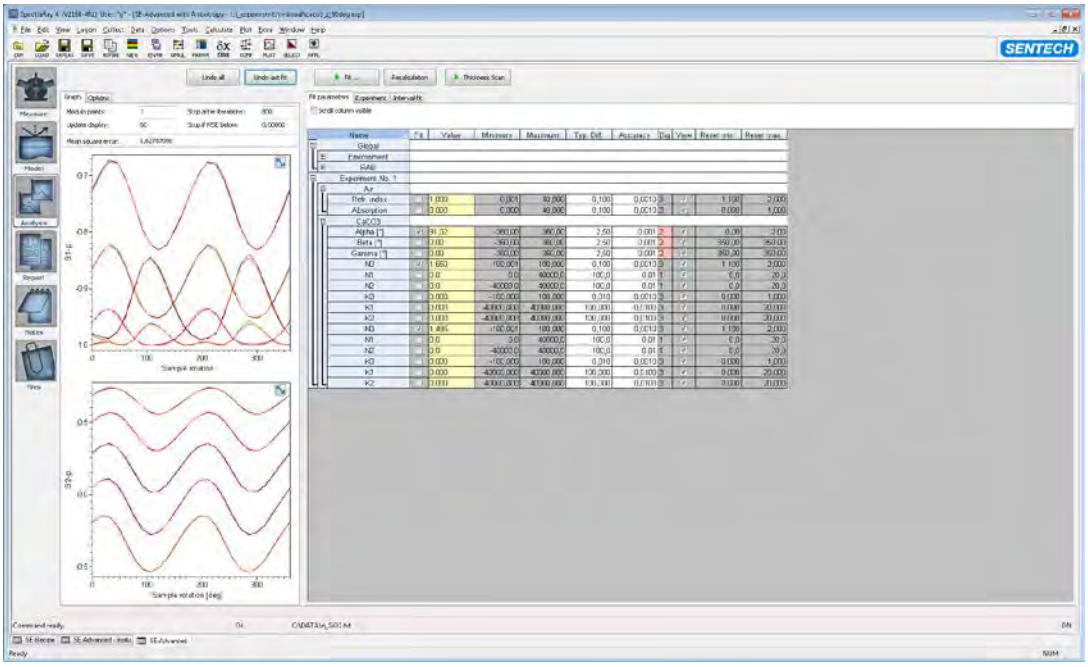


Fig. 8-123 Fit results

For comparison a rotation angle of 10 degrees less (α=81°) is shown. It can be seen, that the structures are shifted by 10 degrees. So the information of the rotation is included in the phase of the sinusoidal structure.

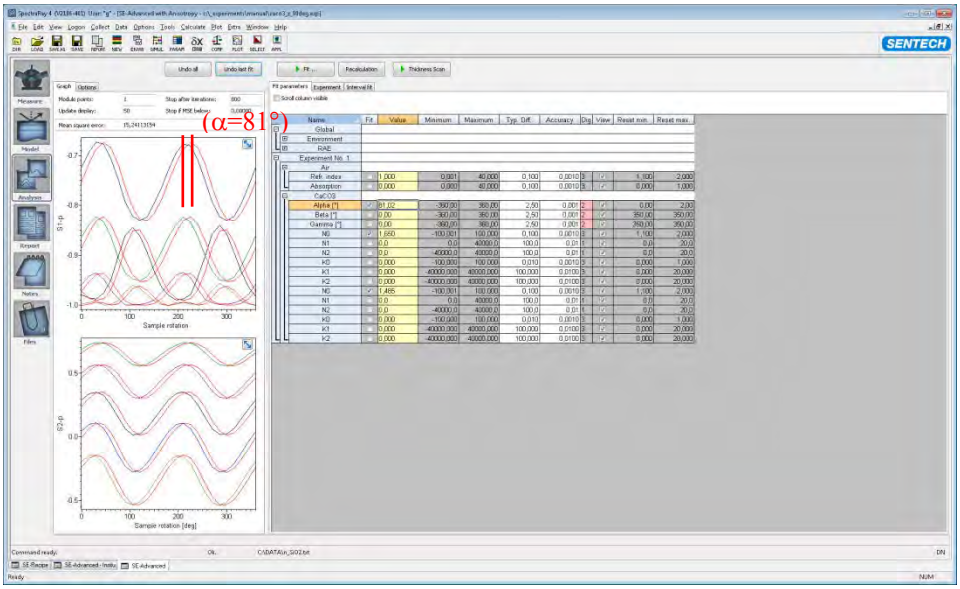
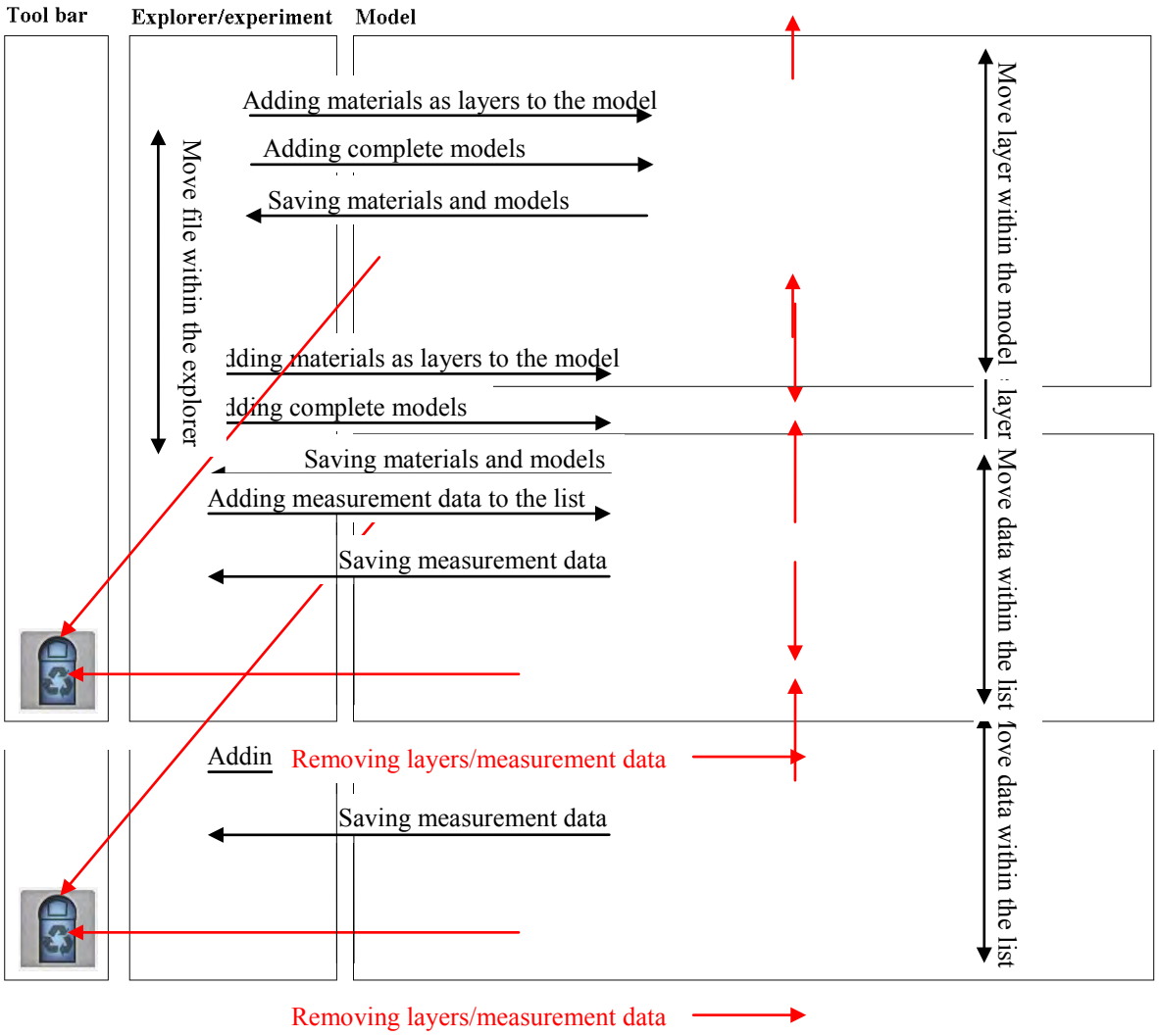


