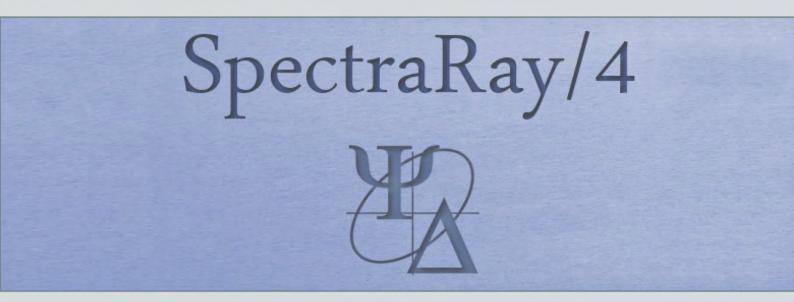


SpectraRay/4

Software Manual





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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

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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 every-thing 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:

🐌 Config	15.01.2016 09:05	Dateiordner	
😽 Sentech Setup V2196-401.exe	29.01.2016 14:27	Anwendung	546.353 KB
📄 2016-03-01 SpectraRay [964AA5FE].lic	01.03.2016 15:11	License	2 KB

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 specific 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.

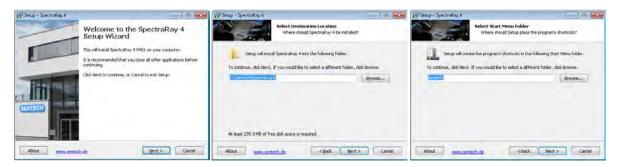


Fig. 2-3 Installation setup

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.

j§J Setup - SpectraRay 4 Ready to Install Setup is now ready to begin installing SpectraRay 4 on your computer,
Click Install to continue with the installation, or click Back iF you want to review or change any settings. Destination location: Ct/Senetch/SpectraRayv4 Setup type; Full installation Selected components; Mapping Apping SpectraRay Start Menu folder: Sentech -

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 .

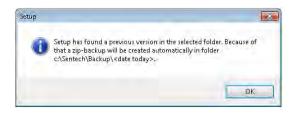


Fig. 2-5-2-6 Message box

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)
 - o 32 or 64 Bit operating system version for secondary licenses
 - o 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.

Application frame 3

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.

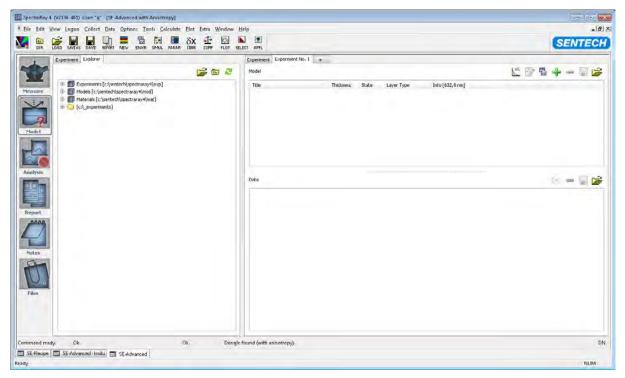


Fig. 3-1 Application frame with start view

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.

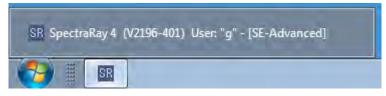


Fig. 3-3: Icon in the Windows task bar for the application frame.

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.

■ <u>File</u> <u>Edit</u> <u>View</u> <u>Logon</u> <u>Extra</u> <u>Data</u> <u>Options</u> <u>Tools</u> <u>Calculate</u> <u>Plot</u> <u>Window</u> <u>Help</u> Fig. 3-4-3-5: The main menu of the SE-Advanced-module

> File Edit View Logon Extra Device Window Help 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

SENTECH

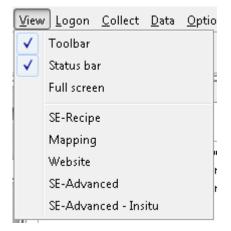


Fig. 3-9 The view menu

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:

ile Edit View Logon Window Help			SENTEC
seed			
			New
			Dekte
			Settings
ights management	Predefined relactions	gast Add predsfred rights	
Name	Publisher	Hinsechical	
G Edit experiment	SpectraRay	Allow to edit experiments	
C Edit layer	SpectraRay	Allow to edit layers	
D Edit high level HT sensor options	SENresearch GUI	Allow editing high level HT sensor options	
Service rights	SpectraRay	Allow service relevant items	
Administrate user management	Framework	Allow create and delete of users and editing permissions for all users	
Run Measure	SENPro GUI	Allow running a complete measurement	
Disteractive GUI	SpectraRay	Enable interactive mode	
6 Edit material	SpectraRay	Allow to edit materials	
> Edit ellipsometer device dependent setting.	SENresearch GUI	Allow editing ellipsometer device dependent settings	
B fdit data	SpectraRay	Allow to edit data / measurements	
	SENresearch GUI	Allow editing low level HT sensor options	
Edit low level HT sensor options	SENsesearch GUI	Alterer loading of recipe via GUI	
		Allow editing measurement, fit and remoting options	
Change recipe	SENPro GUI		
2 Change recipe	SpectraRay	Allow to save experiments	
Change recipe Edit options Sive experiment Remote commands		Allow to run remote commands	
Change recipe Edit options Sive experiment	SpectraRay		
Change respective Edit options Save experiment Remote commands Run fin Show system options	SpectraRay SpectraRay SpectraRay SENPro GUI	Allow to run remote commend; Allow to run fit Allow viewing system option;	
Change recepe Edit options Sove experiment Genete commands Run fit	SpectraRay SpectraRay SpectraRay	Allow to run remote commands Allow to run fit	Lage polyces the

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

Moren		10.000
aut.		Hes
		Delot
		56002
	Fig. 2	3-11: User frame
	1-8. 6	
	11 1	whether hutton New a many some har arrested
In the upper frame	all existing users are shown. Wi	ith the button a new user can be created.
	Create new user	
	Create new user	
	New user name:	new user
	User description:	
	Enter password:	
	Enter password again:	
		Cancel OK
	Fig. 3-1	2: Create new user
	Delete	
With the button	Delete an existing user can b	ne deleted
of the outlon	un existing user eur e	je deleted.



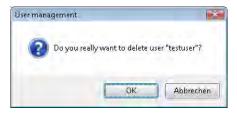


Fig. 3-13: Delete a user

With the button Settings an existing user can be modified.

User settings	
User name:	testuser
User description:	
Enter new password:	•••••
Enter password again:	•••••
	Cancel OK

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

3.2.2 Rights administration

	Predefined selections: no se	election Add predefined rights
Name	Publisher	Description
🚯 Edit material	SpectraRay	Allow to edit materials
🚯 Run fit	SpectraRay	Allow to run fit
🚯 Edit layer	SpectraRay	Allow to edit layers
🙀 Edit data	SpectraRay	Allow to edit data / measurements
🚯 Interactive GUI	SpectraRay	Enable interactive mode
🚯 Remote commands	SpectraRay	Allow to run remote commands
Administrate user management	Framework	Allow create and delete of users and editing permissions for all users
Edit ellipsometer device dependent settings	SENresearch GUI	Allow editing ellipsometer device dependent settings
Edit high level HT sensor options	SENresearch GUI	Allow editing high level HT sensor options
Edit low level HT sensor options	SENresearch GUI	Allow editing low level HT sensor options
Edit system options	SENresearch GUI	Allow editing general program options
Show system options	SENresearch GUI	Allow viewing system options
Edit options	SENresearch GUI	Allow editing measurement, fit and remoting options
🚯 Show options	SENresearch GUI	Allow viewing measurement, fit and remoting options
🕼 Run Measure	SENresearch GUI	Allow running a complete measurement
🔂 Save experiment	SpectraRay	Allow to save experiments
🚯 Edit experiment	SpectraRay	Allow to edit experiments

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

 Add predefined rights

Predefined selections:	no selection 👻	Add predefined rights
	no selection Guest	V Hierarchical
Publisher	Operator Engineer	
SpectraRay	Admin	rials

Fig. 3-17: Predefined right selections

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

Name	Publisher	Description
🖉 🚱 Edit material	SpectraRay	Allow to edit materials
🖉 🚱 Run fit	SpectraRay	Allow to run fit
🖉 🚱 Edit layer	SpectraRay	Allow to edit layers
🖉 🚱 Edit data	SpectraRay	Allow to edit data / measurements
🖉 Interactive GUI	SpectraRay	Enable interactive mode
🖉 Remote commands	SpectraRay	Allow to run remote commands
🚰 Administrate user management	Framework	Allow create and delete of users and editing permissions for all users
Edit ellipsometer device dependent settings	SENresearch GUI	Allow editing ellipsometer device dependent settings
▲ Edit high level HT sensor options	SENresearch GUI	Allow editing high level HT sensor options
▲ Edit low level HT sensor options	SENresearch GUI	Allow editing low level HT sensor options
Edit system options	SENresearch GUI	Allow editing general program options
♪ Show system options	SENresearch GUI	Allow viewing system options
✓ Edit options	SENresearch GUI	Allow editing measurement, fit and remoting options
Show options	SENresearch GUI	Allow viewing measurement, fit and remoting options
🖉 🚱 Run Measure	SENresearch GUI	Allow running a complete measurement
🛛 🚱 Save experiment	SpectraRay	Allow to save experiments
🖉 🚱 Edit experiment	SpectraRay	Allow to edit experiments

Fig. 3-18: Modified user rights

By clicking the button Apply 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.

<u>File Edit View Logon Extra Device Window Help</u> Fig. 4-1 The main menu of the SE-Recipe-module

4.1.1 File menu

File	Edit	View	Logon	Extra	Device	W
	Load					
	Save					
	Save	spectra	as ASCI	[file		
	Save	as SPC	file			
	Direc	tories .				
	Print	Print Setup				
	Shov	v Repor	t			
	Print	Report	:			
	Shov	v/Save i	material	dispersi	ion	
	Exit					

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

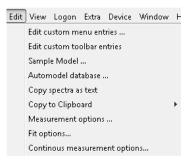


Fig. 4-3 The edit menu

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

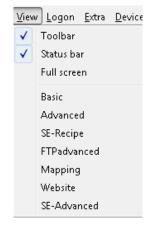


Fig. 4-4 The view menu

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.

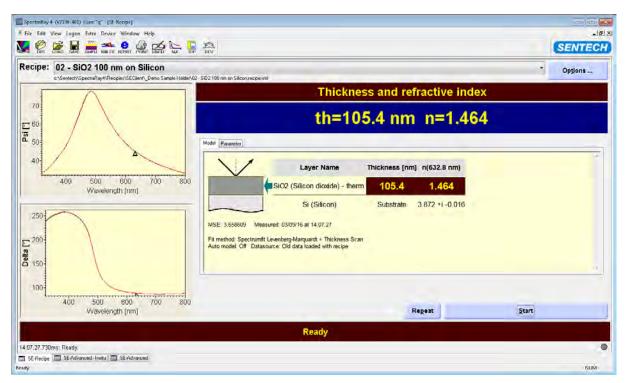


Fig. 4-5: Typical appearance of the frame window with the main user screen for SE-Recipe

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

Logo	on <u>E</u> xtra	<u>D</u> evice	<u>W</u> indow
	User logo	n	
	User logo	off	
	User adm	ninistratio	in

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

<u>E</u> xtra	<u>D</u> evice	<u>W</u> indow	<u>H</u> elp
	Directorie	25	
	Unit opti	ons	
	User inter	rface optio	ns
	Run Fit		
	View last	log file	
	Fig. 4-7	The extra r	nenu

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.

System Option:	5	— ×
Directories S	ystem units options User interface options	
<u>R</u> ecipe:	c:\Sentech\SpectraRay\Recipies\SEClient\Semiconductor Technology\Silicon\Dielectric	
<u>E</u> xperiment	c:\Sentech\SpectraRay\ApplicationFrame\SENClient\Experiment	
<u>M</u> odel:	c:\Sentech\SpectraRay\ApplicationFrame\SENClient\Model	
<u>D</u> ata:	c:\Sentech\SpectraRay\ApplicationFrame\SENClient\Data	
Protocols:	c:\Sentech\SpectraRay\ApplicationFrame\SENClient\Protocols	
	<u> </u>	

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.



rectories S	ystem antis e	aptions User interface options	_
Recipe:	c:\Sentech	\SpectraRay4\Recipies\SEClient_DemoSample Holder	
Experiment	c:\Sentech	Browse for Folder	
Model:	c:\Sentech	Select the recipe directory: C:\Sentech\SpectraRay4{Recipies\SEClient\Semiconductor	IX
Data:	c:\Sentech	Tachaolao Ucilican Diolactric filme	. 11
Protocols:	c:\Sentech	Dielectric films	
		Low k materials Metals, Nitrides Polysilicon	
		Silicides	

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:

System Options		×
Directories System units options	er interface options	
Thickness: Α nm μm mm	Wavelength: A Angle of Rad µm 1/cm eV Digits: 2	
Digits: 1	Digits: 1	
Reflectivity:	Percent:	
Digits: 3	Digits: 3 Digits: 2	
	Defaults	
	<u> </u>	

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.

SpectraRay/4

4.1.5.3 User interface options

SENTECH

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

System Options	x
Directories System units options User interface options	_
 Show (old) measurement after loading recipe Interactive GUI mode Use measurement device state (door, slider position) for GUI accessibility Invalidate last results after start single measurement State Log display detail level 	
Use user profiles Use preselected recipes Configure preselected recipe lists Allow only execution of preselected recipes	
 Recipe selection box will be filled from general directory; User directories (recipe, experiment,) are not active; No recipe change after logon 	-
<u> </u>	

Fig. 4-11: The user interface options tab

Show (old) measurement after loading recipe

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

Interactive GUI mode

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.

Model Parameter				
	Layer Name	Thickness [nn	n] n(632.8 nm)	
	SiO2 (Silicon dioxide) - therm.	105.4	1.464	
	Si (Silicon)	Substrate	3.872 +i -0.016	
MSE: 3.658609 Me	asured: 03/09/16 at 14:07:27			
	fit Levenberg-Marquardt + Thickness Scan isource: Old data loaded with recipe			
1				

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.



	Layer Name	Thickness [nn	n] n(632.8 nm)
(SiO2 (Silicon dioxide) - therm.	105.4	1.464
	Si (Silicon)	Substrate	3.872 +i -0.016
MSE: 3.658609 Measu	red: 03/09/16 at 14:07:27		
	evenberg-Marquardt + Thickness Scan urce: Old data loaded with recipe		

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

Vise measurement device state (door, slider position) for GUI accessibility

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).

State 👻 Log display detail level

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.

<u>R</u> ecipe:	SiO2 (< 5 μm) on Silicon -
	Al2O3 on Silicon
1	HfO2 (100 nm) on Silicon
30-	HfO2 (high k) on native SiO2 on Silicon
307	Si3N4 (230 nm) on silicon
	Si3N4 on native oxide on silicon
	Si3N4 on silicon
[] ²⁵	SiO2 (< 30 nm) on Silicon
20	SiO2 (< 5 μm) on Silicon
	SiO2 (> 5 μm) on Silicon
15-	SiO2 (gate oxide) on Silicon
	SiO2 on Si3N4 on Silicon
4	SiON (Si excess) on silicon
	SiON on silicon
	TiO2 on Silicon
	ZrO2 on Silicon

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.

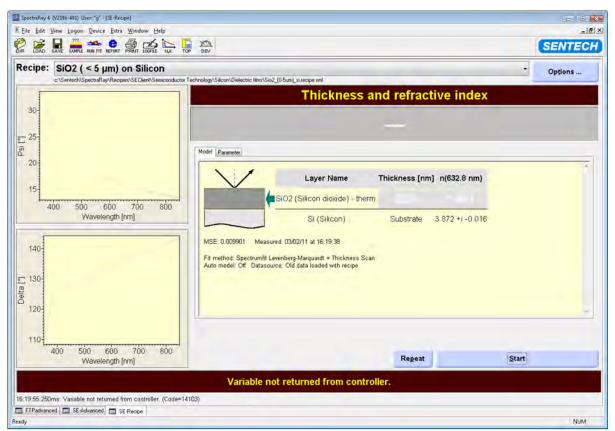


Fig. 4-16: Main screen with information in the model window in case of problems.

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.

Change observation wavelength	
0	-
Obs. wavelength [nm] 632.8	ור

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.

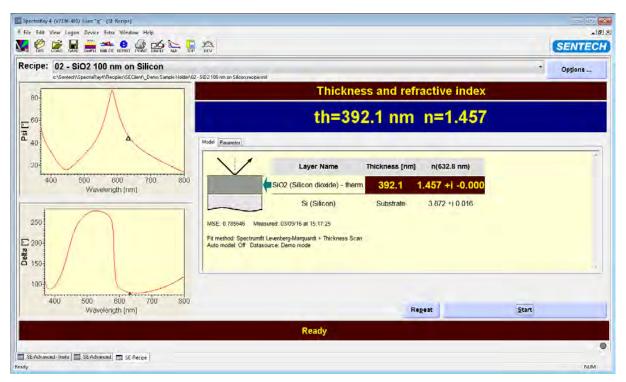


Fig. 4-19 Display of results after a successful measurement.

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.

		SENTECH
Recipe: 02 - SiO2 100 nm on Silicon c\Sentech\SpectralTay1\Recipies\SECient_Demo Sample Holder\/	2 - SiQ2 100 million Silicon recipe smi	· Options
390.90	Thickness and refractive index	
E 390.803 390.75	th=390.9 nm n=1.460	
E 390 75	Layer Name Thickness [nm] n(632.8 nm)	
1 46015-	Si (Silicon) Substrate 3 872 +i 0 016 MSE 4.789445 Measured: 03/09/16 at 15:21;59 Average thickness: 390.8 ± 0.16 nm (3 Sigma) Minimum: 390.7 nm Maximum: 390.9 nm Minimum: 390.7 nm Maximum: 390.9 nm	
1.46010	Fit method: SpectrumM Levenberg-Marguardt + Thickness Scan Auto model: Off Datasource: Demo mode	
0.02 0.04 0.06 0.08 0.10 Time [min]	Regent	Start
	Ready	

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:

Continued Measurement	Finished	×
The continued	d measurement has been finished.	
Run time: 8 s	Measurements: 25	
	OK	

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

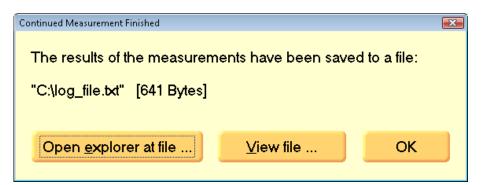


Fig. 4-23: Message if logging is enabled

Datei E	Bearbeiten	Format	Ansicht ?	
0.300	390.71	1	0.023664	
0.602	390.70	2	0.026775	-
0.903	390.95	23	0.024365	E
1.218	390.79		0.028682	
1.520	390.56		0.026533	
1.821	390.26	6	0.027487	
2.124	391.03	6 7	0.021857	
2.431	390.77	8	0.027799	
2.751	390.26	9	0.024036	

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

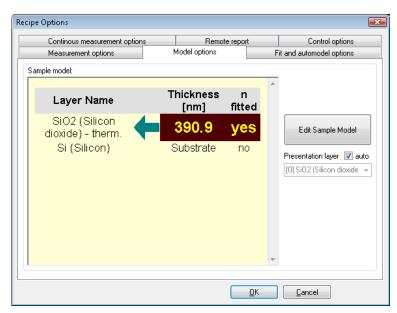


Fig. 4-25: The "Model options" tab in the recipe options

Clicking the button 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" \rightarrow "Measurement options ...".

Continous measurement options Remote report Control options					ol options
Measurement options	Model options Fit		it and automodel options		
Display Image: Measurement Image: Measurement Image: Show N,k Image: Polarization	Show roug	·	Apply settings		efaults
Wavelength Wavelength range [nm]: 370 Device settings Measurement mode: Psi, Delta	. 930	Set rang	e to maximum	limits: 43	5 850 n (bit):16
Integration time [ms]: 2.2 Polarizer position (*): 45 Angle of incidence (*): 70		Calc. degree of Use yellow filter Use polarizer tra Use fast mode Demo mode (de	cking	Steps: Scans: Rounds:	48
Height/Tilt settings					
Save results of single measureme	nts to logging fi	le (see settings (on continued	page)	

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:

Measurement mode:	Psi, Delta 🔹
	Psi, Delta
	S1, S2

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

ADC-Resolution [bit]:16

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

Calc. degree of polarization



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

Integration time [ms]: 2.2

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 (\geq =500 ms), it is possible that there is no sample on stage.

Polarizer position (*): 45

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

Angle of incidence [*]: 70

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.

📃 Use yellow filter

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

🔲 Use polarizer tracking

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.

📃 Use fast mode

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).

Steps: 8 Scans: 48

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.

Rounds: 1

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

V Demo mode (device)

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.

Show manual align window

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" \rightarrow "Fit options ...".

Continous measurement options	Remote repo	ort	Control options	
Measurement options Model options		Fit and automodel options		
utomodel				
AutoModel detects known samples before f	ting and selects a mo	del from the	predefined database	
Name of database: Scanner		•	Edit AutoModel database	
it settings				
<u>Fit Method:</u> Spectrumfit Leve	nberg-Marquardt			
🔲 Use Simplex ir	stead Levenberg-Mar	quardt		
Max. fit iterations: 100	<u>O</u> bserv.	wavelength	[nm]: 632.8	
Wavelength filter [nm]: 400.0	:00.0	Calc. errors		
Spectrum fit optimization	dFo	urier 0.001		
Allow to stop using accuracy limits		dPsi 0.05	dDelta 0.1	
Allow to stop if model is stable at observ. w.	velength	ui ai 0.00	dDieka	
Allow to reduce fit parameters				
Reduce data: Take each 4 th data	point CB	ehavior		
Report dispersions Run the fit twice		Set load values before each fit		

Fig. 4-27 The "Fit and automodel options" tab

4.5.3.1 Frame "Automodel"

AutoModel detects known samples before fitting and selects a model from the predefined database

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"

Eit Method: Spectrumfit Levenberg-Marquardt

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.

Observ. wavelength [nm]: 63	2.0	В
-----------------------------	-----	---

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.

Max. fit jterations: 100

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.

Wavelength filter [nm]: 400.0 ... 800.0

Ŧ

The wavelength filter allows selecting the range used for fitting.

- Allow to stop using accuracy limits
- Allow to stop if model is stable at observ. wavelength
- Allow to reduce fit parameters
- <u>Reduce data: Take each</u> 4 th data point

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.

Report dispersions

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.

🔲 Run the fit twice

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.

📃 Calc. errors

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.

Behavior
🔲 Set load values before each fit
Set load values on errors
📰 Handle too many iterations as error

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.

Continous measureme	ent option	s	Remote repo	rt			Contr	ol options
			ions		Fit	t and a		el options
Automodel								
AutoModel detects kno	wn sample	es before fitting and	selects a mo	del fr	rom the j	predefi	ined dat	abase
Name of database: S	canner			•	•	<u>E</u> dit	AutoMa	del database
Fit settings	_							
<u>F</u> it Method	d: Specti	umfit Levenberg-Ma	arquardt					-
Max. fit iterations: Max. fit iterations: Max. fit iterations: Max. fit iterations: Max. fit iterations: Mo Fit Measurement Combined Fourier Tra- No Fit Measurement Combined Thickness: Spectrum fit optimization Allow to stop using accuracy limits Allow to reduce fit parameters Beduce data: Take each 4 th data point Report dispersions Run the fit twice Defaults		Transformation hed Fourier Transfor (Measurement only hed Thickness Scar	mation and S n and Spectru dFou	ımfit ırier				
		th data point	B	ehav D	Set loa Set loa	d value	es on er	e each fit rors ations as error

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

4.5.5 Continuous measurement options

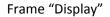
The "Continuous measurement options" window can be accessed also by choosing "Edit" \rightarrow "Continuous measurement options".

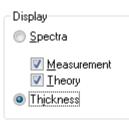
Measurement options		Model options Fit		t and automodel options		
Continous measur	rement options	Remote re	port	Control options		
				Defaults		
Display	Stop continous m	ieasurement	Height/Tilt s	ettings		
Spectra	le on "repeat" re	lease only				
V Measurement	after 5	measurements	_ on hret	measurement		
V Theory	after 20	seconds	 eVe)// 	T measurement		
Thickness	on errors		_ even	0 second		
Timing						
ivanber of pending	measurements: 1	1 1 200	Shew mar	nual align window		
Use <u>d</u> elay between i		0 seconds				
Log file						
Saye to: C:\buffer\t	est2.txt			-1-		
Header:				17		
Eormat: \$Runtime::	s\$\t\$thickness:nm\$\t\$	No\$\t\$mse\$\n		7		
🔲 log errors 🛛 🔲 Apr	pend always			_		

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.





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"

Stop continous measurement				
on "repeat" release only				
) <u>a</u> fter	5	measurements		
⊚ aft <u>e</u> r	20	seconds		
on errors				

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"

Timing		
Number of pending measurements:	1	(1 20)
Use delay between measurements of	10	seconds

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"

Height/Tilt settings				
rieigno riic se	stangs			
🔘 on first	measurem	ent		
		1		
🎯 every	1	. measurement		
-				
🔘 every	0	seconds		
		,		
Show manual align window				

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.

Log file		
🔲 Sa <u>v</u> e to:	C:\buffer\test2.txt	
<u>H</u> eader:		
<u>F</u> ormat:	\$Runtime:s\$\t\$thickness:nm\$\t\$No\$\t\$mse\$\n	ŕ
🔲 log errors	Append always	

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:

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

lecipe Options		
Measurement options	Model options	Fit and automodel options
Continous measurement options	Remote report	Control options
Report options		
Report thickness, n, k		
Report all fitted parameters		
Report reflectivity	Spectral data	
Report transmission	📃 Report dispersion sp	ectra
Report color values	Report polarization	
Report MSE		
Report tolerances		
Report tolerance summary		
Report special values		
		?
Defaults		
	<u> </u>	IK <u>C</u> ancel

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.

📝 Report thickness, n, k

Fitted values of thickness, n and k are reported.

Report all fitted parameters

All fitted parameters are reported.

Report MSE

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

Report tolerances

If checked, the values of tolerances will be reported.

Report tolerance summary

If checked, a summary of tolerances will be reported.

Report special values

If checked, special values will be reported.

4.5.7 Control options

lecipe Options		X
Measurement options	Model options	Fit and automodel options
Continous measurement options	Remote report	Control options
User info input		
Ask for user start notes		
Ask for user completion notes		
Report options		
🔲 Generate report after measurement at	utomatically	
🔲 Insert user info in report		
Insert pictures in report		
Use matching offsets		
Script file:		
	ew script	
Defaults		
		<u>O</u> K <u>C</u> ancel

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.

Measurement Info			×
Measurement ID:			
Start notes:			*
🔲 Don't ask again in th	nis program session	Cancel	ОК

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.

Measurement complet	ion notes		×
Completion notes:			*
			-
🔲 Don't ask again in this	program session	Cancel	ОК

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"

C 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

🔲 Use matching offsets

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.

Script file:			
	Edit script	New script	

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

a-Ge (Amorphous Germanium) a-Si (Amorphous silicon) - Jellison a-Si (Amorphous silicon) - Jellison AF 45 (Schott glass) Ag (Silver) Air Al (Aluminum) - Aspnes Al (Aluminum) - Delli			File	ichy ichy	*	Select jibrary Import NK table Delete material
Insert layer above	Insert l <u>a</u> y Repl <u>a</u> c	e layer	<u>S</u> a Minimum	ert <u>n</u> ew layer we material Maximum	Тур.	I <u>n</u> fo properties
Air		[nm]	[nm]	[nm]		Edit fit parameters
SiO2 (Silicon dioxide) - therm.	×	390.65	0.00	25000.00		Load from file
Si (Silicon)					-	
						Sa <u>v</u> e to file
						Clear <u>m</u> odel

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:

Suchen in:	Analysis		🕲 🗷 📑 🛄 🐑	
(he	Name		Änderungsdatum	Тур
1	Experiments		10.02.2016 08:49	Dateiordr
Zuletzt besucht	📕 Material		09.03.2016 15:18	Dateiordr
-	📕 Oxide on Si		10.02.2016 08:49	Dateiordr
	🌗 Oxides or Nitrides on Si		10.02.2016 08:49	Dateiordr
Desktop	📕 Scanner		09.03.2016 15:12	Dateiord
Computer				
	*	10		
Netzwerk	Folder name: C:\Sentech\Spectra	aRay4\Analysis\Mater	ial 👻 🔽	OK
	A CONTRACTOR OF			911

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.

Material library: c:\Sentech\SpectraRay\Analysis\Material		
a-Ge (Amorphous Germanium) a-Si (Amorphous silicon) - Jellison a-Si (Amorphous silicon) - Palik AF 45 (Schott glass) Ag (Silver) Air Al (Aluminum) - Aspnes Al (Aluminum) - Aspnes Al (Aluminum) - D	File File Cauchy File Cauchy File File File	Select library Import NK table Delete material

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.

Insert layer above	Insert layer below	Insert <u>n</u> ew layer	Info properties
<u>R</u> emove layer	Repl <u>a</u> ce layer	Save material	

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.

Info Device Properties	5	X
Info Device Properti	es:	
Device type: Device name:	3 Measurement device. All features enabled.	
Thicknesses fit:	multiple layers	
Datatypes: Materials:	Psi,Delta S152 S1CS2C NK Reflectivity	
NK Fix	new load edit fitNK	
NK Table Sellmeier	new load new load edit fitNK	
Cauchy	new load edit fitNK	
Oscillator	new load edit fitNK	
EMA Leng	new load edit fitNK new load edit fitNK	
Forouhi-Bloomer	new load edit fitNK	
Schott transp.	new load edit fitNK	
Tauc-Lorentz	new load edit fitNK	
	ОК	

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:

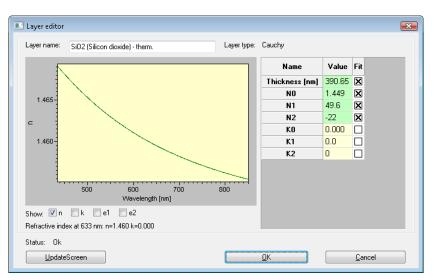


Fig. 4-37: The layer editor window

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:

Name	Value	Fit	Digits	Accuracy	Derive	Typ. Diff.	Minimum	Maximum	Reset
[0] SiO2 (Silicon dioxide) - therm Thickness [nm]	390.65	×	2	0.0010	0.0010	1.00	0.00	25000.00	0.00
SiO2 (Silicon dioxide) - therm - NO	1.449	X	3	0.00100	0.00100	0.100	-100.001	100.000	1.100
SiO2 (Silicon dioxide) - therm - N1	49.6	×	1	0.010	0.010	0.1	-100000.0	100000.0	0.0
SiO2 (Silicon dioxide) - therm - N2	-22	X	0	0.10	0.10	0	-100000	100000	0
SiO2 (Silicon dioxide) - therm - KO	0.000		3	0.00010	0.00001	0.100	-100000.000	100000.000	0.000
SiO2 (Silicon dioxide) - therm - K1	0.0		1	0.010	0.010	0.1	-100000.0	100000.0	0.0
SiO2 (Silicon dioxide) - therm - K2	0		0	0.10	0.10	0	-100000	100000	0
Straylight - Psi Offs.	0.000		3	0.01000	0.01000	0.100	-360.000	360.000	-350.00
Straylight - Psi Linear	0.0000		4	0.010000	0.001000	5.0000	-3000.0000	3000.0000	-3000.0
Straylight - Delta Offs.	0.000		3	0.01000	0.01000	0.100	-360.000	360.000	-350.00
Stravlight - DELTA Linear.	0.0000		4	0.010000	0.001000	5.0000	-3000.0000	3000.0000	-3000.0
Katus: Ok				(ŌK			Cancel	•

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 \leq

Value \leq 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 Save to file 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.

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Sentech + Backup Backup SentPM SectomBay Secto	Nims Material Dade on S Stanter CuttEquited and Si Stanter	Andersongsföhlern 1647-2016 98-84 9685-2045 5239 1047-2016 98-84 1047-2016 98-84 1047-2016 98-84 1047-2016 97-52 95-62-2016 95-52	Typ Dataiothar Dataiothar Dataiothar Dataiothar Dataiothar Notepad ++ Datai	Gella		
Dateigame:						
Distant on Francis	ment files (*.exp.xml)					

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).

obern Typ 648 Dataionthor 510 Dateionthor 648 Dateionthor 648 Dateionthor 749 Dateionthor 749 Notepaulee D	Gettin Dota 15348	8. 0	0
649 Dateiordner 518 Dateiordner 549 Dateiordner 549 Dateiordner 510 Dateiordner			
			• Expremnint files (*exp.umf) Offnen [v] Abbrech

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):

Create new material	×
Cauchy Drude-Lorentz Oscillator Effective Medium (EMA) Fixed NK Formula Forouhi-Bloomer Fraction Table Harmonic Oscillator ITO Hamberg ITO Sernelius Leng oscillator NK table Schott transparent Sellmeier Tauc-Lorentz	E encel

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_0 , n_1 , and n_2 have been typed in.

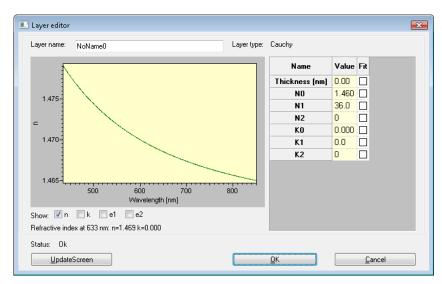


Fig. 4-42: Example for parameters of a new Cauchy layer with arbitrarily set values.

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).

SpectraRay/4

SENTECH

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Sentech *	Name	Anderungsdatum	Тург	Griffe	
di Backup	AF 45 (Schott glass) Cauchy matural	25/FL2082 18-36	Notepade - Docu_	148	
a, log	Ag (Silver) DL matami	04 11 2013 10:07	Noteped - + Docu.	23 875	
SenPM	Ag (Silver) File matami	75.41.2017 18-18	Nobrand + + Docu-	AKE	
SpectraRay	a-Ge (Amorphous Germanium) Filemat	25,81,2002 10:38	Notepad Docu-	DED	
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🔔 Analysia 🔤	Al (Aluminum) - Aspnes File.mat.uml	25/01/2002 35:38	Notepad ++ Dilla-	0.62	
🐇 Expenier 💡	Al (Aluminum) - Palik File mataml	75,01,2012 18:38	Notegied ++ Diacu	5.08	
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Applicati-	AI.596a.41As File matxml	25/01/2012 18:58	Notepad + + Doci.	588	
intribute	ALTOGa 30As File matumi	25.81.2002 56:38	Notepade + Docu-	898	
AL DOC	Al 80Ga 20A: File.mat.xml	23.41.2007.16:38	Notepad + + Docs.	0.02	
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is external	AUIO3 (Sapphire) - e-beam Cauchy,mato	25,41,2092 18,29	Notepad+= Docu.	3/2	
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Dateigame:					
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Fig. 4-43: Saving the material in a file

Edit Sample Model						
Material library: c:\Sentech\Spectra	aRay∖An	alysis\Material				
Ni (Nickel) NiCr			File Ler	ng-Osc	*	Select library
NoName0 Os (Osmium)			File			Import NK <u>t</u> able
p-Si (Polysilicon) - 540°C p-Si (Polysilicon) - 540°C p-Si (Polysilicon) - 600°C			File	uchy uchy		Dele <u>t</u> e material
p-Si (Polysilicon) - 600°C - C: (Delysilicon) - 600°C Selected material file: NoName0.mat.>	ml			acity	Ŧ	
						
	nsert l <u>a</u> ye Replace			ert <u>n</u> ew layer		Info properties
<u>R</u> emove layer	<u>S</u> ave material					
Material	Fit	Thickness [nm]	Minimum [nm]	Maximum [nm]	Тур.	<u>E</u> dit layer
Air		[nm]	[nm]	[nm]	Тур.	Edit layer Edit fit <u>p</u> arameters
	Fit				Тур.	
Air NoName0		[nm] 0.00	[nm] 0.00	[nm] 100000.00	Тур.	Edit fit parameters
Air NoName0 SiO2 (Silicon dioxide) - therm.		[nm] 0.00	[nm] 0.00	[nm] 100000.00	Тур.	Edit fit parameters
Air NoName0 SiO2 (Silicon dioxide) - therm.		[nm] 0.00	[nm] 0.00	[nm] 100000.00	Тур.	Edit fit parameters
Air NoName0 SiO2 (Silicon dioxide) - therm. Si (Silicon)		[nm] 0.00	[nm] 0.00	[nm] 100000.00		Edit fit garameters

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.