Fig. 8-124 Results for a wrong rotation angle

Appendix A: Drag&Drop Overview

SpectraRay has rich built in drag&drop features for model design and data setup. The following sketch describes the drag&drop path and associated functions:



Appendix B: Icon reference

Layer types:

 Afromovitz III-V layer
 Biaxial anisotropic layer
 Cauchy layer
 Effective medium and index gradient layer
 Formula layer
 Harmonic oscillator layer
 In(1-x)GaxAsyP(1-y) layer
 In(1-x)GaxP layer
 ITO Hamberg layer
 Leng oscillator layer
 Nucleus growing layer
 Periodical layer
 Schott layer
 Silicon epitaxial layer
 Tanguy III-V layer
 Uniaxial anisotropic layer

 AlxGa(1-x)As layer
 Brendel oscillator layer
 Drude-Lorentz oscillator layer
 File layer
 Forouhi-Bloomer layer
 Homogeneous growing layer
 In(1-x)GaxAsyP(1-y)on InP layer
 InxGa(1-x)As layer
 Ito Sernelius layer
 NK layer
 Parametric file (2D) layer
 Polynomial layer
 Sellmeier transparent layer
 Spectral combination layer
 Tauc-Lorentz layer

Icon bar functions:

 Directories for materials and data
 Save and export (*exp, *.csv,...)
 Open report window
 Edit environment
 Fit parameter list
 Plot with current experiment
 Open application window

 Load and import (*.spc, *.exp,...)
 Save the actual experiment
 Create new material
 Simulation
 Compare selected data
 Select data columns

Data selections:

 all columns selected
 no column selected

 some columns selected

Appendix C: Parameters and supported units

Parameter type	Units
thickness	“Å”, “nm”, “µm”, “mm”, “inch”
wavelength	“Å”, “nm”, “µm”, “mm”, “eV”, “cm-1”
growth rate	“Å/s”, “nm/s”, “µm/s”, “Å/min”, “nm/min”, “µm/min”
temperature	“°C”, “K”, “F”
angle	“°”, “deg”, “rad”, “grad”
time	“ms”, “s”, “min”, “h”, “d”, “a”
fraction	“”, “%”
diameter	“mm”, “inch”
thickness variation	“A/mm”, “nm/mm”, “µm/mm”

Tab. 0-1 Supported physical units

Appendix D: Miscellaneous functions

Material name edit fields and buttons

The effective medium, index gradient, uniaxial anisotropic and all growing layers use or combine other materials and have special edit-fields and buttons to edit and specify these “sub”-materials. The functioning of such edit field-button combination is described below.

If you want to select another material the button 

opens a material select box listing all materials available in the current material directory. You can select one and its name is returned to the “name” edit field. The specified material has been loaded and can be edited by pressing the button 

. This opens the related materials editor.

If you want to change the associated material to a material currently present in the model (this is the case when creating interface layers) you could click the button 

to open a popup menu of available materials. Selecting one of these materials changes the associated layer to the selected one.

If you do not specify a material a default material with fixed refractive index and absorptions is added after the new layer has been saved and loaded.

A change of the material name without pressing the edit button changes the materials name. It is recommended to avoid to rename a material to a different existing material and to avoid duplicate names (a duplicate name creates a copy of the previously named material and destroys the current material).

Physical number edit fields

A special functionality is supported by physical number edit fields. The standard user interface of Windows does not support <number>+<unit> combinations as required for input of physical numbers. All fields labeled as physical number edit fields work as follows.

The standard output uses a physical unit appended to the current value. The edit field uses the default unit defined in the environment “units”-page to display current values. You can enter your values in any unit allowed. For example thicknesses can be entered in “nm” as well as in “µm”. A complete overview of the allowed units for each type of physical number is contained in Appendix C.

A click with the right mouse button opens a popup menu offering a conversion of the current number into any new unit.

If you delete the unit or do not enter a physical unit the last correct unit entered or displayed is assumed and used when the display is refreshed when the edit field looses the input focus.