500	1200	00/00	1.20	70.52	-0.0	34700	17
202	.000	0065	9,27	6122	-0.	0460	la:
309	1000	00400	9.25	5128	-0.0	145.10	211
1200	.000	2200	9,35	545.	-0.1	0403*	17
309	.000	0000	4,24	SILL	-0.1	04272	12
100	0.000	2200	9,23	\$561	-0.1	04162	12.
542	.000	0000	4.22	5660	-0.1	94963	15
314	.000	2200	5/21	6541	-0.1	04011	0
514	.1206	9000	4.20	6973	-0.1	1986	16
545	1.000	2200	9,19	7617	-0.1	2302-	15
520		0000	4.10	0159	-0.1	1877.	ñ
3122	.000	0000	5/17	2070	-0-1	03490	15
5.29	1.000	0060	4. 17	0822	-0.	11612	a,
2126	F, 000	0000	6.16	2436.	-0.	335 45	ŵ
526	.000	2000	4.15	4269	-0.1	27485	16
15.00	1000	200	1.14	646 L	-9.	33425	11
523	.000	2000	1.12	0100	-0.	22372	9
324	L D00	000	8.13	1505	-9.1	33316	14

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:

Organisieren 🔻 🏢 A	nsichten 🔻	Neuer Ordner	_	-
ikfavoriten	Name	Anderungs Typ	Größe	
Dokumente	NewM	aterial_nk.txt		
Zuletzt besuchte Orte				
Desktop				
Weitere »				
dner 🗸 🗸				
Desktop				

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:

Save converted data to	material file				×
00- 📕 « 14]	Lsi0508 (C:) 🕨 M	aterials 🗸 🗸	Such	ien	٩
🦉 Organisieren 👻	Ansichten	Neuer Ordner	_	-	0
Linkfavoriten Dokumente Weitere » Ordner Desktop	Name	Änderungsdatum Es wurden keine S	Typ Suchergebnis:	Größe se gefunden.	
Dateiname: Dateityp:	NewMaterial_nk Material files (*.n n			Speichem	+ +

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 $\varepsilon(\lambda)$ 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 $\epsilon(\lambda)$ using coefficients for n and k (the wavelength λ given in nm): n

n

$$n(\lambda) = n_0 + C_0 \frac{n_1}{\lambda^2} + C_1 \frac{n_2}{\lambda^4}$$
$$k(\lambda) = k_0 + C_0 \frac{k_1}{\lambda^2} + C_1 \frac{k_2}{\lambda^4}$$

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

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 <u>single wavelength</u> devices. Since at a fixed wavelength the dielectric function degrades to a dielectric constant

 $\widetilde{\epsilon} = \epsilon_1 + i\epsilon_2$ $\widetilde{n} = n + ik$ $\widetilde{\epsilon} = \widetilde{n}^2$

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:

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

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 $\tilde{\epsilon} = 1 + \tilde{\chi}_{ve} + \tilde{\chi}_{ph} + \tilde{\chi}_{fc}$ 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 $\tilde{\epsilon} = 1 + \tilde{\chi}$ a high frequency dielectric constant $\epsilon_{\infty} = 1 + \chi_{ve}$ 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
$$\widetilde{\chi}_{ph}(\nu) = \sum_{k=1}^{k=n} \frac{\Omega_{pk}^2}{\Omega_{ok}^2 - \nu^2 - i\Omega_{\tau k}\nu}$$

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 $\chi_{fc} = \frac{\omega_p^2}{-v^2 - i\omega_\tau v}$, 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

$$\omega_{\rm p} = \sqrt{\frac{ne^2}{\epsilon_0 m^*}}$$
 and $\omega_{\tau} = \frac{e}{m \mu}$, where n is the concentration, μ the mobility and m^* the effective mass

of the carriers and $\boldsymbol{\epsilon}_0$ 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.

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

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:

$$n(E) = n(\infty) + \frac{B_0E + C_0}{E^2 - BE + C}, \ k(E) = \frac{A(E - E_g)^2}{E^2 - BE + C},$$

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

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 = A₀ + A₁m +
$$\frac{A_2}{m}$$
 + $\frac{A_3}{m^2}$ + $\frac{A_4}{m^3}$ + $\frac{A_5}{m^4}$, k = 0,
m = $\left(\frac{\lambda}{1000}\right)^2$, [λ] = 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):

$$\varepsilon_{2}(E) = \begin{cases} \frac{AE_{0}CE(E-E_{g})^{2}}{\left(\left(E^{2}-E_{0}^{2}\right)^{2}+C^{2}E^{2}\right)\left(\left(E-E_{g}\right)^{2}+E_{p}^{2}\right)} & E > E_{t}\\ \frac{E_{1}}{E}\exp\left(\frac{(E-E_{t})}{E_{u}}\right) & E \le E_{t}\\ \varepsilon_{1}(E) = \varepsilon_{1}(\infty) + \frac{2}{\pi}P\int_{E_{g}}^{\infty}\frac{x\varepsilon_{2}(x)}{x^{2}-E^{2}}dx \end{cases}$$

This layer type has 7N+1 constants 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 <u>E</u>dit or in the Recipe options. It allows generating, modifying, or deleting the databases for the AutoModel feature.



Active database: Oxide on	Si	•		Learn	current sample stack
Learned within selected stack Experiments: 1 Entries : 201	(\$)				eriment(s) to database
Air / 4990.0 nm SiO2 (Silicon	odioxide) - therm elete database			10.0 nm 4 eate new d	
Lerning preferences					
Lerning preferences Lower limit (0 T1) T <u>1</u> :	30.0	Step:	3.0	[nm]	De <u>f</u> aults
		Step: Step:	3.0 10.0	[nm] [nm]	De <u>f</u> aults
Lower limit (0 T1) T <u>1</u> :	50.0				Defaults

Fig. 4-48 The AutoModel Database editor.

To create a new database type a name right to the button "<u>C</u>reate new database" and click the button. If you have just performed a measurement, you may click "<u>L</u>earn 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 "<u>M</u>ake 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).

Suchen in:	👋 AR coatings		🧿 🕸 🐸 🖽 🔹			
Name	2	Änderungsdatum	Тур	Größe	Markierun	
SiO2 on	n Ta2O5 on glas	12.09.2008 11:12	Notepad++ Docu	74 KB		
Datei <u>n</u> ame:	SiO2 on Ta2O5 (on glass (cauchy), recipe,	xml			Öğmen
Datei <u>n</u> ame: Dateityp:	SiO2 on Ta2O5	a the second second	xml		•	Öjfnen Abbrechen

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.

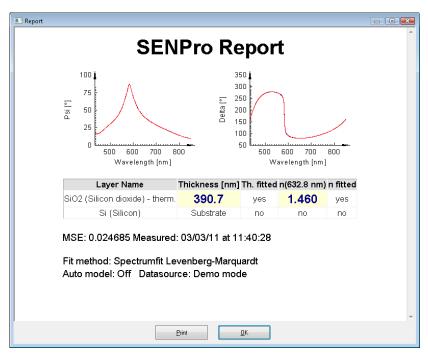


Fig. 4-50: Preview of a print report of a measurement showing the (Ψ, Δ) versus wavelength and the layer stacks with the used and fitted parameters. Click Print to select a printer, OK to leave without printing.

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.

D	ruckeinricht	ung		×
	Drucker			
	<u>N</u> ame:	\\SENTECHS\HP LaserJet 4050 Seri	ies P(🔻	Eigenschaften
	Status:	Bereit		
	Тур:	HP LaserJet 4050 Series PCL 6		
	Standort:	Flur 3.Etage (vor dem Fahrstuhl)		
	Kommenta	r: SW Laserdrucker allgemein		
	Papier		Ausrichtu	ing
	<u>G</u> röße:	A4 •		O Hochformat
	Q <u>u</u> elle:	Auto Select 🔹	Α	© Querformat
	Network	,	ОК	Abbrechen
	Netzwerk	•		Abbrechen

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.*

LOAD SARAS SAVE REDORT NEV ENVIR SMAL PARAM UMM COMP PLOT SEL	ECT AVPL	SENTECI
Reflectivity via Spectrocelli Transmission via Spectrocelli Marketing Vialante Spectrocellia Transmission via Spectrocellia Marketing Vialante Sorght dalups Sorght dalups Denvice Setup Marketing Marketing Denvice Setup Denvice Setup Marketing Denvice Setup Denvice Setup Denvice Setup	Diversion Model 10 0 05 0 05 0 10 -1.0 -1.0 -0.5	Name
Angle of inodesco: # sngle angle 70,00 * multiple angles from \$6,00 * to 70,00 * \$200 : 5,00 *	Defa range:n0*200*RT nange: O display all data row: @ display current. data row Current Experiment: Rad/DushjiBook Defa	🗹 show used only
Rufes Nufes Files Repettons <u>Serge</u> Inter between two measurements: 0.6 s		

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.

Reflectivity via SpectroElli	Transmission via S	PoortroElli	Grating Hardware
Spectroscopic Ellipsometry	Reflectivity	Transmissio	
Name of the sample:	Reneeding	T CHIEFE C	benprendidgo
Measure			Device Setup
			bencebetap
Measure data type:			
Psi, Delta			•
Spectral range:			
from 400,0 nm	to	800,0) nm
Predefined spectral rang	jes:		
Select a pr	edefined Spectral r	ange	-
Angle of incidence:			
 single angle 	70,00 °		
 multiple angles from 		70,00 °	Step: 5,00 °
0		,	
Tools XY-Map HT stage	Repetitions Scri		
AT hop I'm stage	Repetitions Scri		
Goniometer			Position In: 90,00
Angle of incidence:	70,00 °		Out: 90,00
Move sender arm	Move both arms	Move	receiver arm
Before measure move go	niometer to	60,00 °	
After measure move gon	iometer to	70,00 °	

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.

Nam	e of the sample:
	400nm SiO2 on Si

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

Data	
400nm SiO2 on Si / Psi, Delta / Spectral range: 400,0 to 800,0 nm / Angle of incidence: 70,0° / 24.03.2011 09:49:02	

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

	Psi, Delta								-
	Psi, Delta								
	Psi, Delta and degree of polarisation S1, S2 Intensity S1CS2C Mueller matrix Mueller matrix with Psi, Delta								
the selected spectral ra	ange, Spectral range:								
	from	400,0 nm		to	800,0	nm			
the angle of incidence	(or range of angles Angle of incident		ence)						
	🧿 single and	gle	70,00 °]					
	🔘 multiple a	ingles from	50,00 °	to 70,	00 °	Step:	5,00 °		
and date and time of the	ne measurement.								
It is also possible to se		ctral rang d spectral ranges:	ges.						
		Select a predefi Maximum Spect Default Spectra DUV Spectral ra UVVIS Spectral	ined Spectral rang ned Spectral rang ral range (190.0 - I range (320.0 - 93 nge (190.0 - 400.) range (400.0 - 93) nge (790.0 - 2500	e 2500.0) 30.0) 0) 0.0)		•			

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).

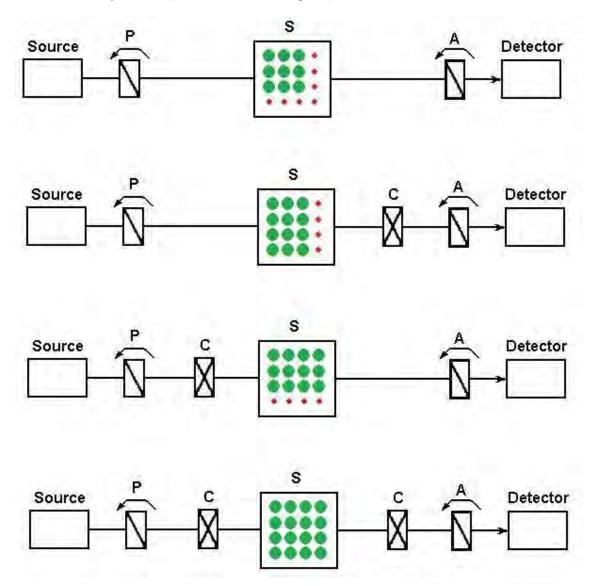


Fig. 5-3 Setups for Mueller matrix measurements

Fig. 5-4 shows the Mueller matrix measurement mode. For measuring the Mueller matrix the Fouriercoefficients 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.

Refle	ctivity via SpectroElli		Hardw	are
Spectr	oscopic Ellipsometry		Script dia	logs
Name of the sam	ple:			
Measure Measure data ty	pe:		Device	e Setup
Mueller matr	ix		▼ Pol. steps:	30 ° 🔽
Spectral range:	DUV 🗸	UVVIS 🗸]	45 ° 30 °
from	190,0 nm	to	1700,0 nm	15° 10°
Predefined s	pectral ranges:			5° 2°
	Select a predefined	Spectral rar	nge	•

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").

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-Axis:	Wavelength		·			lse al		Use	none					
Col	or y-Axis		z-Axis		z-Value	Use	View	Mod.	Minimum	Maximum	Device ty	pe	Rotatio	n type
	S1	Ŧ	Polapos	-	89,987				-1,00440	-0,99681	NONE	-	RAE	•
	S2	Ŧ	Polapos	-	89,987	×			-0,00438	0,00382	NONE	•	RAE	-
	Intensity	•	Polapos	-	89,987	V			0,09865	2,53976		•	RAE	-
	S1	_	Polapos	•	-44,973				-0,94069	-0,42249		-	RAE	-
	S2	_	Polapos	•	-44,973				0,21109	0,39377		•	RAE	-
	Intensity	•	Polapos	•	-44,973				0,05174	1,29766		•	RAE	-
	S1	•	Polapos	•	0,012				0,98355	1,00731		•	RAE	
	S2	•	Polapos	•	0,012				-0,01501	0,01408		•	RAE	
	Intensity	_	Polapos	•	0,012				0,00358	0,88741		•	RAE	
	S1	•	Polapos Balanas	•	45,005				-0,94055	-0,42118		•	RAE	
	S2	•	Polapos Deleneo	•	45,005	2	V		-0,39312	-0,20896		•	RAE	
2	Intensity S1o	-	Polapos Polopos	•	45,005 -44,973				0,05011	1,30922		-	RAE RAE	
	S1c S2c	_	Polapos Polanos	• •	-44,973 -44,973				-0,94554 -0,89842	-0,38721		-	RAE	
		• •	Polapos Polapos	• •	-44,973				-0,89842	-0,22355 1,28497		• •	RAE	
;	Intensity S1c	Ŧ	Polapos Polapos	• •	-44,973 45,005	V V			-0,93936	-0,44759		• •	RAE	• •
·	S2c	Ŧ	Polapos	•	45,005			-	0,93938	0,86599		•	RAE	
}	Intensity	_	Polapos	Ŧ	45,005			-	0,04414	1,35656		• •	RAE	
	S1c	Ŧ	Polapos	•	-44,973			Ē	-0,92605	-0.48699			RAE	
	S2c	_	Polapos	Ŧ	-44,973			Ē	-0,85689	-0,25612		•	RAE	•
	Intensity	Ŧ	Polapos	•	-44,973			Ē	0,04772	1,21103		•	RAE	•
2	S1c	_	Polapos	•	45,005			Ē	-0,95442	-0,34332		•	RAE	-
	S2c	_	Polapos	Ŧ	45,005			Г	0,19222	0,90790		-	RAE	-
	Intensity	Ŧ	Polapos	Ŧ	45,005			Г	0,04512	1,16108		-	RAE	
;	S1c	Ŧ	Polapos	-	89,987			Г	-1,00174	-0,99393		-	RAE	-
;	S2c	•	Polapos	-	89,987			Г	-0,03569	0,07227		-	RAE	•
·	Intensity	•	Polapos	-	89,987			Г	0,08950	2,29865	NONE	-	RAE	-
1	S1cc	•	Polapos	-	45,005				-0,93710	-0,48976	PCSCA	-	RAE	-
	S2cc	•	Polapos	•	45,005				0,18564	0,50442	PCSCA	•	RAE	-
)	Intensity	Ŧ	Polapos	•	45,005	×			0,03994	1,10297	NONE	•	RAE	-
	Retphase	•	None	-					-93,03712	-86,88820	PSCA	•	RAE	-
2	Retaxis	_	None	-					-2,08436	0,95679		•	RAE	-
;	Retgamma	_	None	•					-0,00730	0,00641		•	RAE	
	Retphase	_	None	•					-93,60159	-83,78555		•	RAE	-
	Retaxis	_	None	•					-0,80197	1,35687		•	RAE	-
	Retgamma	_	None	•					-0,00984	0,00305		•	RAE	
	M11	_	Phi	•	70,00				1,00000	1,00000		•	RAE	
	M12	-	Phi	•	70,00				-0,93861	-0,42190		•	RAE	
	M13	•	Phi Dhi	•	70,00 70.00	V	V V		-0,02075	0,01929		-	RAE	
	M14 M21	-	Phi Phi	•	70,00 70,00				-0,02426	0,02212 -0,42241		• •	RAE	
2	M22		Phi Phi	• •	70,00				-0,94029 0,99716				RAE	
	M23		Phi	•	70,00				-0,01482	0,01833			RAE	• •
	M24	_	Phi	•	70,00				-0,01402				RAE	
	tx-Axis: fron Trim fron		350,273 350,273		to 980,380 to 980,38			" ead	n 1					

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

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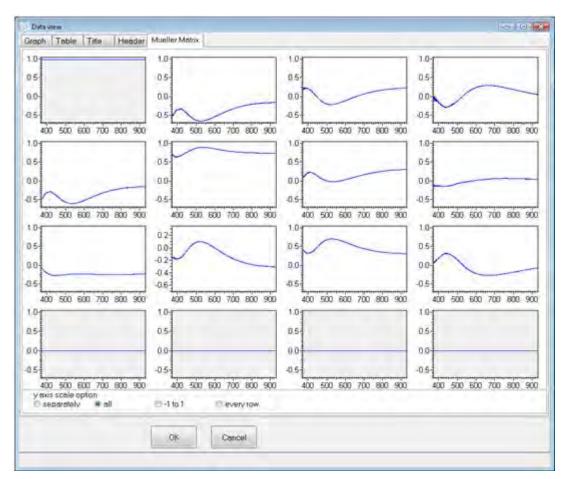


Fig. 5-7 Mueller matrix spectra

The 16 graphs in Fig. 5-7 show the 16 Mueller matrix elements in dependence of the wavelength. Depending on the measurement device 12 (PCSA³ 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).



SpectraRay/4

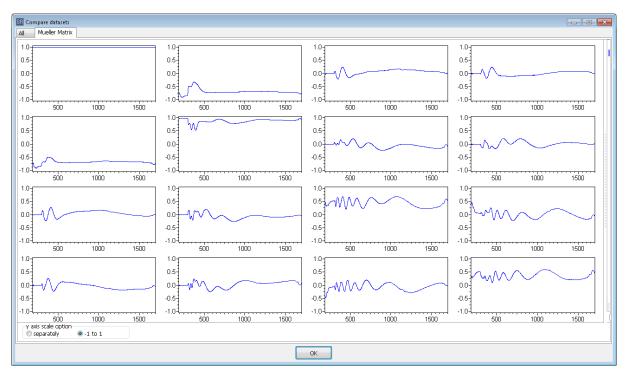


Fig. 5-8 Mueller matrix measurement with a PCSCA device

5.1.1.3 Reflectivity

Reflectivity	via SpectroElli	Transmission	n via SpectroElli	Hardware
Spectroscop	ic Ellipsometry	Reflectivity	Transmission	Script dialogs
Name of the :	sample:			
400nm Si	iO2 on Si			
Measure re		Measure dark	Measu	re reflectivity
Spectral rang				
from	400,0 nm	to	800,0 nm	
Predefine	ed spectral range	s:		
	Select a prec	defined Spectral r	ange	•
Number of sc	ans:			
1				

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 Measure reference and Measure dark. 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 north. For the dark maggingment you need a gracial teal which reflects all of the light out of the light not

1

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

Transmission	Script dialogs
ission	
ission	
nission	
to 800,0 nm	
l range	•
	to 800,0 nm al range

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 Measure transmission you have to

you have to measure a background

spectrum without any sample in the light path by clicking Measure background. 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 (dia-gram).



5.1.1.5 Script dialogs



Fig. 5-11 Script dialogs tab

When you click on $\boxed{}$ 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.

Spectroscopic Ellipsometry Reflectivity Transmission Script dialogs C:\Sentech\SpectraRay\ApplicationFrame\Measure_LineScan.scr Line Scan Ellipsometer Th in nm center distance position start position end Step[mm]: x: -2.000 x: 2.000 0.100 y: 0.000 y: 0.000	Reflectivity via SpectroElli	Transmission	n via Spectro	Elli	Hardware
Line Scan Ellipsometer Th in nm Center distance position start position end Step[mm]: x: -2.000 x: 2.000 0.100	Spectroscopic Ellipsometry	Reflectivity	Transmissi	ion	Script dialogs
x -2.000 x: 2.000 0.100	Line Scan Ellipsometr	er 🔹 Th	in nm 🔻	Cer	nter distance
0.100					
				0.100	
Measure					

Fig. 5-12 Example for a script dialog

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



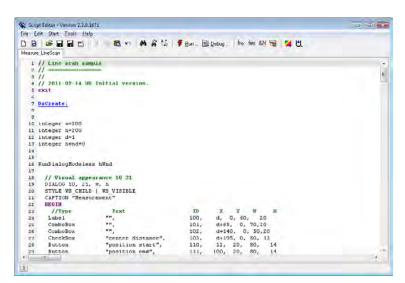


Fig. 5-13 Scripting example

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

5.1.1.6 Reflectivity via SpectroElli

Spectroscopic	Ellipsometry	Reflectiv	ty	Trans	mission	9	cript dialogs
Reflectivity vi	ia SpectroElli	Transr	Transmission via SpectroElli				Hardware
Name of the sar	nple:						
				_			
Measure Refe	rence	Measure Rel	lectivit	У		Device	: Setup
Spectral range:							
from	400,0 nm		to		800,0	nm	
Predefined	spectral range	s:					
Select a predefined Spectral range 🔹							
Angle of inciden	ce:						
 single an 	gle	70,00 °					
🔘 multiple a	angles from	50,00 °	to	70,0	0 °	Step	5,00 °
Polarization:							
s-polarizati	on (90°)	-					
Intensities for re	eference meas	urement:					
Overflow:	95	,0 %					
Target:	85	,0%	Ĩ.				
Underflow:	10	,0 %	ĩ				

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

gle of incidence:							
💿 single angle		70,00 °					
multiple angles	from	50,00 °	to	70,00 °	Step:	5,00 °	

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

Polarization:

s-polarization (90°)	-
s-polarization (90°) p-polarization (0°) s- and p-polarization	

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	Measure Reflection
Underflow:	10,0 %
Target:	85,0 %
Overflow:	95,0 %
Intensities for reference m	easurement:

you have to measure a reference spec-

trum by clicking Measure Reference. 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

Spectroscop	ic Ellipsometry	Reflectivity	Transmission	Script dialogs
Reflectivity	via SpectroElli	Transmissi	on via SpectroElli	Hardware
Name of the s	ample:			
Measure Ba	ckground Me	easure Transmi	ssion D	evice Setup
Spectral rang	e:			
from	400,0 nm		:o 800,0 nr	n
Predefine	d spectral ranges	:		
	Select a prede	efined Spectral	range	-
Intoncitu for l	background measu	rement		
Target:	65,0			
rargoti	00,0	5 10		

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 Measure Transmission you have to measure a background

spectrum without any sample in the light path by clicking Measure Background. 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

Spectroscopic Ellips	sometry	R	eflecti	vity	Scrip	t dialogs
Reflectivity via Spectro	Elli Tra	ansmission '	via Spe	ectroElli	Grating	Hardware
Name of the sample:						
Reflectivity with refere	oce mode	əl				
Kenecowcy warrerer		-1				
Measure Reference	Me	asure Refle	ectivity		Device	Setup
Spectral range:	, <u> </u>					
from 250,0	nm		to	850	,0 nm	
Predefined spectra	I ranges:					
Selec	t a predef	ined Specti	ral ran	ge		•
Angle of incidence:						
single angle	70	0,00 °				
🔘 multiple angles	from 50	0,00 °	to	70,00 °	Step:	5,00 °
Angle of reflection:						
single angle	7	0,00 °	1			
multiple angles	_	0,00 °	to	70,00 °	Step:	5,00 °
Polarization:						
s-polarization (90°) •	-				
Intensities for reference	e measure	ement:				
Overflow:	95,0	%				
Target:	85,0	%				
Underflow:	10,0	%]			

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.

,	
Reflectivity with reference model	-
Reflectivity with reference model	
Reflectivity without reference model	
Transmission	
Psi/Delta	
5152	
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).

Angle of incidence:						
single angle		70,00 °]			
multiple angles	from	50,00 °	to	70,00 °	Step: 5,0	° 0
Angle of reflection:						
single angle		70,00 °				
multiple angles	from	70,00 °	to	70,00 °	Step: 5,0	0 °

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 Measure Reference 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 Measure Reflectivity.

Device Setup

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.

Polarization:	
s-polarization (90°)	•
Intensities for reference m	easurement:
Overflow:	0,950
Target:	0,850
Underflow:	0,100

5.1.1.8.2 Reflectivity without reference model

Spectroscopic	Ellipsometry	y Reflectiv	/ity	Transmiss	ion So	ript dialogs
Reflectivity via	SpectroElli	Transmissio	n via Sp	ectroElli	Grating	Hardware
Name of the sa	mple:					
Reflectivity wit	hout refere	nce model				•
Measure Refe	erence	Measure Re	flectivity	/	Device !	Setup
Spectral range:						
from	400,0 nm		to	800	,0 nm	
Predefined	spectral rar	nges:				
	Select a p	predefined Spe	ctral ran	ge		-
Angle of incider	ice:					
 single an 	gle	70,00 °				
🔘 multiple a	angles fro	om 50,00 °	to	70,00 °	Step:	5,00 °
Angle of reflect	tion:					
single ar		70,00 °				
multiple	-	om 70,00 °	to	70,00 °	Step:	5,00 °
Polarization:						
s-polarizati	ion (90°)	•				
Intensities for r	eference m	easurement:				
Overflow:		0,950				
Target:		0,850				
Underflow:		0,100				

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 Measure Reference. 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).

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5.1.1.8.3 Transmission

Spectroscopic E		Reflectivi		Transmissio		ript dialogs
Reflectivity via S	SpectroElli	Transmission	i via Sp	ectroElli	Grating	Hardware
Name of the sam	ple:					
Transmission						•
Measure Backg	round	Measure Tran	nsmissio	n	Device	Setup
Spectral range:						
from	400,0 nm		to	800,	0 nm	
Predefined s	pectral rang	es:				
	Select a pre	edefined Spec	tral ran	ge		-
Angle of incidence	e:					
single ang		70,00 °	1			
multiple ar			to	70,00 °	Step:	5,00 °
Angle of reflecti						
single and		70,00 °				
	-		۲.		_	
multiple a	ingles fron	n 70,00 °	to	70,00 °	Step:	5,00 °
Polarization:						
s-polarizatio	n (90°)	•				
Intensity for bac	kground mea	asurement:				
Target:	0	,650				

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

Spectroscopic E	Ellipson	netry	Reflectiv	ity	Transmiss	ion S	cript dialogs
Reflectivity via	Spectro	Elli	Transmissio	n via Sp	ectroElli	Grating	Hardware
Name of the sam	ple:						
Psi/Delta							-
raijoetta)			_		
Measure		J				Device	Setup
Spectral range:							
from	400,0	nm		to	800	,0 nm	
Predefined s	pectra	l range	s:				
	Selec	t a prec	defined Spe	ctral rar	nge		•
Angle of incidence	e:						
single ang	le		70,00 °				
🔘 multiple ar	ngles	from	50,00 °	to	70,00 °	Step:	5,00 °
Angle of reflecti	on:						
single and	gle		70,00 °				
🔘 multiple a	angles	from	70,00 °	to	70,00 °	Step	5,00 °

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

Spectroscopic Ellipsometry	Reflectivity	Transmission	Script dialogs
Reflectivity via SpectroElli	Transmission	n via SpectroElli	Hardware
Refresh			
Measurement Devices			
Spectroscopic ellipsometer	SE 850 (UV/VIS Driver OK	HNIR)	
Laser ellipsometer	not available -		
FTPadvanced	FTPadvanced Driver OK		
General			
Goniometer type	Automatic goni	ometer	
Status	available, initia	lized	Init
Stage	Automatic xy n	napping stage	
Status	available, initia	lized	Init
Turn table	none		
Status	not available		
Auto alignment	Video based he	ight system	
Status	available, initia	lized	Init
Objective slider	found		
Status	moved in		

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

Tools	XY-Map	HT stage	Repetitions	Script	pt	
Goniome	eter			_	Position	
Angl	e of incide	ence:	70,00 °		In: 90,00 Out: 90,00	
Mov	ve sender	arm	Move both a	arms	Move receiver arm	
🔲 Befo	re measu	re move gor	niometer to	6	60,00 °	
🔲 Afte	r measure	move goni	ometer to	7	70,00 °	

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: 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.

		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

SENTECH

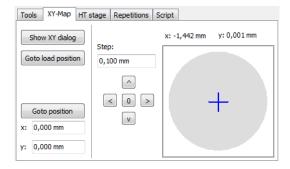
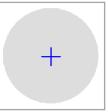


Fig. 5-22 XY-Map

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

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

	Goto position
x:	0,000 mm
y:	0,000 mm

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

SENTECH S

leight and tilt stage		XY mapping stage		XY mappin	ng stage with coor	dinate systems an	d sample frames	1
Alpha tilt angle	Beta tilt angle	× position	Y position	Coordinal	e systems and sa	mple frames: Di	sabled	
0.000 deg	0.000 deg	-1.442 mm	0.001 mm	Active sa	mole frame: #0	OriaX: 0.000 Ori	ry: 0.000 SizeX	i n
		***				1.000 Angle: 0.000		
0 deg	0 deg	0 mm XYGota	a 0 mm	Coordinal	re system: 0	Mapping stage (st	andard system)	•
Height (at C-axis, negative)	Z Height (at meas spot, negative)	Radius (R)	Angle (Theta)	Move o	urrent point from (old CS to new CS	Auto mos	ve
-0.663 mm	-0.663 mm	1.442 mm	179.9603 deg	XY M	ove current point i	in CS to camera	[]	
··· ·· · · + +++	··· · · · + ++ +++	··· · · · + + ++	· · · * ++ +++	×	Y Go to genter po	sition in CS	1	
0 ABH Got	a 0 ABZ Go to	0 mm RTGote	i O deg	X in CS:	-1.442 mm	Yin C	S: 0.001	mm
HT Store position	HT Go to stored position	XY Store position XY Go to	stored pos.		0 mm	XY in CS Go to	0	mm
HT Go to load position	Const. height at meas. spot	XY Go to load position XY Go to F	efi Rei pos.: 0 Standard 🔹	BinCS:	1.442 mm	Theta in C	6: 179.9603	deg
ample pos Get und Goto	Backstep before goto	XY Go to genter position XY Go to Tr	ans Ref pos.; 0 Standard 🔹	•	0 mm	RT in CS Ga to	0	deg
		XY Go to repair position XY Go to	Dark pos. DStandard 🔹	IsXouto	if frame: 0	Is Yout o	if frame: 0	
IT Go to reference (initialize)	Is initialized	XY Go to reference (init.)	initialized	X Out dis	tance: 0.000	mm YOut dis	tance: 0.000	m
HT Uninitialize		XY Uninitialize		XYM	ove from border o	r exclusion into sa	mple frame	
Jpdate position	148	Teach coordinate syste	ms and sample frames					
ommand: Finished.	Reset Communication	CoSys origin xy (negati	ve of current pos.): 0	0	Get CS or	igin Se	t CS origin to co	onfig
TOC	Heset Communication	Sample frame top left x	y. 0	0	Get SF top	left Set SF	origin (center) t	o config
101.		Sample frame bottom ri	ght xy: 0	0	Get SF botto	m right Se	et SF sizes to co	nfig
		Exclusion top left xy:	0	0	Get exclusion	top left Set exc	Lorigin (center)	to config
<< Show less	ОК	Exclusion bottom right	хо [.] П	0	Get excl. botto	and the second	clusion sizes to	

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

Show	alignmer	nt dialog	Auto align	Close camera
Step:	0,	100 mm		
Position	z; -	-27,768 mm		
		~		5 0
				_diakini
Goto refe	rence	V		= V

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.
snow alignment dialog	opens an advanced alignment dialog.

1 ·	AutoFocus	Stage movement
	Substrate thickness [mm]	Current height [mm]: 0.000
25'	1	Go to Down 0.50 mm 🔻 Up
15' —	Height scanning range [m	m]: Current Tilt vertically: -0.0 '
	20' 25' 30 0.50	Up 10' V Down
5'	relative to current p	
	🔘 absolute	Current Tilt horizontal: 0.0
	relative around subs	
1 30' 25' 20' 15' 10' 5' W		Right 10' V Left
1. E	Height offset after scan [[mm]: 0.000
- 15'	Reset tilt before heigh	Goto parallel Initialize stage
	Camera	Turntable
	Gain for viewing:	25 motorized turntable Init
Video heig	ht Video tilt Exposure Time [ms]:	10.00 Position [°]: Goto
age not available or not setup.	V Auto exposure for vie	ewing AutoTilt
	Gain for scanning:	0 V Show ROI
	Scan details	
Run Autoalign	More <-> Less	Tilt with only one step (fast)
(Focus and Tilt)	Provide the second seco	Setup tilt

Fig. 5-25 Sample alignment

It is also possible to move the sample stage "manually" one step into the desired direction by clicking on \square . 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.

0,100 mm
z: -27,768 mm

Goto reference

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

5.1.1.13 Repetitions

Tools	XY-Map	HT stage	Repetitions	Script
Number	rofmeasu	rements:		
1]	
Time be	tween two	measurem	ients:	
0,	0 s			

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

Tools	XY-Map	HT stage	Repetitions	Script		
📃 enat	ole script				all options are script labels	
					😰	
	OnStart			Onl	UserAbort	
	OnFinish			OnE	Error	
	OnBeforeS	SingleMeasu	rement	On/	AfterSingleMeasurement	
	OnBeforeT	urnTable		On/	AfterTurnTable	
	OnBeforeGoniometer			OnAfterGoniometer		
	OnBeforeA	AutoAlign		On/	AfterAutoAlign	

Fig. 5-27 Script

The script tab allows using additional scripts for your measurement. By checking \square enable script you can use a script which you have loaded by clicking on \square . \square 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.

ConStart	OnUserAbort
🔲 OnFinish	OnError
CnBeforeSingleMeasurement	📝 OnAfterSingleMeasurement
OnBeforeTurnTable	🔲 OnAfterTurnTable
OnBeforeGoniometer	OnAfterGoniometer
🔲 OnBeforeAutoAlign	🔲 OnAfterAutoAlign

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.

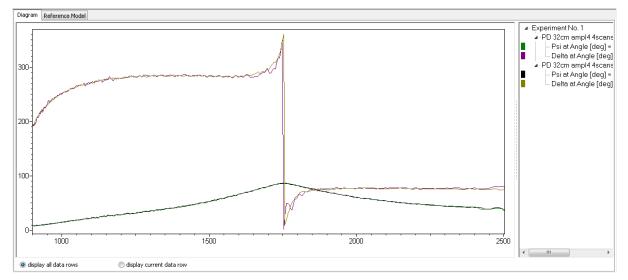


Fig. 5-28 Diagram - display all data rows

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

PD 32cm ampl4 4scans steps 8/2 fourier 1 - 1:12

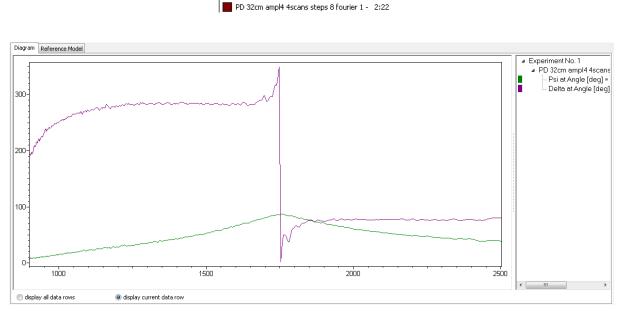
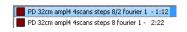


Fig. 5-29 Diagram – display current data row

If ^(a) 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 measure-

ments (see Fig. 5-30). Clicking on \cong allows loading a model. Clicking on \cong allows editing layers of a selected model.