Appendix E: Color setup

The color scheme of the SpectraRay is predefined in PModell.Ini:

```
[Colors]
Theory=000000FF                 theory curves (PLOT) and smoothed curves
Grayed=00C0C0C0                 disabled x-regions
Fit=00000080                    theory curves in the fit dialog
Back=00FFFFFF

Curve0=00808000                 color of first curve of experiment
Curve1=00800000
Curve2=00008000
Curve3=00800080
Curve4=00000000
Curve5=00008080
Curve6=00FF0000
Curve7=00000080
Curve8=0000FF00
Curve9=00FF00FF
Curve10=00808080
Curve11=00808000
Curve12=00800000
Curve13=00008000
Curve14=00800080
Curve15=00000000
...
Curve50=00FF0000

Layer0=00739894                 Color of layer 0
Layer1=0073A994
Layer2=00525FA9
Layer3=006F84A9
Layer4=00949852
Layer5=00CAD6DE
Layer6=009CD6DE
Layer7=009CBDDE
Layer8=00949894
Layer9=00BDCEDE
Layer10=00BDCEAD
Layer11=00B9C19C
Layer12=00C5B59C

grcntl_Shadow=white             3D frame background
grcntl_Light=gray               3D frame foreground
grcntl_CurveBk=gray             curve area background
grcntl_AxisBk=lightgray         axis background
grcntl_Scale=black              color of scale
grcntl_LegendText=black         text color
grcntl_AxisName=black           axis description
grcntl_AxisTick=black           tick color

Ed_N=00800000                   n - curves in layer editors
Ed_K=00000080                   k - curves in layer editors
Ed_E1=00FF0000                  ε1 - curves in layer editors
Ed_E2=000000FF                  ε2 - curves in layer editors
```

Appendix F: Functionality of 2D-plots within dialogs

Many dialogs contain a 2D-plot of one or more curves. All these plots can be zoomed by clicking in the curve area and dragging a rectangle. After releasing the left mouse button the plot is redrawn using the zoomed floating point range. The original floating point range is easily set by clicking in the draw area and releasing the left mouse button without dragging a rectangle.

Appendix G: Frequently asked questions

My printer does not appear in the printer list during Windows setup and the same applies for the control panel. How can I print my data?
Your printer may require a non-standard printer driver. The package of your printer should contain a printer driver floppy disk/CD/DVD. Insert this disk/CD/DVD into your floppy/CD/DVD drive and run the printer installation from the control panel with printer type "Other" and follow the instructions you get. If you have no printer driver disk/CD/DVD contact your computer dealer or look for a driver within a mailbox (for example CompuServe). If nothing helps you could only use a supported printer.

My print outs have a strange lookout. How can I improve the quality?
If printing quality is bad change the setup of your printer by means of the control panel. Another reason could be the selected font size. When directly printing 2D-plot-controls you have to set the size in pixels or percent. Most other printer settings (for example the PLOT program) are in Pica points (Windows standard).

When I open the editor of certain file layers the curves are not visible. Is the layer corrupted?
No it isn't. The editor of the file layer displays the wavelength range of its data trimmed by the wavelength range defined in the environment. The result can be an empty range if there is no overlap. Check the settings of the environment, because you need to have the overlap before fitting.

The simulation does not calculate anything when I pressed "Calc", but all parameters seem to be ok?
The simulation does not start if any of the parameters in the dialog is no valid number or if there is a file I/O error. If you selected "curve" or "multicurve" as type there may be hidden parameters wrong. Change to "net" and control the additional parameters.
When the filename for output is invalid the simulation stops immediately. This could be a wrong directory path, a locked file name (network access) or a related problem. It is recommended to use an appropriate name instead.

Always when I start a simulation the error message "Cannot create fit ..." occurs but everything seems to work?
This message occurs when it is not possible to calculate a figure of merit from the data/model/environment combination. If you do not use the scanner function this does not influence your simulations, otherwise this informs on the disabling of the scanner.

I have an in-situ ellipsometer and want to fit the angle of incidence from a measurement of my known sample, but the fits make no sense. How can I fit it?
You set up your model with your known sample and load a single (Ψ, Δ)-measurement. Open the data editor and set the z-axis type to "none". Check the angle of incidence to be fitted within the environment and run the fit.

Appendix H: Shortcuts

The following keyboard shortcuts can be used:

F2	Open measurement panel
F3	Open model panel
F4	Open environment editor
F6	Open simulation window
F7	Open compare data window
F9	Open Analysis panel
F10	Open Script Editor
Ctrl+Shift+S	Save current experiment
Ctrl+S	Save as ...
Ctrl+N	New Experiment
Ctrl+Shift+O	Open Experiment
Ctrl+O	Open ...
Ctrl+I	Create an interface layer between the selected layer in the model and the layer below
Ctrl+R	Create an roughness layer between the selected layer in the model and the layer below
Shift+F3	Open the selected node in the explorer
Shift+F5	Refresh the selected node in the explorer
Shift+F7	Create a new folder in the selected position in the explorer
Shift+F8	Delete the selected file or folder in the explorer
Ctrl+Dragging	a layer inside a model: layer will be copied after dropping inside the model with the same name (copied and original layer will always have the same parameters)
Ctrl+Shift+Dragging	a layer inside a model: layer will be copied with a new name after dropping inside the model (copied and original layer can have different parameters)
Ctrl+Dragging	a data set in the list will create a copied data set at the end of the list after dropping it into the list
Ctrl+Dragging	a file in the explorer will copy the file to the directory where you dropped the file in the explorer