Diagram	Reference Model					
reference	e model for reflectivity meas	urement				😰 📂
Title		Thickness	State	Layer Type	Info [799,9 nm]	
Air	\checkmark			NK layer	n=1,0000	
	Cau-SiO2 (therm.)	2,00 nm		Cauchy layer	n=1,4576	
	Silicon VIS+NIR			File layer	n=3,6819 k=0,00448	
I						

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.

Current Experiment Ref/Dark/Back	
Data	📐 🗕 📕 🎽
PD 32cm ampl4 4scans steps 8/2 fourier 1 - 1:12	
PD 32cm ampl4 4scans steps 8 fourier 1 - 2:22	
D D 32cm ampl4 16scans steps 8 fourier 1 - 4:18	
DPD 32cm ampl4 16scans steps 8 fourier 4 - 16:16	

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.

Dat	ā
	2 nm / Psi, Delta / Spectral range: 370.3 nm - 970.2 nm / Angle of incidence: 70.0° / 04.09.2013 09:17:56
	100 nm / Psi, Delta / Spectral range: 370.3 nm - 970.2 nm / Angle of incidence: 70.0° / 04.09.2013 09:13:08
	20 nm / Psi, Delta / Spectral range: 370.3 nm - 970.2 nm / Angle of incidence: 70.0° / 04.09.2013 09:11:08
Ē	400 nm / Psi, Delta / Spectral range: 370.3 nm - 970.2 nm / Angle of incidence: 70.0° / 04.09.2013 09:15:21
	Copy: 2 nm / Psi, Delta / Spectral range: 370.3 nm - 970.2 nm / Angle of incidence: 70.0° / 04.09.2013 09:17:56

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

ype	Waverange	goniometer angle	polarization	time
10 01 transmission background	190,1 nm - 919,9 nm	90,00	s-pol.	3/24/2011 3:01:19 PM
10 01 transmission dark	190, 1 nm - 919, 9 nm	90,00	s-pol.	3/24/2011 3:01:24 PM

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.

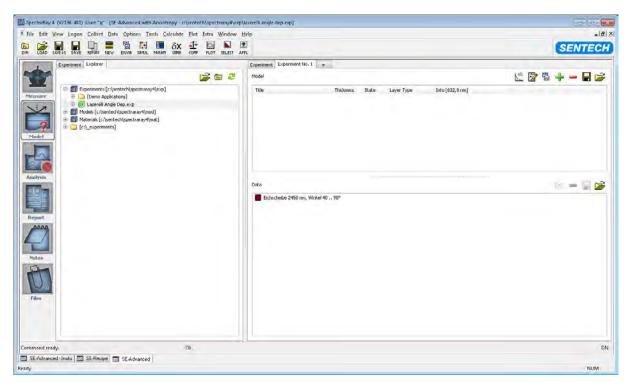


Fig. 5-33 Main screen with "Laserelli Angle Dep.exp" loaded and a new (empty) model created

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. SiO₂". This can be done by dragging the material name and dropping it onto the model box at the desired position⁴. 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 dis- played 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					

⁴see also Appendix A: Drag&Drop Overview

Experiments directory	this directory is used to search for experiment files *.exp which are dis- played 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

Directories		BX
Materials:	c:\sentech\spectraray4\mat	
Measurements:	c:\sentech\spectraray4\data	
Models:	c:\sentech\spectraray4\mod	
Experiments:	c:\sentech\spectraray4\exp	
Recipes:	c:\sentech\spectraray4\icp	
Applications:	c_applications	
Custom Directones:	C:_experiments	
	DK	

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.

Die d	SpectraRay 4 (V/2196-401) User: "g" - (SE-Advanced with Ar		
Personer Perso	a 🚅 🖬 🖬 🖬 = 🖏 🗃 I	🕷 δχ 💤 🖾 🔍 🔳	SENTECH
	In LOAD SAVES GAVE INFORMATION OF DAVID GAVE, DAVID GA	Experiment reprint reprint	L" 🕼 🖶 🗕 🖬 🚁
3 SE-Advanced - Insta J 🔤 SE-Recupe 🔤 SE-advanced	Command ready.	OF.	DN
90y NUM			

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.

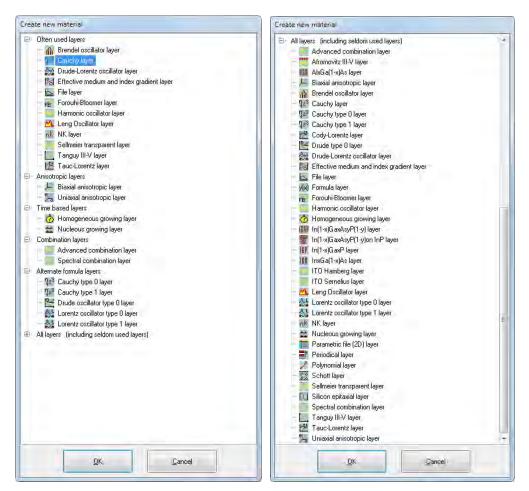


Fig. 5-36: Available layer types

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
Н	Fixed n and k	Constant dispersion	Only air
Н	Cauchy	transparent dielectric materials Photoresist Glass	SiO ₂ , Al ₂ O ₃ , Si ₃ N ₄ , TiO ₂ PMMA BK7, quartz
Н	Tauc-Lorentz	Absorbing dielectric materials amorphous materials	Si₃N₄, TiO₂ a-Si, a-C
Н	Drude-Lorentz	Metals TCO (transparent conductive oxide)	Au, Ag, Cu, Cr, Ni ITO, ZnO:Al
Н	File-Layer	Table of wavelength, n, k, no fit parameters	Good for all
		substrates	Si, Ge, GaAs, quartz
Μ	Leng-Lorentz	Crystalline indirect semiconductors polycrystalline indirect semiconduct. conjugated polymers (OLED, OFET)	c-Si, c-Ge, c-SiGe poly-Si MEH-PPV, P3HT
Μ	Brendel	Absorption (vibration) bands in the \ensuremath{MIR}	SiO2, SiN, CH-bonds
Μ	Sellmeier	Like Cauchy but for broader spectral range (VIS + NIR)	SiO ₂
Μ	Tanguy III/V	Bandgap of direct semiconductors, also II/VI	GaAs, GaN, AlGaN ZnSe
L	Hamberg Sernelius	TCO (transparent conductive oxide)	ITO, ZnO:AI, 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
Н	EMA (effective medium approximation)	Mixture of two materials Roughness Interface Gradient	mixture: Air / layer mixture: layer1 / layer2
М	Biaxial anisotropic	Direction dependent dispersion	Crystalline quartz
М	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 _x Ge _{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.

The kines Image: Solution Image: Solution<	Dispersion - Tauc-Lorentz layer	Name	FR.	Value	Scroll value	Minimum	Maximum		a ler	Later -				leii	Scre
Chronic DB nm More Imm Imm Consol 9 99999 999909 0.0000<	syer name: Zr02 · [DUVN]					hinmum .n nn		Typ, Diff	Accuracy Dig	Vien	Reset Min	Bobbo BD Anim	Scroll Step		
Character Column			-	1.00000						4					
Int Marchy 1.0000 400 V 16.0000 C 0.0000 <td< td=""><td>Z Thickness: 0.00 nm More</td><td></td><td></td><td>4.5327</td><td>1 1</td><td></td><td>1000,0000</td><td></td><td></td><td></td><td></td><td>8 0000 Ani</td><td>0.2100</td><td></td><td>120</td></td<>	Z Thickness: 0.00 nm More			4.5327	1 1		1000,0000					8 0000 Ani	0.2100		120
No. Use EditV1 AcV EditV1 AcV C(0) ✓ 34433 * * 0.0000 0.2280 0.001018 ✓ 0.0000 Acv 0.00000 Acv	et infinity 1.00000	A(0)										200.000 Am	10.000		
2 00 • • 0<	No Line Estant Arant Entant Chart T	E0(0)	4												
2 00 • • 0<	0 Ves + V 1 5327 V 196 963 V 7 5040 V 3 4043	C(0)	2		1 1					~		8.0000 Ani			
2 00 • • 0<	1 yea + 9 1 1669 9 4 245 9 7 7363 9 4 4210 -	Eg(1)	15												+
	2 no	P4 11	4	7 7363											-
			V	4.4210			1000.0000								
	7 m • • • • • • • • • • • • • • • • • •														

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

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.

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

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 (\mathbf{t}), from a directory with material files (\mathbf{t}) 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 (\square) or deleted (\square).

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.

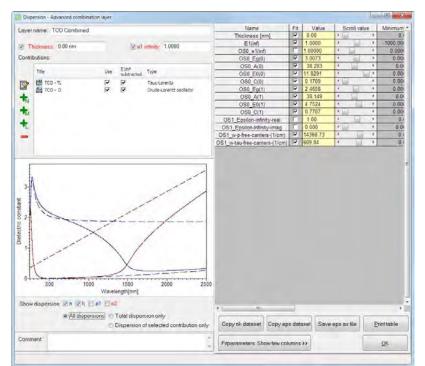


Fig. 5-38 Advanced combination layer editor

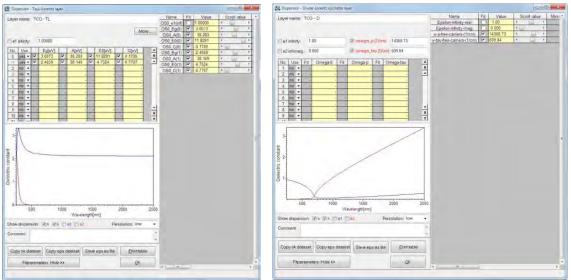


Fig. 5-39 Contributions of advanced combination layer



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:

$$E_g(y) = 1.35 - 0.75 \cdot y + 0.12 \cdot y^2$$

$$E_0(y) = 3.391 - 1.652 \cdot y + 0.863 \cdot y^2 - 0.123 \cdot y^3$$

$$E_i = eV$$

$$E_d(y) = 28.91 - 9.278 \cdot y + 5.626 \cdot y^2$$

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

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

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

$$\begin{aligned} k &= \operatorname{Im}[\varepsilon] & \text{if } E < E_g \\ k &= \operatorname{Im}[\varepsilon] + c(E - E_g) + d(E - E_g)^2 & \text{if } E \ge E_g \end{aligned}$$

Standard values for the parameters and their meaning are:

Parameter	Default value	Description
Gamma	0.001	Damping at E _g [eV]
х	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]
с	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.

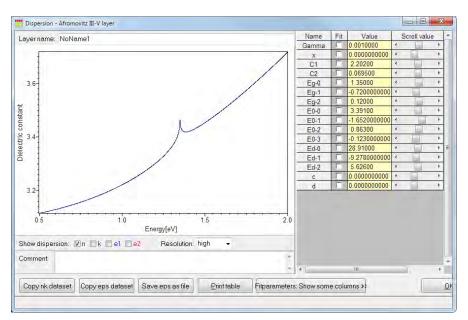


Fig. 5-41 Example for an Afromovitz layer (n)

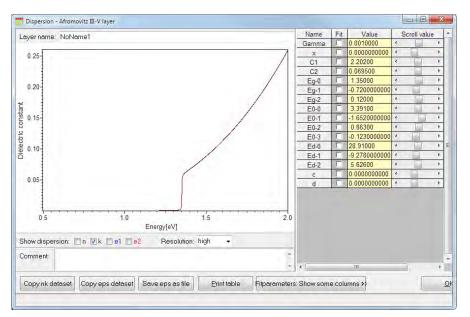


Fig. 5-42 Example for an Afromovitz layer (k)



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.

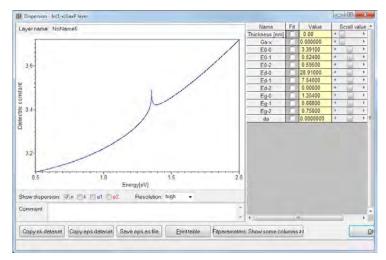


Fig. 5-43 Example for In(1-x)Ga(x)P editor (n)

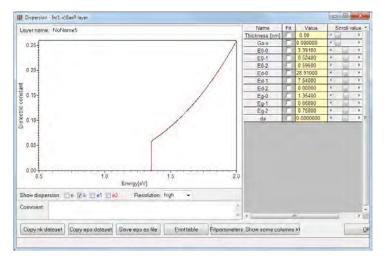


Fig. 5-44 Example for In(1-x)Ga(x)P editor (k)

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:

$$\underbrace{\widetilde{\varepsilon}}_{=Ci} = \begin{pmatrix} \widetilde{\varepsilon}_{xi} & 0 & 0 \\ 0 & \widetilde{\varepsilon}_{y_i} & 0 \\ 0 & 0 & \widetilde{\varepsilon}_{z_i} \end{pmatrix}$$

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.



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Fig. 5-45 Example for biaxial layer



Fig. 5-46 Definition of observation values for display

Title	Thickness	State	Layer Type	Info [633.0 nm]
Air 📝			NK layer	n=1.0000
CaCO3			Biaxial anisotropic	n=1.5950
CaCO3 o			Cauchy layer	n=1.6500
CaCO3 e			Cauchy layer	n=1.4850
CaCO3 o			Cauchy layer	n=1.6500

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



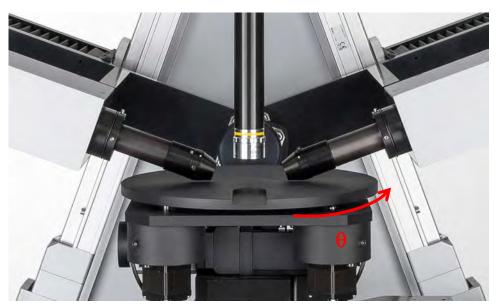


Fig. 5-48 Sample on rotatable sample stage and angle $\boldsymbol{\theta}$

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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

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.

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

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

Susceptibility of the Brendel oscillator k χ_k

Resonance frequency / cm⁻¹ V_{0k}

- $v_{\mathrm{T}k}$ Damping of the oscillator / cm⁻¹
- Oscillator strength / cm⁻¹ V_{Pk}
- Standard deviation of the centre frequency / cm⁻¹ $\sigma_{\scriptscriptstyle k}$
- 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

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An example for the Brendel oscillator with damping of the oscillator term $v_{Tk} > 0$ 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 v_{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 .

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							nu-p(0)	F	1000.00	*		0.10
							Sigma(0)	Г	100.000	4		0.010
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Fig. 5-50 Brendel oscillator with damping and standard variation



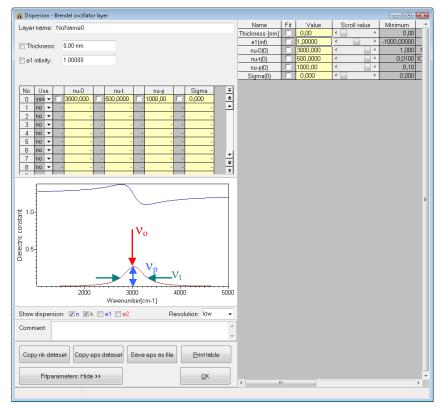


Fig. 5-51 Brendel oscillator with standard deviation equal to 0 (like Lorentz-oscillator)

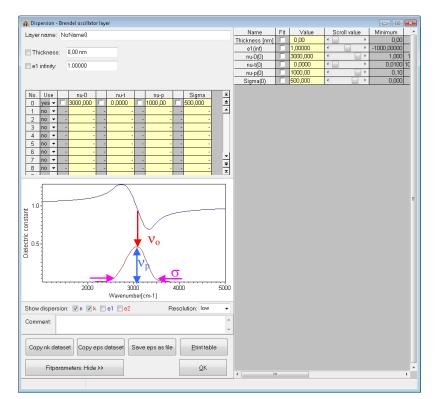


Fig. 5-52 Brendel oscillator with damping equal to 0 (like Gaussian-oscillator)

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 SiO₂, Al₂O₃, Si₃N₄ and TiO₂. 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:

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

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

$[n_i], [k_i]$: 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.



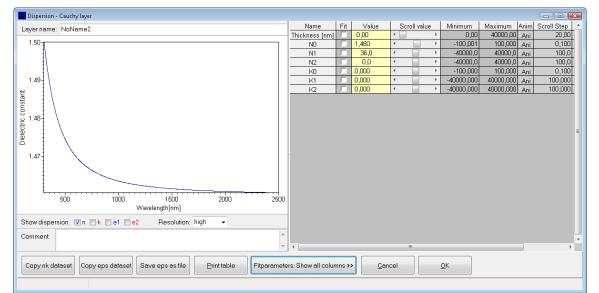


Fig. 5-53 Cauchy layer editor

Name	Fit	Value	Тур.	Minimum	Maximum	Reset	Reset	Accuracy
			Diff.			Min.	Max.	
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 SiO₂. 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 SiO₂

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



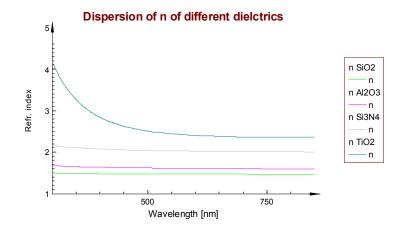


Fig. 5-55 Cauchy dispersion of different dielectrics

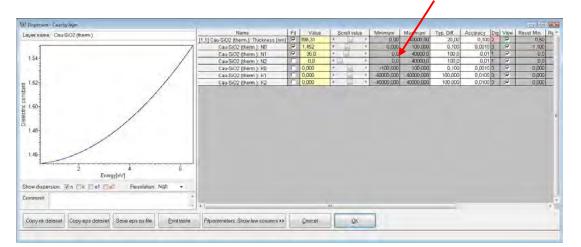


Fig. 5-56 Cauchy layer minimum values

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.

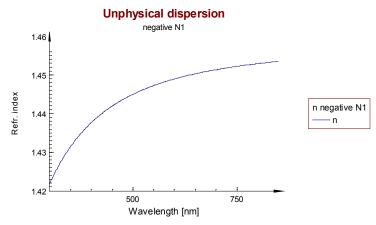


Fig. 5-57 Cauchy layer unphysical solution



Anormal dispersion:

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

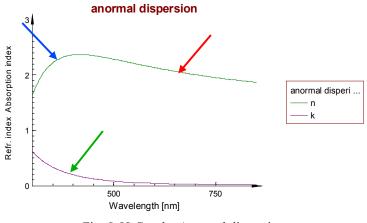


Fig. 5-58 Cauchy Anormal dispersion

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:

$$n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4} \qquad [\lambda] - \mu m, \ [A_n]: \text{ dimensionless, } \ [B_n] - \mu m^2, \ [C_n] - \mu m^4$$
$$k(\lambda) = A_k \cdot e^{B_k(E-C_k)} \qquad [E] - eV, \ [A_k]: \text{ dimensionless, } \ [B_k] - eV^{-1}, \ [C_n] - eV$$

Cauchy-type1-layer:

$$n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4} \qquad [\lambda] - \mu m, \ [A_n]: \text{ dimensionless, } \ [B_n] - \mu m^2, \ [C_n] - \mu m^4$$
$$k(\lambda) = 10^{A_k} \cdot e^{B_k(E-C_k)} \qquad [E] - eV, \ [A_k]: \text{ dimensionless, } \ [B_k] - eV^{-1}, \ [C_n] - eV$$

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.

							00
Levername, Cout)	Name	Fit	Value	S	crall value	Meimum	Maximum
	DS0 An	10.1	1.450		- hal-	100.001	100.000
15	OS0 Bri	15 1	0.01000		Aug	1.00000	
	OS0_Cn	10	0.000000	100	And in	* -1 989000	1,000000
	OS0 Ak	C1	0.100	10	And in the	-10.000	
1	OS0 BK	(Γ)	0.750	1	100		
	DS0_Ck	101	3.100		1011	* -10.000	10.000
500 1500 1500 V/zeviengst(rm)							
Vlavelengst(nm) Show dispersion (V,n (V):k □ e1 □ e2 Resolution: low •							
Wavelength[nm]							

Fig. 5-59 Cauchy type 0 layer editor



										(c)B	×
Layer name: NoName1			Name	Fd	Value		iciol valu		Minimum	Maximum	
A state of the sta			 Alt	101	1.450	10	100-	1	100.001		
15			Bø	101	0.01000	15		- 31	-1.00000		
			Ça	10	0.000000	0	1		-1.000000		
1			Ak	10.1	0.001	1.5	100	1	+1.000		
1			Bk.	100	0 750	A	of the local sectors.		-10 000		
			Ck	10	5.100	1	140	•	-10 000	10 000	
10- 10- 10- 10- 10- 10- 10- 10- 10- 10-											
	100	tree .									
500	1000 Wavelengthjom]	1500									
Show dispersion: If in I k in e1	Wavelength(nm)										
	Wavelength(nm)										
Show dispersion: If in I k in e1	Wavelength(nm)		 *								

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:H⁵.

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

$$\varepsilon_{2}(E) = \begin{cases} \frac{AE_{0}CE(E-E_{g})^{2}}{\left(\left(E^{2}-E_{0}^{2}\right)^{2}+C^{2}E^{2}\right)\left(\left(E-E_{g}\right)^{2}+E_{P}^{2}\right)} & E > E_{t} \\ \frac{E_{1}}{E}\exp\left(\frac{(E-E_{t})}{E_{u}}\right) & E \le E_{t} \end{cases}$$
$$\varepsilon_{1}(E) = \varepsilon_{1}(\infty) + \frac{2}{\pi}P\int_{E_{g}}^{\infty}\frac{x\varepsilon_{2}(x)}{x^{2}-E^{2}}dx$$

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:

$$\varepsilon_{2}(E) = \begin{cases} \frac{AE_{0}CE(E-E_{g})^{2}}{\left(\left(E^{2}-E_{0}^{2}\right)^{2}+C^{2}E^{2}\right)\left(\left(E-E_{g}\right)^{2}+E_{p}^{2}\right)} & E > E_{g} \\ 0 & E \le E_{g} \end{cases}$$
$$\varepsilon_{1}(E) = \varepsilon_{1}(\infty) + \frac{2}{\pi}P\int_{E_{g}}^{\infty}\frac{x\varepsilon_{2}(x)}{x^{2}-E^{2}}dx$$

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

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

SENTECH

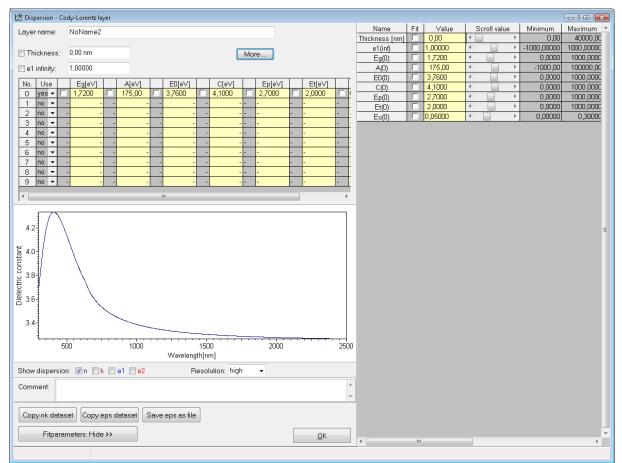


Fig. 5-61 Cody-Lorentz layer editor

Name	Fit	Value	Typ.	Minimum	Maximum	Reset	Reset	Accuracy
			Diff.			Min.	Max.	
Thickness [nm]	0	0.0	20.00	0.0	40000	0.5	30000	0.1
Eg	0	1.720	0.100	0.0	100	0.1	8.0	0.001
А	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
С	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
Et	0	2.000	0.010	0.0	1000	0.100	8.0	0.001
Eu	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 Ω_p gives the strength, Ω_0 gives the center frequency, and Ω_τ 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 ω_p gives the strength and ω_τ gives the damping.

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

As usual in infrared spectroscopy the wavenumbers $\boldsymbol{\nu}$ [cm⁻¹] are used for the spectral scale, and all parameters $\boldsymbol{\Omega}_{\mathbf{p}}$, $\boldsymbol{\Omega}_{\mathbf{0}}$, $\boldsymbol{\Omega}_{\tau}$, $\boldsymbol{\omega}_{p}$ 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 $\omega_p = \sqrt{\frac{Ne^2}{\varepsilon_0 m^*}}$ and $\omega_\tau = \frac{e}{\mu m^*}$ where **N** is the concentration, μ the mobility, **m*** the effective mass of the carriers and ε_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 Ω_p etc. of the oscillator parameters are shown as Omega_p etc. The names ω_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.



			-		-	-		_	Name	Fa	Value	Scroll value	Min
Loye	nome:	1,10	4						Thickness (um)	17	2.426	r r	
									Epsilon infinity real	100	2.150		
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	namy					h (i) bi	ny. 0.000		w tau free carriers (1/cm)	1-	0.000	2 4	-
02	inf imag	g: 0.0	00		_ omega_	tou (1/c	cm)= 0.000		(1)Omega_O (1/cm)	0.1	447.915	1 1	
-			-	_		_		-	(1)Omega_p (1/cm)	5	444 709	1	
No	Usa		Omega-0	Fit	Отнеда-р	Fé	Omega-tau	× 0	(1)Omega_tau (1/cm)	10	38.720	8 9	
1	yes -		447.915	1.5	444,709	171	35 720	-	(2)Omega_O (1/cm)	11.1	809.856	×	
2	yes -		809.856	101	211.226	0	48.542	-	(2)Omega_p (1/cm)	15 1	211 226	1 1	1
3	yes +		075.753	1.1	848 933	1.1	13.670		(2)Omega_tau (1/cm)	15-1	48.542	× +	
4	yes +	1	222.035	1.1	109 443	12.2	12.358		(3)Omega_O (1/cm)	10	1075.753	10	1000
	no: •		-	100	-				(3)Omega_p (1/cm)	0.1	848.933	e	
6	00) -			-					(-3)Omega_tau (1/cm)	101	13.670	× 1 ×	
1	00/ +	1		1.00				-	(4)Omega O (1/cm)	101	1222.035	4	
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9	nő: +	-	-	-		-		÷.	(4)Omega tau (1/cm)	1.1	12 358	A 10 4	1100
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4 3 2 1	A disperi	sion: S			enumber[cm-	-							
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Fig. 5-62 Drude-Lorentz-oscillator layer editor for SiO_2 in the MIR

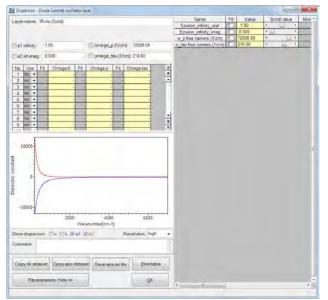


Fig. 5-63 Drude-Lorentz-oscillator layer editor for Au in the MIR

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:

$$\varepsilon_{Drude_type0}(E) = \varepsilon_{1\infty} - \frac{Amp \cdot Br}{E^2 + i \cdot Br \cdot E}$$
 [E] - eV, [Amp] - 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 $\mathcal{E}_{1\infty}$, 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.

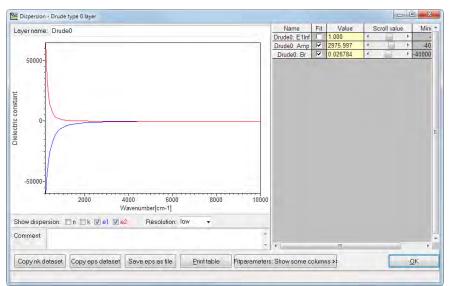


Fig. 5-64 Drude-type 0 layer editor for Au in the MIR

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)
$$\frac{\widetilde{n}_{e}^{2} - \widetilde{n}_{h}^{2}}{\widetilde{n}_{e}^{2} + 2\widetilde{n}_{h}^{2}} = \sum_{i=1}^{N} f_{i} \frac{\widetilde{n}_{i}^{2} - \widetilde{n}_{h}^{2}}{\widetilde{n}_{i}^{2} + 2\widetilde{n}_{h}^{2}} \qquad \text{N-number of constituents}$$

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 interactions⁶⁷. 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)
$$\frac{\widetilde{n}_{e}^{2}-1}{\widetilde{n}_{e}^{2}+2} = \sum_{i=1}^{N} f_{i} \frac{\widetilde{n}_{i}^{2}-1}{\widetilde{n}_{i}^{2}+2}$$
 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)
$$\frac{\widetilde{n}_e^2 - \widetilde{n}_h^2}{\widetilde{n}_e^2 + 2\widetilde{n}_h^2} = f_1 \frac{\widetilde{n}_1^2 - \widetilde{n}_h^2}{\widetilde{n}_1^2 + 2\widetilde{n}_h^2} \qquad \text{Maxwell-Garnett model}$$

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.

⁶C.G.Grandqvist and O. Hunderi, Phys. Rev. B, 16, 3513 (1977)

⁷R. 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)

⁸Harland G. Tompkins, in "A User's Guide to Ellipsometry", Academic Press, New York (1993), p. 247 ⁹D.E:Aspnes, J.B. Theeten, and F. Hottier, Phys. Rev. B, 20, 3292 (1979)

To deal with this matter, Bruggeman¹⁰ suggested making the "host" the effective medium itself, i.e., making $n_h=n_e$. With this formulation, equation (1) becomes

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

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 (ϵ =n²) with the volume fractions:

(5)
$$\widetilde{n}_{e}^{2} = \frac{\sum_{i=1}^{N} f_{i} \widetilde{n}_{i}^{2}}{\sum_{i=1}^{N} f_{i}}$$
 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)
$$n_{i} = n_{b} + \frac{1}{2a} \left(a \tan\left(\frac{3\pi}{N} - \frac{3\pi}{2}\right) + a \right) (n_{t} - n_{b}) \quad \text{arctan-Gradient}$$
$$a = a \tan\left(\frac{3\pi}{2}\right)$$

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.

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



Effective medium layer						• 💌
Lavername: NoName1	0.010	Name	Fit	Value	Scroll value	Mir *
Edjormane. Hernaner		Thickness [nm]	1	0,00	4 T +	1.00
Thickness: 0.00 nm	1	Fraction of inclusion		0,500	4 🔲 F	
		Inclusion:n(inf.)	1	1,930	* E +	-10
Inclusion material		Inclusion:A	V	0,677	4	-10
a-Si (Fit Jellison) Edit		Inclusion: B	1	5,712	3 L I	-10
	0.005-	Inclusion:C	V	9,444	*	-10
From materials From layers	A	Inclusion:Eg	V	0,442	18 11 F	-10
Host material	ар 	1000				
Silicon (Aspnes) Edit	E 0.000-					
From materiels From layers						
EMA	<pre>< c > bottom </pre>					
Type of Effective Medium Approximation:	Di la companya di la					
Bruggeman (small inclusions in layers)						
Gradient Neme -	-0.005-					
Variables						
IZ Fraction inclusion. 0,500	-0.010 4.620 4.625 4.630 4.635 Fraction, Dielectric constant					
	Show dispersion: In the konstant of inclusion					
	Display at wavelength: 550.0 nm Refractive index: 4.626 + i * 0.670					
Comment	(at 550.0 nm. fraction 0:500)					
Copy profile datasets Save profile as file Print table	Fitparameters: Hide >> QK	-4				

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.

Create new file layer 💽
Do you have the data for the new file layer
as a file - then press Yes or do you want to enter data manually - then press No
Yes <u>N</u> o <u>C</u> ancel

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

C:\buffer\e1e2_test.dat - Notepad++ [Admin	istrator]			SE Load file I	ayer table			×
Datei Bearbeiten Suchen Ansicht Kodier Ausführen Erweiterungen Fenster Z	ung S <u>p</u> rachen <u>E</u> in	stellungen <u>M</u> akro	×	<u>S</u> uchen in:	buffer	- G 🗊 🖓 🐨		
e1=2_test.dat 🛛	20182	* * @ @ [1 *	Name ele2_te	st.dat	Anderungsdatum 09.03:2016 16:03	Typ DAT-I	Datei
: ; WAVELENGTH EPSILON1 EPSI	LON2		-					
2 400.00000 5.18591 0.06454								
3 406.71141 5.16259 0.06161								
4 413.42282 5.14065 0.05885								
5 420.13423 5.11999 0.05624								
£ 426.84564 5.10049 0.05377								
1 433.55705 5.08207 0.05143								
8 440.26846 5.06464 0.04921								
9 446.97987 5.04812 0.04710						m		
10 453.69128 5.03246 0.04510				DAL				
11 460.40268 5.01758 0.04319				Dateiname:	e1e2_test.dat		•	Öffnen
12 467.11409 5.00344 0.04137				Dateityp:	ASCII data files (*.dat)		+	Abbrechen
13 473.82550 4.98998 0.03964								(
14 480.53691 4.97716 0.03799			*	Selected: e1				
ler Ln:12 Col:27 Sel:0 0	Dos\Windows	ANSI as UTF-8	INS	Siz	re: 47 Bytes			

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



SE Edit data of new file layer Wavelength n k	×
: WAVELENGTH EPSILON1 EPSILON2 400.00000 5.18591 0.06454 406.71141 5.16259 0.06161 413.4228 5.14065 0.05885 420.13423 5.11999 0.05624 426.84564 5.10049 0.05377 433.55705 5.08207 0.05143 440.26845 5.06464 0.04921 446.97987 5.04812 0.04710	* III *
<	F.
Load Save Save as OK Cancel	

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.

SR Edit data	of new file layer	Wavelength n l	k			
300 3.85 0 400 3.76 0 500 3.63 0 600 3,54 0						•
						-
						Þ
	Load	<u>S</u> ave	S <u>a</u> ve as	<u>D</u> K	<u>C</u> ancel	

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

Deta vier	Date view
Graph Teble Title Hoeder	Graph Table Tria Header
e-Naz (Wex-strong) Dije et Use Ivan tone Celor p-Aus type (p-Aus datat z-Aus type) z-Value (Vae (Vae)/Mot Memour (Maxmun Celor type Rock 1 Epster 1 + Nete + Value (Vae)/Mot Memour (Maxmun Celor type Rock 2 Enster 2 + Nete + Value (Vae)/Mot Memour (Maxmun Celor type Rock 2 Enster 2 + Nete + Value (Vae)/Mot Memour (Maxmun Celor type Rock 2 Enster 2 + Nete + Value (Vae)/Mot Memour (Maxmun Celor type Rock 2 - Vae)// - Vae)	solas Woodangth . Uta ali Uta noia Cotr yokus type pAns dital zolas type a Valie Uta Noia Uta Minimum Utazmum Descritype Roz 1 Utaz jelesta = <u>Here</u> = <u>→</u> <u>P</u> <u>P</u> <u>1</u> 3438 32771902E = Roz 2 Utaz jelesta = <u>Here</u> = <u>→</u> <u>P</u> <u>P</u> <u>1</u> 6450 0000 000139/02E = Roz 2 Utaz jelesta = <u>Here</u> = <u>P</u> <u>P</u> <u>1</u> 65000 000139/02E = Roz
* Cartent Alon Tom, json: 400.000 to 1400.000 Tom, json: 400.000 to 1400.000 each 1	T Currem-Akis for 400.000 to 1400.000 Trim foor 400.000 to 1400.000 each 1
OK. Danal	OK. Cascal

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

hange (n,k) data			X
Do you want to			
convert (n,k) data to (Epsil then press (>YES<)	on1,Epsilon2) data		
or switch the unit identifie unchanged then press (>NO<)	r from (n,k) to (Epsilon	1,Epsilon2) and	leave the data
or cancel?			
	Ja	Nein	Abbrechen

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'.

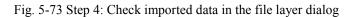
If the imported dataset contains refractive index data (n, k) select 'Mat_refractive_index' for column 1 and 'Mat_absorption' for column 2.

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).