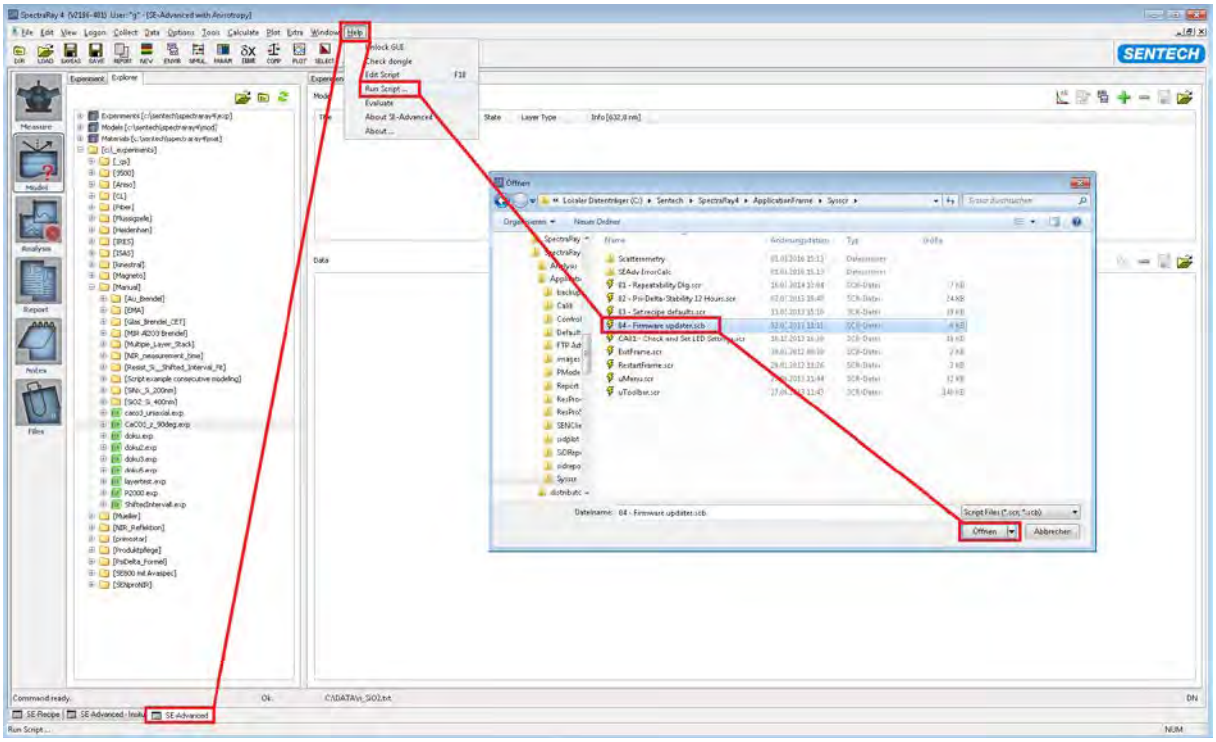
Appendix I: Firmware Updater

The firmware update utility is intended for service purposes only. **If the firmware is updated during the warranty period of a SENTECH device without expilicit permission from SENTECH the warranty is lost!**The utility for firmware update should be used for diagnostic purposes and on request by SENTECH service.

Each ellipsometer or reflectormeter which is supported by SpectraRay is equipped with a controller which is attached to the PC via network. It has a small computer built in running a Linux operating system and the firmware controlling the SENTECH hardware connected to the controller. From the PC the controller is a network device and runs a server program to fulfill all the required actions related to hardware. It is responsible for all low level hardware actions and for implementing security issues (as a door lock should disable xy-stage movements).

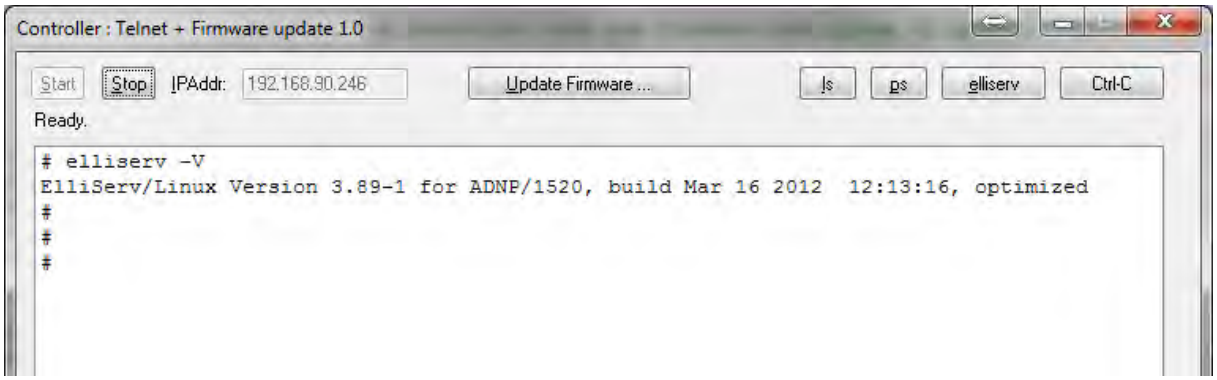
The firmware is a combination of both the operating system and the software running on the controller. It does not include the controller configuration file which defines the connected hardware settings. If you update the firmware there is no need to save the configuration file first, it saved in a different location on the flash memory on the controller. However it is a good policy to save the file before updating. When you run the utility from within SpectraRay/4 this function is already built in, since SpectraRay checks on each startup whether there is a change of the controller configuration file and keeps a current copy as well as a history of changes.

How do you run the utility?



After you have launched the firmware updater utility the screen shown below should appear. The buttons on the top allow to connect to the controller, update the firmware and to perform basic maintenance tasks by running commands directly via telnet on the controller. Since this may harm the controller function use this only on detailed instructions from SENTECH service.

The only setting required to here is the IP address of the controller. This is by default the SENTECH standard 192.168.0.199 and is different only for special purposes. So in most cases there is no need to setup a IP yourself and the utility should start up as shown below. It will connect and list the firmware version of the controller and the move the input prompt to the edit field on the bottom expecting commands to be entered. If there is no connection (i.e. “Start” is not grayed), check whether the controller is powered on, running at least for a minute (allow it to finish booting) and if the network cables are connected to the right input (some computers have multiple network plugs).



After you have connected, you can run the main job of the utility which is to update the firmware. This is done fully automatic if you press the button “Update firmware”. It does the following steps:

1. Select a firmware file (typically bimage*): This is either submitted by SENTECH service or if you need to roll back you may select one from “c:\Sentech\SpectraRay4\external\Controller”.
2. Upload this file to the controller (typ. 10..20 sec)
3. Write the firmware to the flash (typ. 35.55 sec)
4. Reboot the controller (typ. 40..50 sec)

There are some controllers which do not allow to reboot automatically. In such case after waiting the utility presents a message requesting to power off and on again. This is a normal behavior and no failure. Since a firmware is a complex piece of software SENTECH does extensive tests before delivery. However it is recommended to run a deeper test before the service action is closed (keep in mind, if the update does not solve a problem or causes other problems it is always possible to roll back the firmware to the delivery state which was working correctly.