Dispersion - File layer			(a)	e 8
Layer name: NoName0	Name //	7 Value	Minimum Ma	aximum
Report spectral points as fit parameters Date range: 400.0 nm _ 1400.0 nm / Points: 150.				
angue ang				
1 1 1 8 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	-			
400 500 800 1000 1200 Wavelength[cm]	1400			
400 500 800 1000 1200				
400 500 800 1000 1200 Wavelength[om] Show dispersion: □n □k ⊘et ⊘e? Resolution Iow •				



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.

Dispersion - File layer						
Layer name: Si	Name Thickness [nm]	Fit	Value 0,00	Scroll value	Minimum 0,00	Maxin ^ 40000
 Thickness: 0.00 nm Report spectral points as fit parameters Data range: 187,9 nm 6200,0 nm / Points: 636 Display limited by environment settings (300,0 nm 2500,0 nm) 			0,00		0,001	40000
te 6 5 4 5 500 1000 1500 2000 2500 Wavelength(nm)	=					E
Show dispersion: Vn Vk el el e2 Resolution: high -						
Comment.						
Copy nk dataset Copy eps dataset Save eps as file Print table						
Fitparameters: Show all columns >> QK	•	111				

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:

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

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

1

١

Schott:

$$n^{2} = A_{0} + A_{1}\lambda^{2} + \frac{A_{2}}{\lambda^{2}} + \frac{A_{3}}{\lambda^{4}} + \frac{A_{4}}{\lambda^{6}} + \frac{A_{5}}{\lambda^{8}}$$

$$k(\lambda) = 0$$
[\lambda]: \mum [A0] - dim.-less, [A1] - \mum m^{-2}, [A2] - \mum m^{2}, [A3] - \mum m^{4}, [A4] - \mum m^{6}, [A5] - \mum m^{8}

Sellmeier transparent:

$$n^{2}(\lambda) = 1 + \frac{A_{1}\lambda^{2}}{\lambda^{2} - B_{1}} + \frac{A_{2}\lambda^{2}}{\lambda^{2} - B_{2}} + \frac{A_{3}\lambda^{2}}{\lambda^{2} - B_{3}}$$

$$k(\lambda) = 0$$

[\lambda]: \mummath{\mu}m [A_{1}], [A_{2}], [A_{3}]: dimensionless, [B_{1}], [B_{2}], [B_{3}]: \mummath{\mu}m^{2}

1

1

1

Sellmeier absorbing with N=1

SENTECH

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

$$k = \frac{C}{n \cdot D \cdot \lambda + \frac{F}{\lambda} + \frac{1}{\lambda^{3}}}$$
[\lambda]: nm [A], [C]:dimensionless, [B]:nm², [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.

					Fé	Value			Manman
ayername: NoName	1			Name Thickness [nm]	4	200.00	1	croll value	
				N0	-	1 4520000	4	14	-
/ Thickness: 200.00	nm			N1	m	36.0000000	1	11.1	
Formula for n or epsilo	into			NŽ	101	0.0000000	4		-100000.0000
N(L)-N0-N1-10-2/L/L+	N2*10^77.J.J.J.J.			KÖ	8 1 1	0 0000000	4	10	
and the second second				K1	10-1	0 0000000	1		
Formula for k or epsilo				K2	(d. 3)	0.0000000	. e	14	-100000 0000
K(L)=K0+K1*10*2/L/L+K	2*10"7AAAA								
Load standard formula:	Cauchy								
Company to make		destition of a		1					
Save as new formula	Erase star	ndard formula							
148									
1.45		ength[nm]	2000 250	5					
1.47 1.45 500	Wavel	engto[nm]	2000 2500 olution: Iow -						
Show dispersion: 2 n Comment	Waved	engto[nm]							

Fig. 5-75 Editor for formula type layers

Cauchy	•
constant e1(E), e2(E)	
Cauchy	
Forouhi-Bloomer	
Schott glass	
Sellmeier transp.	
Sellmeier absorb.	
Custom	

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 all
--

- 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 $\tilde{\epsilon}$ 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< td=""></b<>
	>	larger	a>b
	\diamond	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
	1	wavelength [nm]	1/1
	w	wavenumber [cm ⁻¹]	w-w0
	Phi	angle of incidence [°]	sin(phi*pi/180)
	Theta	rotation of sample [°]	theta/2/pi
	Т	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
А	0	0.2177	0.100	-100000	10000	0.000	10.000	0.001
С	0	12.711	0.100	-100000	10000	0.000	10.000	0.001
В	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:

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

$$Q = \frac{1}{2}\sqrt{4C - B^{2}}, \qquad B_{0} = \frac{-AB^{2}}{Q(2 + E_{g}B - E_{g}^{2} + C)}, \qquad C_{0} = \frac{AB(E_{g}^{2} + C)}{Q(2 - 2E_{g}C)}.$$

[A] $[n(\infty)]$ - dimensionless, [B], [E_g] - eV, [C] - eV²

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.

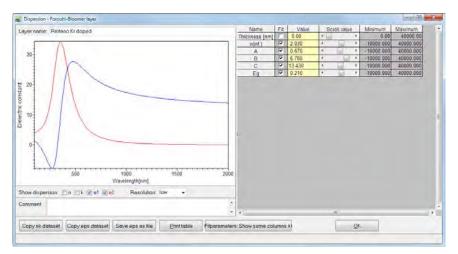


Fig. 5-77 Example for Forouhi-Bloomer layer

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 Ω_p gives the strength, Ω_0 gives the center frequency, and Ω_{τ} gives the damping of each resonance.

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

As usual in infrared spectroscopy the wavenumbers $\boldsymbol{\nu}$ [cm⁻¹] are used for the spectral scale, and all parameters $\boldsymbol{\Omega}_{\mathbf{p}}, \boldsymbol{\Omega}_{\mathbf{0}}, \boldsymbol{\Omega}_{\mathbf{r}}$, 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 Ω_p etc. of the oscillator parameters are shown as Omega_p etc.

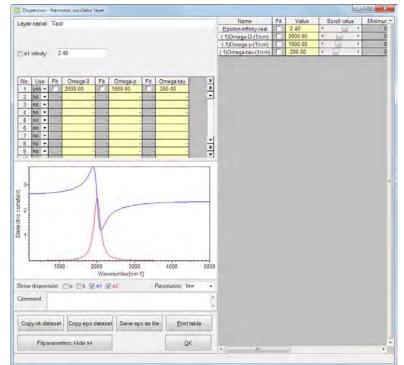


Fig. 5-78 Harmonic-oscillator layer editor

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.

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

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

		Name	Fit	Value	S	croll valu	ie	Minimum	
ayer name: NoName0		Thickness [nm]	V	2,00	1		F.	00,00	
Material		Rate [nm/s]	V	1,0000	*			-1000,0000	
SiO2	Edit material	ND	11	1,452	E.		F.	-100,001	
3102	Edit material	N1	J.T.I	36,0	*	11	+	-40000,0	
Select from directory	Select from existing layers	N2		0,0	*	100		-40000,0	
		KO		0,000	*	-		-100,000	
Layertype		K1		0,000	*		N.	-40000,000	-
 Growing layer th(t) = th(tstart) + G * Min(Etched layer th(t) = th(tend) + E * Min((K2	12	0,000	1			-40000,000	4
This layer grows in the time interval between Start time (tstart): 0.0 s and End time (tend): 100,0 s									
The final thickness at 100,0 s is 102,00 nm		2							

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:

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

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

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

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

Standard values for the parameters and their meaning are:

Parameter	Default	Description	Unit
	value		
Epsilon-infinity	3.29	\mathcal{E}_{∞}	dimensionless
Effective electron mass (relative)	0.21	m_c^*	dimensionless
Epsilon background	1.266	\mathcal{E}_0	dimensionless
Charge number	0.111	Ζ	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.



_ayer name: NoName1	Name Fit Value Scroll value
	Thickness [nm] 0.00 *
Mare	Epsilon-infinity 5.290 *
	effective electron mass (relative) 0.210 <
	epsilon background 🔲 1.266 *
	charge number 0.111 ·
1.5-	free carrier density (1E21 cm^-3) C 0.252 *
	impurity density (1E21 cm^-3) 5.579 *
0.5	
0.5- 500 1000 1500 200 Wavelength[nm]	2500
0.5 500 1000 1500 200	2500
0.5- 500 1000 1500 200 Wavelength[nm]	2500

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	Description	Unit
	value		
Epsilon-inifinity-real	1	\mathcal{E}_{∞}	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	$\omega_{ au 0}$	eV
w-tau-1-free-carriers	0.12	ω_{τ^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.

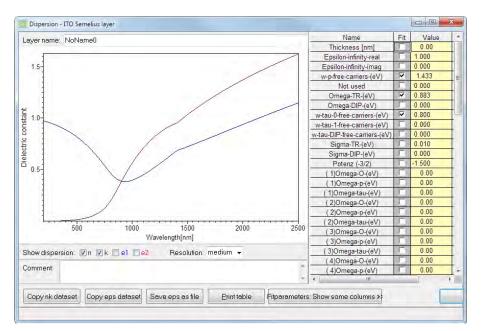


Fig. 5-81 Example for ITO Sernelius layer

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.

$$\varepsilon(E) = \varepsilon_{\infty} + \sum_{i=1}^{N} \left[\frac{C_{0_{i}}}{E^{2}} \left[e^{j\beta_{i}} (E_{g_{i}} - E - j\Gamma_{i})^{\mu_{i}} + e^{-j\beta_{i}} (E_{g_{i}} + E + j\Gamma_{i})^{\mu_{i}} - 2\operatorname{Re} \left[e^{-j\beta_{i}} (E_{g_{i}} + j\Gamma_{i})^{\mu_{i}} \right] - 2j\mu_{i} \cdot E \cdot \operatorname{Im} \left[e^{-j\beta_{i}} (E_{g_{i}} + j\Gamma_{i})^{\mu_{i-1}} \right] \right] + m_{0}E^{x_{0}} + jk_{0}$$

$$\begin{split} & [\mathcal{E}_{\infty}], [\beta_i], [\mu_i], [x_0], [k_0] : & \text{dimensionless} \\ & [E], [E_g], [\Gamma_i] : & \text{eV} \end{split}$$

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.

aver name:	Silang osci						Name	Fit	Value	Scroll value	Minimum	Maxi
ayer nome.	or congressi						E1(inf)	151	0.3972	•	-1000.0000	100
							MO		-0.033029	*	-10.000000	10.0
							XO		1.012892	< -	-10.000000	10.0
e1 infinity:	0.3972		I x0:	1.01	2892		K0	5	0.0241	*	-100.0000	10
							C0(0)	F	56.320	< 🗌 🗆	0.000	1000
_ m0:	-0.033029		📄 k0:	0.02	:41		Beta(0)		-0.45890	*	-100.00000	100
. Dan T	1	TING	1.1.	-	1	-	Eg(0)	$[\Box]$	3.3800	< 🗌	0.0000	100
No. Use	C0 Beta		Gamma		My	*	Gamma(0)	E	0.11500	Link.	-100.00000	100
0 yes -	56.320 -0.458		0.11500		-0.824100		My(0)	F	-0.824100	<	-100.000000	100.
1 yes -	240.900 -0.411		0.30790		-0.396500	1	C0(1)		240.900	× 🗌 🗉	0.000	1000
2 yes -	125.460 0.330		0.20300		-0.950400		Beta(1)	F)	-0.41100	*	-100.00000	100
3 yes -	16.660 0.281	5.3825	0.24100		-0.976100		Eg(1)	171	3.6266	*	0.0000	100
4 no 👻							Gamma(1)	F	0.30790	4	-100.00000	100
5 no 🕶			•				My(1)	1	-0.396500	4	-100.000000	100
6 no 🔻	a (14) a (14)		-		1000	-1	C0(2)	E	125.460	< []	0.000	1000
7 no •		- +			1	ŧ	Beta(2)	5	0.33070	*	-100.00000	100
8 no 🕶		- 8			-	Ť	Eg(2)	F	4 2906	< []	0.0000	100
~ 1 1	a par	1 al	1-1	J.		1	Gamma(2)		0.20300	1	-100.00000	100
1	0						My(2)	10	-0.950400	< []		100
6-	N .						C0(3)	E	16.660	*	0.000	1000
°7 . /	1						Beta(3)	F	0.28160		-100.00000	100
IN							Eg(3)	T	5.3825	1	0.0000	100
1 11	1						Gamma(3)	F	0.24100			100
4- /							My(3)	5	-0.976100	1	-100.000000	
4	500	1 Navelength[nn	000			1500						
how dispersi	on: 🔽 n 🔽 k 🗖 e1			olutii	on: high	•						
Comment:						* *						
Copy nk data	aset Copy eps date	set Save e	ps as file		<u>P</u> rint table							
				_		-						

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:

$$\varepsilon_{Lor_{_lypel}}(E) = \varepsilon_{1\infty} - \frac{A \cdot E_n}{E_n^2 - E^2 - i \cdot B_r \cdot E}$$
[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.



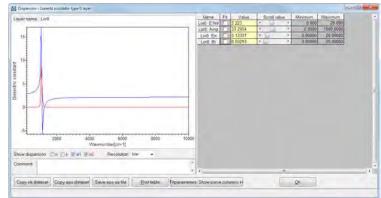


Fig. 5-83 Lorentz type 0 editor

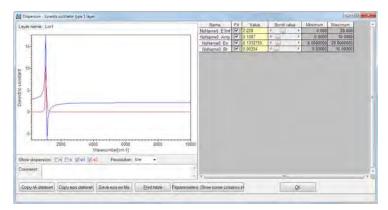


Fig. 5-84 Lorentz type 1 editor

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

$$\widetilde{\epsilon} = \epsilon_1 + i\epsilon_2 \qquad \widetilde{n} = n + ik \qquad \widetilde{\epsilon} = \widetilde{n}^2$$

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.

Layername NoName1		Na		Fit	Value	Scrolly	alue	Minimum	Maximum	Typ. Diff.				Reset Max.		Scroll Step	Scroll Mini	
		Thickne	ss [nm]		0,00	N Lat		0,00		20,00			0,			20,00	0,00	
		Refr.			000,1	1	- F	0,001 0,000	40,000	0,100						0,100	100,0	10,000
2)Thickness	0,00 nm	Abso	ption		000,0	1		0,000	40,000	0,100	0,0010	3 6	0,0	0 1,000	Ani	20,00 0,100 0,100	0,000	10,000
Refractive index n	1.000																	
The months made in																		
Absorption index k:	0.000																	
		-																
Comment																		
		~ r									m							
	1.0	T.																
Fitparameters: H	(ide >>	QK.																
		2.																

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

1.8	4.0
2.6	0
1.510	0
0	
2.38	0.52
2.74	0.27
	0.3472
2.21	4.17
	1.96
	3.3118
	4.36
	0
	3.8182
	3.41
	0.11
	0.0000
	3.3
	0.20 0.0000
	0.0000
	0.0000
	5.24
	0.6059
	0.3796
	0.3790
	0.30
	0.50
	0.0000
	1.8014
	4.61
	5.09
	1.75
1.56	0
1.49	0.00
1.40	0.00
1.735	0
3.70	3.54
4.01	3.86
3.5800	3.7035
0.05	2.64
	0
	0
2.83	2.86
1 0-	
	3.72
	3.8945
	1.66
	1.444
	3.032
	2.8851
	4.060 4.29
	4.15 5.61
	0
	0
	0.0000
	0.0000
	0.010
	0.010
	0
3.95	0.04
	1 2.27
4.206	0.422
	$\begin{array}{c} 1.510\\ 0\\ 2.38\\ 2.74\\ 2.9810\\ 2.21\\ 3.1365\\ 3.58\\ 1.78\\ 0.1337\\ 0.25\\ 2.94\\ 2.4094\\ 2.43\\ 3.86\\ 3.3174\\ 5.4727\\ 1.3315\\ 1.99\\ 3.9621\\ 3.9898\\ 3.54\\ 3.52\\ 0.45\\ 3.5364\\ 4.2544\\ 2.53\\ 2.52\\ 0.05\\ 1.56\\ 1.49\\ 1.40\\ 1.735\\ 3.70\\ 4.01\\ 3.5800\\ 0.05\\ 1.56\\ 1.49\\ 1.40\\ 1.735\\ 3.70\\ 4.01\\ 3.5800\\ 0.05\\ 1.542\\ 1.325\\ 2.83\\ 1.97\\ 2.0671\\ 3.90\\ 4.338\\ 3.97\\ 3.7458\\ 6.352\\ 1.77\\ 2.33\\ 2.15\\ 2.632\\ 2.66\\ 2.021\\ 1.462\\ 1.965\\ 1.542\\ 1.457\\ \end{array}$

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).

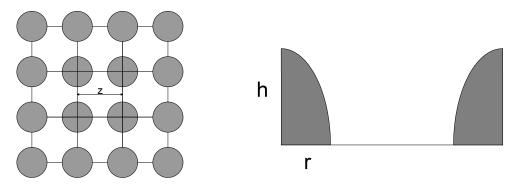


Fig. 5-86 Tetragonal lattice with ellipsoidal nuclei (z-cell width): left top view, right cell view

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)
$$\mathbf{R}(\mathbf{t}) = \mathbf{A}\mathbf{t}^{a} + \mathbf{R}_{0} \qquad h(\mathbf{t}) = Bt^{b} + \mathbf{t}\mathbf{h}_{\text{start}}$$

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



Dispersion - Nucleous growing I			Name	Fit	Value	Scroll value	1	Minimum	Maximum	Typ. Diff.	Accuracy [
Layername: NoName1			Init.Thickn. [nm]	I	0,00	<		0,00		20,00	0,100 2
Nuclei material			growth rate [nm/s]	IT.	1,0000	*		0,0000		4,0000	0,01000 4
amorphous Silicon			growth exp.	Г	1,000	*		0,000	5,000	0,100	0,0010 3
amorphous Silicon		Edit	nuclei rate [nm/s]	F	1,0000	*		0,0000		4,0000	0,01000 4
	From materials	From layers	nuclei exp.	F	1,000	1	1	0,000	5,000	0,100	0,0010 3
			init radius [nm]		50,00	*	+	0,00	10000,00	4,00	0,010 2
Filling material			cell width [nm]	-	100,00		*	0,00 0,001	10000,00	4,00 0,100	0,010 2
Air		Edit	fill-Refr. index fill-Absorption	1	1,000	11		0,001		0,100	0,0010 3
	From materials	Cashedanana		100	10,000	121.1	-	0,000	40,000	0,100	0,00101
	From materials	From layers									
EMA Type of Effective Medium App	provimation:										
Bruggeman (small nuclei in la											
ibraggeman (smarmacierin ic	yers)										
Initial thickness th (tstart):	0,00 nm										
Growth rate B:	1,0000 nm/s										
- A MARKAN COLOR											
Growth exponent b:	1,000										
Nuclei radius rate A:	1,0000 nm/s										
Nuclei radius exponent a:	1,000										
Initial radius R0:	50,00 nm										
Cell width z:	100,00 nm										
Subdivision: 1,00 nm											
This layer grows in the time inte	erval between										
Start time (tstart): 0.0 s	and										
End time (tend): 1000.0 s	cinci										
Lind diffe (dend). Tobo, o s											
The final thickness at 1000,0 s i	s 1000,00 nm										
Comment			-								
			-								
Fitparameters: Hide >>	Printtable	OK									

Fig. 5-87 Nuclei layer edit screen

Editor description

The th_{start}, B, b, A, a, R₀, 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.