Appendix J: Configuration of Custom Menu Entries

SpectraRay has a powerful script engine included and allows adding actions implemented by script to the applications main menu. The following guide explains how this is setup properly. The standard SpectraRay setup only provides the built-in functionality.

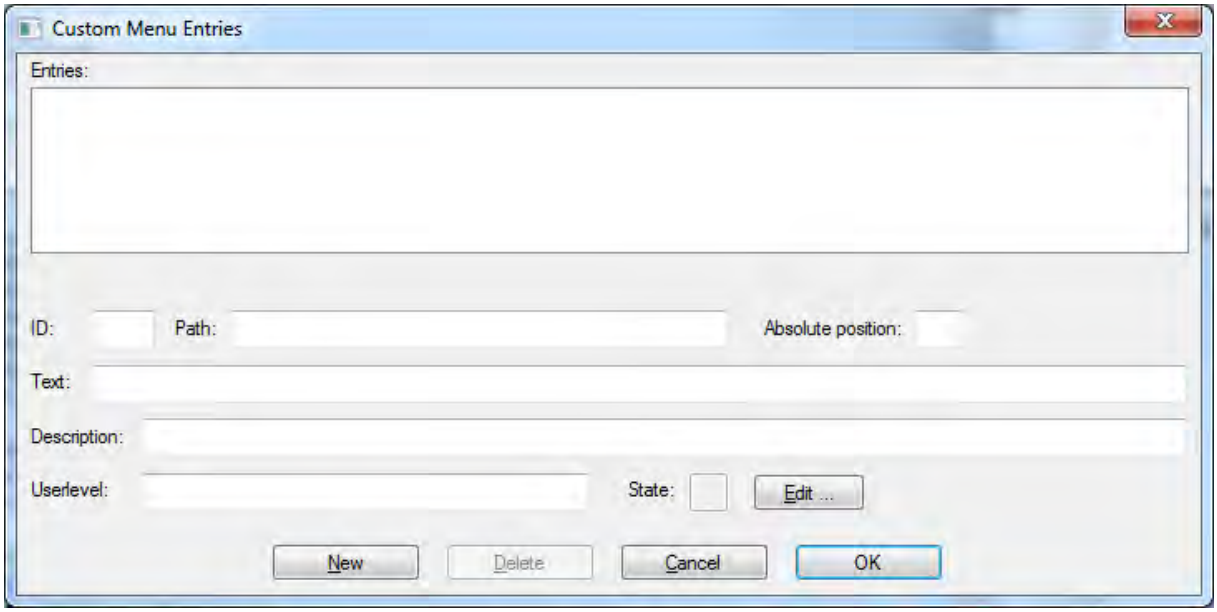
For older setups than 102 (see in the SpectraRay caption an expression like "V1868-**111**") the following procedure is needed, since the update installation does not change configuration files. If your existing setup is newer or you have installed a new version, you may skip this section and continue with part 2.

Part 1: Prepare functions (on older setups only)

In the following steps we will add two functions:

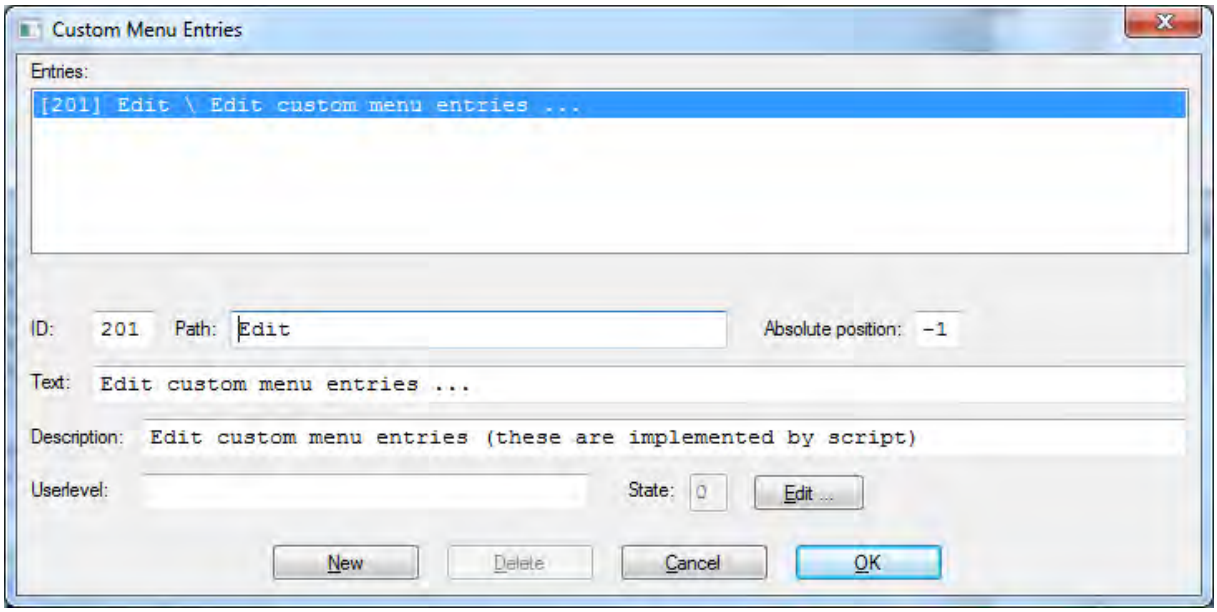
1. Add the menu editor to the "Edit" menu
2. Add an "Exit" menu to the "File" menu

When SpectraRay is running, please click in the menu "Help\Edit Script" to open the script editor. Within the editor load the file "uMenu.scr"[14] and click in "Run". The following window should appear:

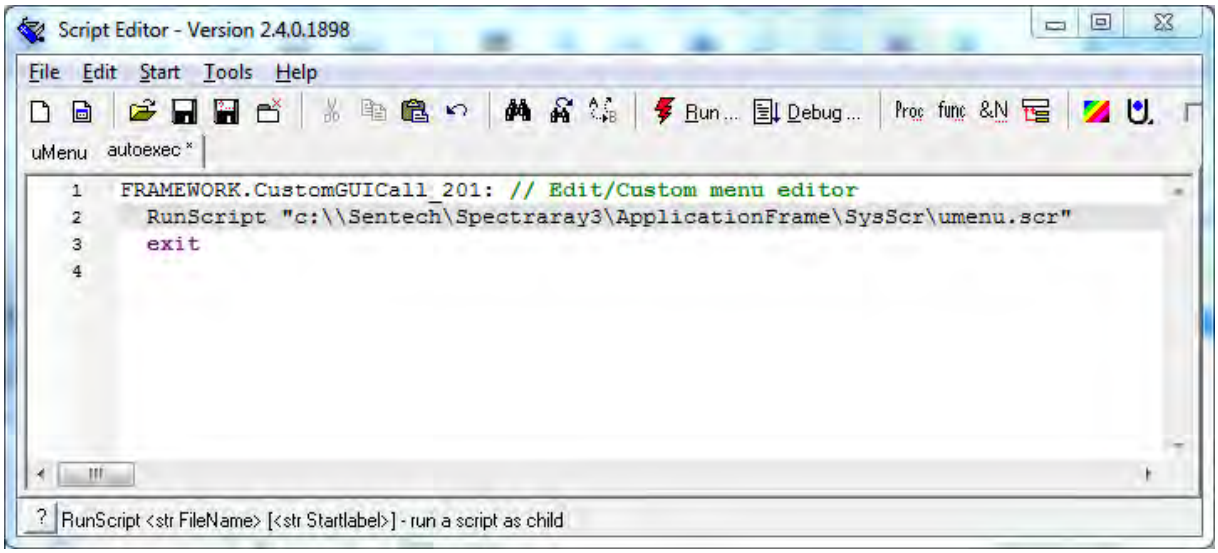


Click on "New" to add a new entry and fill the text fields as follows below. This defines the "Edit" menu as the root for the new entry "Edit custom menu entries …". The description may contain a longer text and is displayed when selecting the menu in the status bar on the bottom of SpectraRay. The user level may be one of the predefined categories as "Guest", "Operator", "Engineer" or "Admin". The "ID" must be an unused ID in the range 150 .. 250. You see the IDs on the left in the entries list.

[14] this is usually located in "c:\Sentech\SpectraRay4\ApplicationFrame\Sysscr"

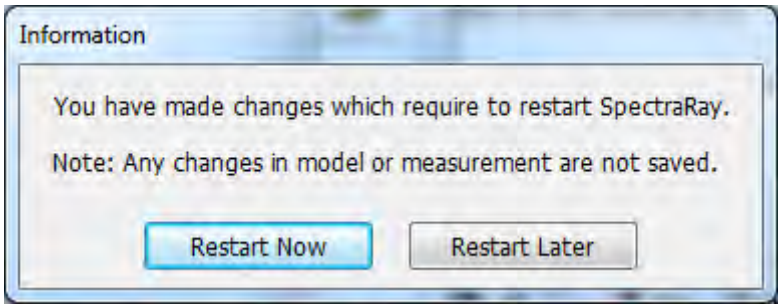


This defines the menu entry, next is to add the function. When we define an ID=201, it is routed to the script autostart.scr (near SiAFrame.exe) and the script is executed from the start label "Frame-Work.CustomGUICall_201:". For other events the value of ID is used to build the starting label, which allows to have all events handled in the same file.
Since the editor is implemented in a separate file "uMenu.scr". Using the command "RunScript" the call to the daughter script is easily setup – see below.

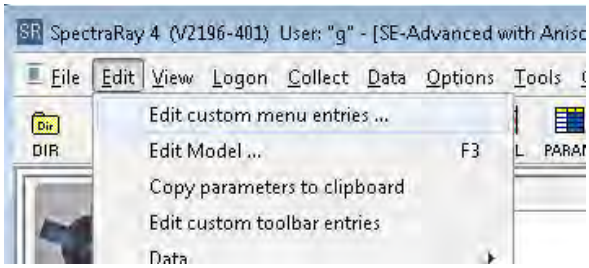


Close the editor to return to the menu editor and click on "OK" to accept the changes. The editor closes and checks whether there are changes in the menu. If there are changes, a restart of SpectraRay/4 is required for it builds the menu only at startup. The following box appears[15]:

[15] For setups newer than 102, this is no longer necessary and no message appears.



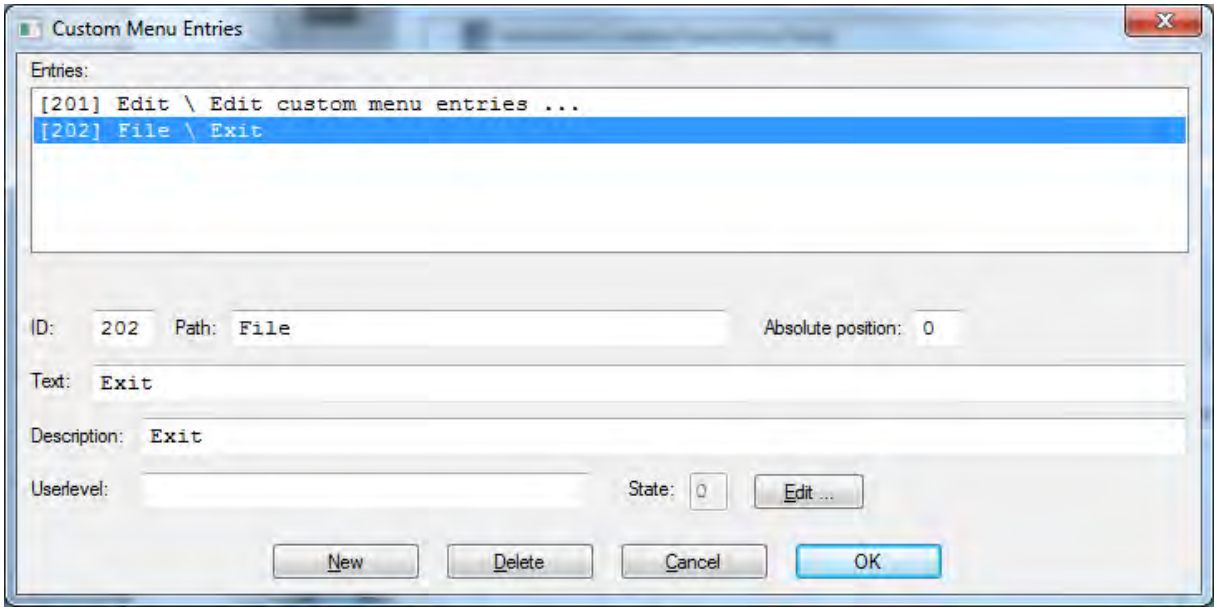
When you press “Restart Now” SpectraRay is restarted in a way which discards any data measured or modified. If in doubt, select “Restart later” to finish manually. After SpectraRay has restarted, the menu entry becomes visible and allows to directly open the editor.



We test the new menu entry and open the editor directly via menu. If the editor does not open properly, use the method above (‘Help\Edit Script” and “Run”) to correct the input.

Part 2: Configure an additional sample function

In the next sample we will add an “Exit” function to the “File” menu. Please add a new entry as shown below:



If this is verified after clicking “OK” and restarting SpectraRay, you should “Edit …” the autoexec.scr file and add the following code:

```
FRAMEWORK.CustomGUICall_202: // File\Exit w/o questions
  shell {..}Launch.exe "/NoAddins /Spawn /Run:{.}SysScr\ExitFrame.scr"
  exit
```

The code looks a bit complicated, but does the following. The shell command runs the utility “Launch.exe” which opens another instance of the scripting engine. With the parameters given no addins are loaded and the called shell process immediately terminates and starts another independent task. This task will run the script “ExitFrame.scr”. Since this script is running outside SpectraRay the “Process.Kill” commands may be used to stop SpectraRay. The application is stopped with a 20 second timeout, but without waiting for message boxes “Do you want to save …”. With the code given, this acts as a hard close in a friendly manner. If you want to ensure all the data are saved before exiting, you may either add a question or a save of the current experiment to the script before the “shell” is called.

Please note, that this is only a sample and in general it is possible to have any sequence that can be scripted available via menu or toolbar.

This is too complicated? Use drag and drop:

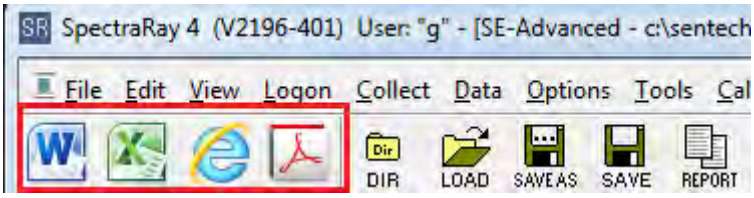
The script editor also allows to drop files on its window. When you drag a file from the Windows Explorer onto the editor the following happens for each file in the drop:

- Generate a default entry in the Tools menu: The name is derived from the file name, the ID is automatically generated.
- Delete any existing section in autoexec.scr for the new ID.
- Add a new section in autoexec.scr for the new ID as follows:
    - if the file is a script (*.scr), it is executed via “RunScript …”
    - if the file is a program (*.exe), it is run via “Shell …”
    - otherwise it will be treated like a document and opened via “ShellExecute …”

After a drop the files can be executed without any changes. However, if you want to place the files to individual menus, you may change the generated entries as explained before.

Appendix K: Configuration of Custom Toolbar Entries

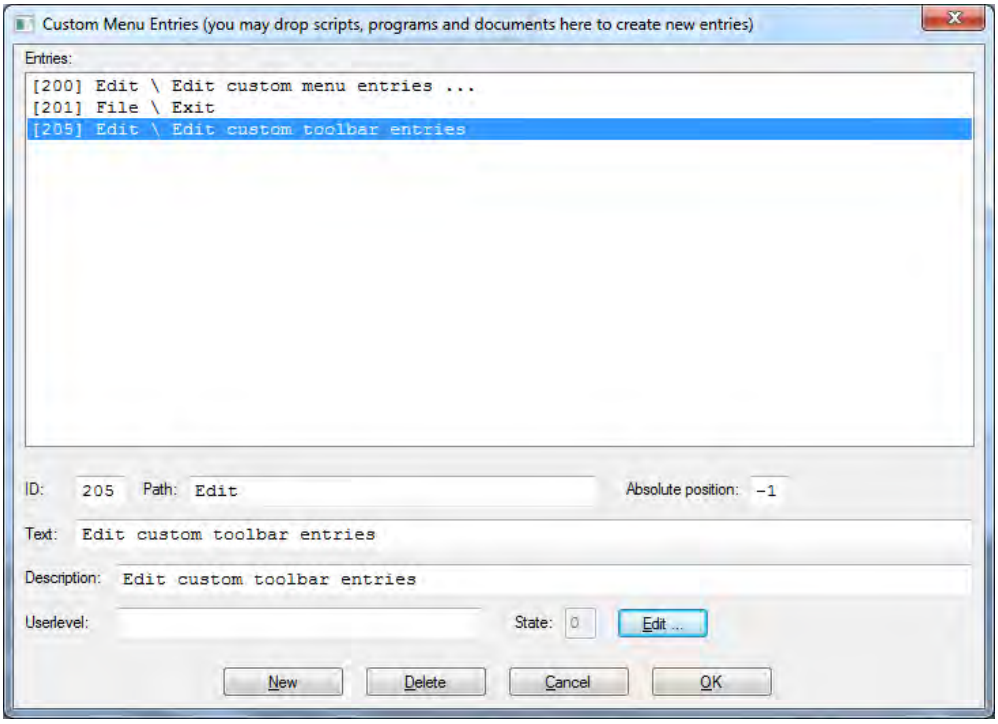
The toobar in SpectraRay can be extended in a very similar manner compared to the method used for menus. Here we used the script “uToolbar.scr” which opens an editor for toolbars. As you see below, the toolbar can contain any icons and may be used to run applications, scripts or to open documents.



For older setups than 102 (see in the SpectraRay caption an expression like “V1868-**111**”) the following procedure is needed, since the update installation does not change configuration files. If your existing setup is newer or you have installed a new version, you may skip this section and continue with part 2.

Part 1: Prepare functions (on older setups only)

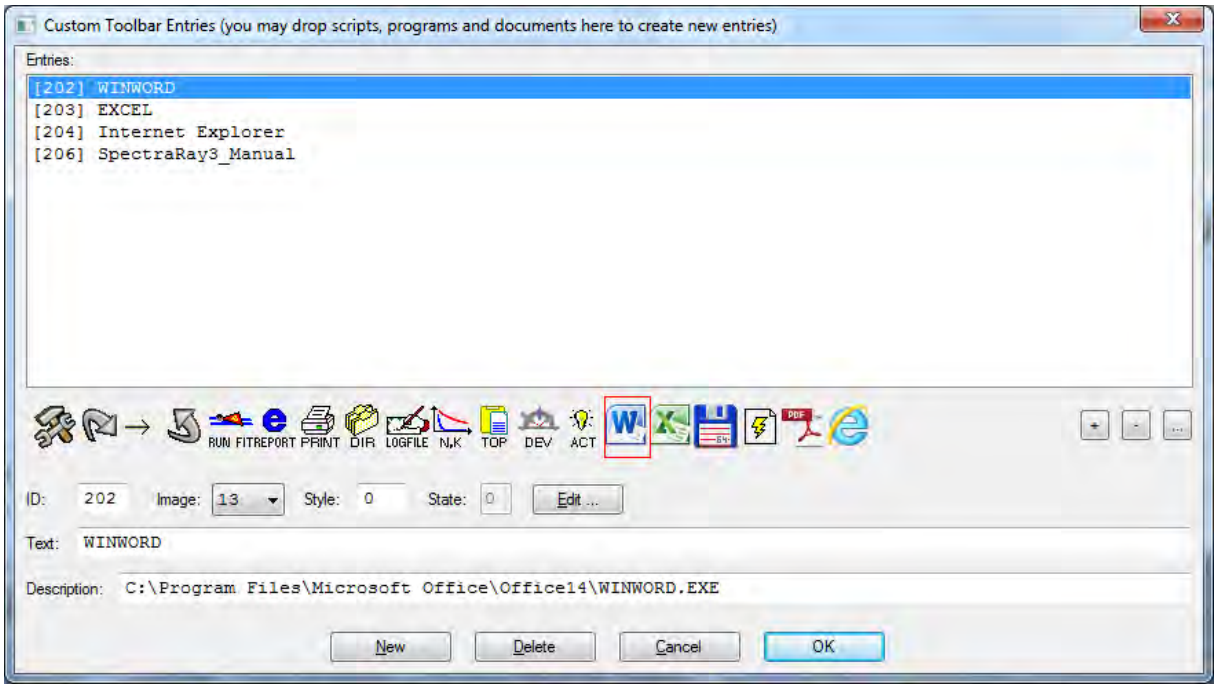
The best method is to add the editor to the menu in a first step. Please fill out the window as shown below (or just drag the file “uToolbar.scr” from within the windows explorer and drop it onto the menu editor). Close the editor, allow a restart and use the “Edit” menu to open the toolbar editor.



If you have edited the menu setting manually, you may need to add the following script to the “autoexec.scr” (click on “Edit …” to open the editor for this file):

```
FRAMEWORK.CustomGUICall_205:
  RunScript "C:\\Sentech\\SpectraRay4\\ApplicationFrame\\Sysscr\\uToolbar.scr"
  Exit
```

If you successfully finished the setup of the toolbar editor via the menu editor, you can open the toolbar editor to see a window as shown below (except the entry list can be empty):



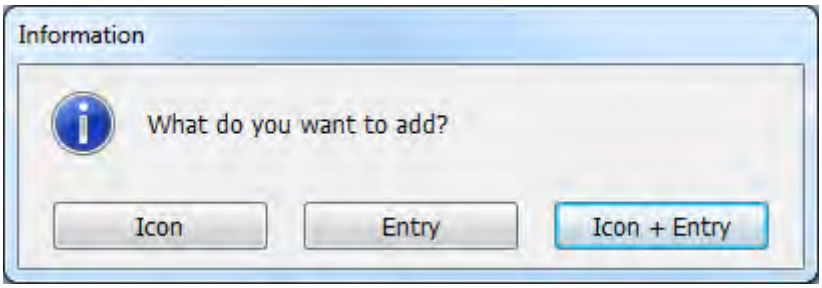
Part 2: Adding items to the toolbar

The toolbar editor resembles the menu editor, but has a list of images which can be used on the toolbar (if you ever destroy the toolbar, you may delete the file "SiAFrameCustomToolbar.bmp" – on startup of any of the two editors a new default toolbar is created).
On the top is the list of toolbar entries currently in use. In the lower pane of the window, the current toolbar item is edited. The buttons on the bottom have general functions.
The image list shows the icon used for the selected item with a red rectangle. If you click on an icon, the associated image (with the red marker) is changed. Keep in mind that you have a list of images and entries and you select for each toolbar item a single icon out of these images.
On the right of the image list there are three buttons. The "+" button selects an image file which is added to the list (you may select for example a photo which is resized and added). If you have the ALT-key pressed while you add the image, it is resized with full area keep proportions. Otherwise the image is zoomed so that the square shape cuts some area of the image (the proportions are kept the same). The button "-" is intended for error corrections and allows to remove the most right image from the image list. If you press "…" the software launches "mspaint.exe" with the bitmap containing the toolbar images for specific editing.
When you click on "New", a new toolbar entry is added and you have to edit the settings and the autoexec.scr script yourself (there is little help by finding a new unused ID and adding a new section to the autoexec.scr file).
The button "Delete" removes the selected entry from the toolbar entry list, but does not touch the image list (use "-" or "…" for modifying the images).

Support for Drag and Drop:
You may use drag&drop also for toolbars. Sources for dragging are the start menu, the desktop and the Windows Explorer. When you drop files onto the editor the following is allowed.

- Programs or Links: The target will be executed (by default) and an image can be added.
- Images (*.bmp, *.tif, *.png, *.jpg): The images will be added to the image list as icons after resizing.
- Scripts (*.scr): a new toolbar entry is added and the autoexec.scr is extended to run the script.
- Documents and other files: a new toolbar entry is added

The use of drag&drop is the simplest way to add your favorite external programs and documents to SpectraRays toolbar. If such a drop allows to add an image AND a toolbar item, you have to decide:



For example when you want to add a program the typical answer is “Icon+Entry”. If you add multiple PDF files, you might choose “Entry” for all but the first additions.

Note: After any change to the toolbar the editor asks on closing on older versions (before setup 102) to restart SpectraRay for this is updated only at startup. If you restart, all current data will be lost (if in doubt: select “Restart later”).