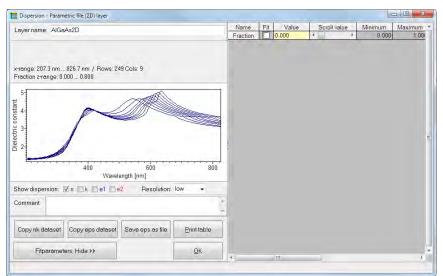


Fig. 5-88 Parametric file (2D) layer editor

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 $(SiO_2 \text{ and } TiO_2)$

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.

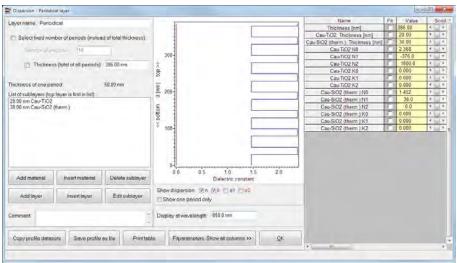


Fig. 5-89 Periodical layer editor with example of 2 sublayers



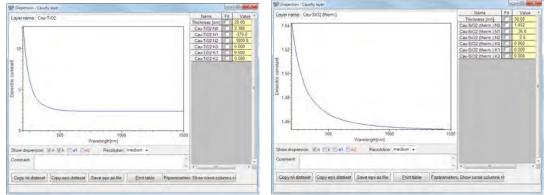


Fig. 5-90 Alternating sublayers

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

Wavelength	632.8 nm	Temperature	235 °C	Devicetype	PSCA	1
Angle of Incidence	70.00 *	Process tree:	0.0 s	Flatationtype	RAE	1
Angle of Rotation.	0.00 *	Environme	of Settings	P/A engle	45.00 '	
Curve parameter	5	-				-
1 Patronican The						
From 0.000	K	1000.000				
	Curve step	1.000				
			Value 1	Velue 2	Туре	
			179.405	10510	Curve	12
Celc unit Delta	Ead	2				
Celc unit Deba	F%()					
Celc unit Deher	F30					
2) Add simulated d	ala to experimer	C\SenPModel\Spectr				
2) Add simulated d	ala to experimer	C\SenPModell\Spectre	Add line o	olon 🗆 Merk tra		
2) Add simulated d Name of transfer like	alla to experiment	C\SenPModell\Spectre	Add line o	olon 🗆 Merk tra		
2) Add simulated d	ala të experimeri k	C\SenPModel\Spectr	Add line o	olon 🗆 Merk tra		

Fig. 5-92 Simulation with thickness as curve parameter

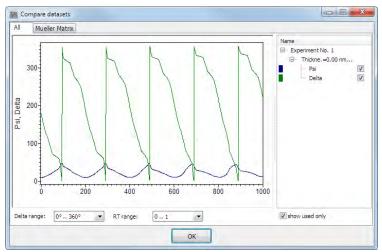


Fig. 5-93 Resulting dependence of Ψ and Δ from total thickness.

5.2.4.28 Polynomial-Layer

Theoretical assumptions:

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

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

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.

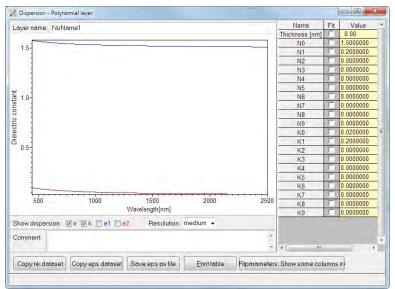


Fig. 5-94 Polynomial layer editor

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.

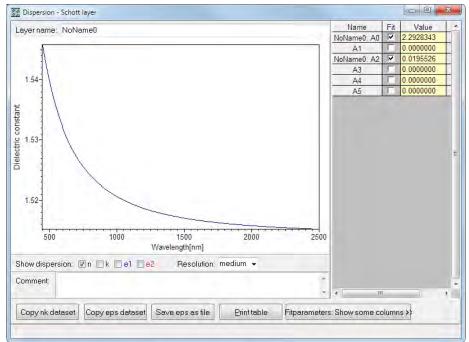


Fig. 5-95 Schott layer editor

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.

$$n^{2}(\lambda) = 1 + \frac{A_{1}\lambda^{2}}{\lambda^{2} - B_{1}} + \frac{A_{2}\lambda^{2}}{\lambda^{2} - B_{2}} + \frac{A_{3}\lambda^{2}}{\lambda^{2} - B_{3}}$$

$$k(\lambda) = 0$$

$$[\lambda] - \mu m \qquad \left[A_{1}, A_{2}, A_{3}\right]: \text{ dimensionless} \qquad \left[B_{1}, B_{2}, B_{3}\right] - \mu m^{2}$$

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 .

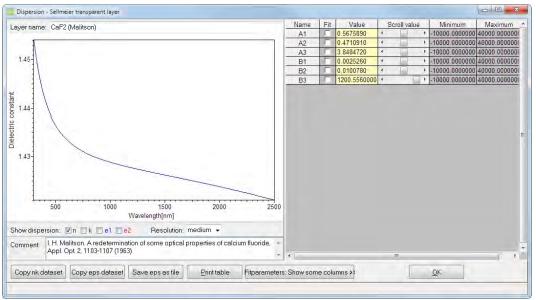


Fig. 5-96 Sellmeier layer editor

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 visible range. But in the near infrared range the Sellmeier formula offers a better description.

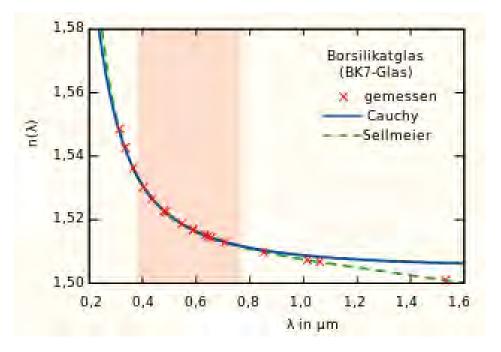


Fig. 5-97 Comparison of Cauchy and Sellmeier dispersion

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.

formatic	n 📃 💆
1	The top and the bottom layer are not an oscillator layer. The silicon profile layer will therefore not work correctly.
	QK

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.

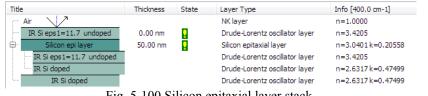
The effective mass can be set. The default value of 0.26 will be fine in many cases.

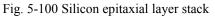
The list of fit parameters contains the effective mass and the parameters of the bottom and the top layer.



Silicon epitaxial layer								0.0
Lavername: Silicon ep	oi laver		50-4			Name	Fit	Value
					+	Thickness [nm]	4	50.00
7 Thickness 50.00 nn	n		1			Effective Mass	1.1	0.260
Top material			1		1	bottom Epsilon_infinity_real	101	11.70
			40-		f.	bottom Epsilon_infinity_imag		0.000
IR Sieps1=11.7 undo	iped	Edit_			1	bottom w_p free carriers (1/cm)	1	1000.00
	From materials	From lavers				bottom w tau free carriers (1/cm) top Epsilon infinity real	100	200.00
	Lifer marginas	ritinitayens	top >>		1	top Epsilon infinity imag		0.000
Eottom material			30-		. 1	top e pailon iminity imag top w p free camers (1/cm)	1	0.00
					1	top w tau free carriers (1/cm)	100	0.00
IR Sidoped		Edit	d mm		1	top in tau new canoes (inclug	10.00	1 0.00
	From materials	From layers _	0		1			
5.3.4			5 20-	1	1			
Gradient			8 **	1	1			
Gradient ArcTan	+ Subdiv	ision: 15	20- 20-	1	1			
			*					
Effective mass			10-	1	t l			
Effective mass	1.26		101	1				
				4				
			0.1	2 4 6	8 10			
			0	Fraction Dielectric				
						-		
			Show dispers	ion: 🗋 n 🗔 k 🗹 el	12 BC			
				El Frection of Tap	0			
			Display at way	velength: 400.0 cm-1				
			Retractive ind (et 400.0 cm-1	ex: 3.040 + 1* 0.206				
Comment			(at 400.0 Cm-1					
			-					
-	10	10	11		10			
Copy profile detasets	Save profile as file	Print table	Fitpara	meters Hide >>	QK			
	1					x = =		

Fig. 5-99 Silicon epitaxial layer editor





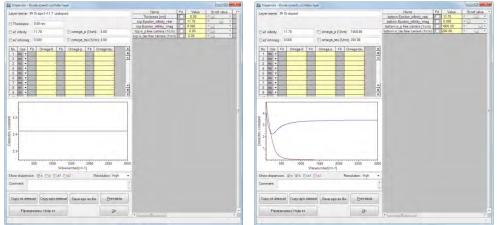


Fig. 5-101 Top and bottom layer

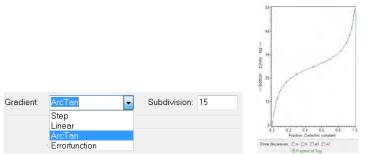


Fig. 5-102 Gradient type, number of steps and resulting fraction versus thickness

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 'partial-ly 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.

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

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.

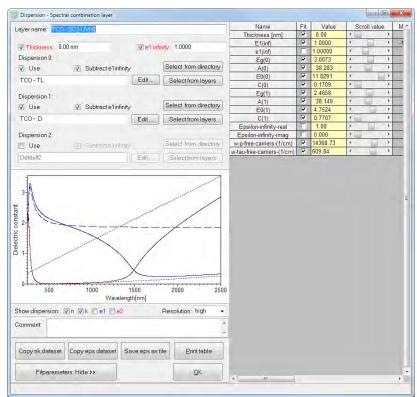


Fig. 5-103 Spectral combination layer editor

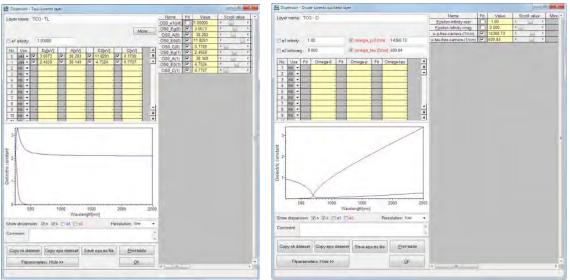


Fig. 5-104 Contributions of spectral combination layer



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.

$$\varepsilon(E) = 1 + \frac{a}{b - E^2} + \frac{CA\sqrt{R}}{(E + i\Gamma)^2} \left\{ g\left[\xi(E + i\Gamma)\right] + g\left[\xi(-E - i\Gamma)\right] - 2g\left[\xi(0)\right] \right\} \right\}$$
$$\xi(z) = \sqrt{\frac{R}{E_g - z}} \qquad g(\xi) = 2Ln(\xi) - 2\pi Cot(\pi\xi) - 2\psi(\xi) - \frac{1}{\xi}$$
$$\psi(z) = \frac{d}{dz} Ln[\Gamma(z)]$$

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 $n=Re(\epsilon)$ but the absorption is expanded by a second order polynomial above the band gap:

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

Standard values for the parameters and their meaning are:

Parameter	Default	Description	Unit
	value		
Eg	1.425	Direct band gap energy	eV
R	0.0034	Binding energy of exciton, typically a few meV^2	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
с	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.

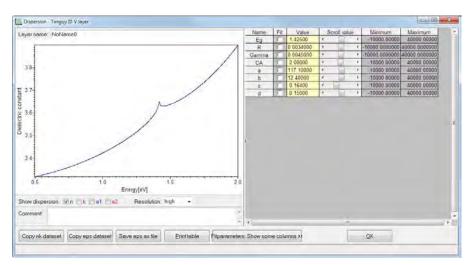


Fig. 5-106 Example for a Tanguy layer (n)

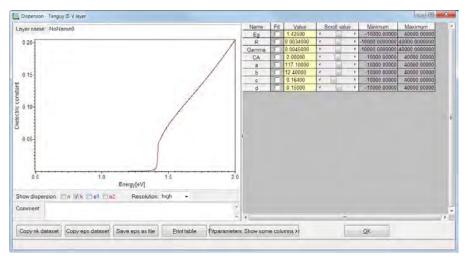


Fig. 5-107 Example for a Tanguy layer (k)

A comparison 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 .

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0C(E-E_g)^2}{(E^2 - E_0^2)^2 + C^2 E^2} \frac{1}{E} & E > E_g \\ 0 & E \le E_g \end{cases}$$
$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_E^{\infty} \frac{x\varepsilon_2(x)}{x^2 - E^2} dx$$

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].AStrength 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)CBroadening of the oscillator [eV]
Small (C < 1.0) values will give sharp oscillators
High (C >> 1.0) will create broad oscillators

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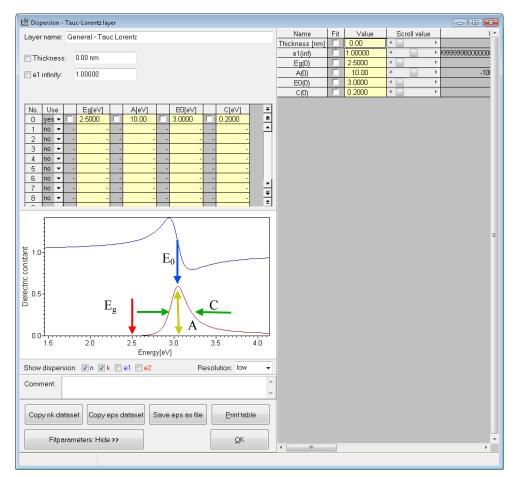


Fig. 5-108 Example of the Tauc-Lorentz-oscillator with effects of the parameters

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).



2 Onpersion - Taux-	Connects Daywe							1010
Lever name: Sinc	hintide - Truc L	orentz.		Name	14	Value	Scroll value	Minimi
				Thickness [hm]	12	534.25		
Thickness 63	H25 mm			et(inf)	10	-1.95400	1 1	
				Eg(0)	10	2.3171		
al infinity -1	96400			(U)A.	1.1	223 29	1	
				E0(0)	C	9.4713	9 F - +	
				C(0)		18.2799	6.1.	
No. Use	EgleV]	Alevi EDIevi	C[eV]					
		23 28 9 4713	C[eV] 2 18.2799					
1 00 -				J.				
2 80 -	4 10 10							
3 10		- 11						
4 10		1000						
5 00 *								
6 10		-						
7 80 -				2				
8 10 -								
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Fig. 5-109 Example for a Tauc-Lorentz layer (x-axis: wavelength / nm)

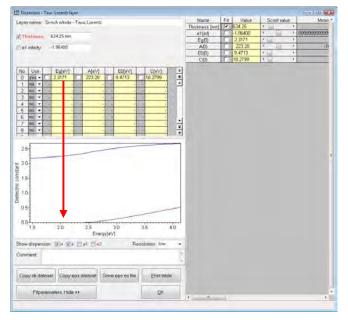


Fig. 5-110 Example for a Tauc-Lorentz layer (x-axis: photon energy / eV)

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)
$$\mathbf{R}_{pp} = \frac{\mathbf{r}_{01pp} + \mathbf{r}_{12pp} e^{-2i\beta_p}}{1 + \mathbf{r}_{01pp} \mathbf{r}_{12pp} e^{-2i\beta_p}} \qquad \mathbf{R}_{ss} = \frac{\mathbf{r}_{01ss} + \mathbf{r}_{12ss} e^{-2i\beta_s}}{1 + \mathbf{r}_{01ss} \mathbf{r}_{12ss} e^{-2i\beta_s}}$$

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

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

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

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

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

where n_0 , n_2 are the refractive indices of the isotropic ambient and substrate and n_{10} , 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)
$$n_0 \sin \phi_0 = n_2 \sin \phi_2$$

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

(18)
$$\beta_{p} = 2\pi \frac{d_{1}}{\lambda} \frac{n_{1o}}{n_{1e}} \sqrt{n_{1e}^{2} - n_{0}^{2} \sin^{2} \phi_{0}}$$

(19)
$$\beta_s = 2\pi \frac{d_1}{\lambda} \sqrt{n_{1o}^2 - n_0^2 \sin^2 \phi_0}$$

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.

Dispersion - Uniaxial anisotropic layer							
Layer name: NoName1		Name	Fit	Value	Scroll value	Minimum 1 ^	
Layer hame. Norvamen		Thickness [nm]	Г	0,00	< >	0,00	
Thickness: 0,00 nm		para-Refr. index	Г	1,000	< 📄 F	0,001	
		para-Absorption		0,000	< 📄 👘 🕨 🕨	0,000	
Dispersion at 0° (E-vector in z-direction perpendicular to surface):		perp-Refr. index		1,000	< 📄 F	0,001	
Default2 Edit perpendicula	ar	perp-Absorption		0,000	< _ +	0,000	
Select from directory Select from existing layers							
Dispersion at 90° (E-vector in x- or y-direction parallel to surface):							
Default1 Edit parallel							
Select from directory Select from existing layers							
1.0							
0.8							
Oleectric constant 9.0 0.0						E	
2 0.6							
Ē 0.4							
8							
0.2							
0.2							
0.04							
500 1000 1500 2000	2500						
Wavelength[nm]							
Show dispersion: V n V k e1 e2 Resolution: low	Show dispersion: In Ik et e2 Resolution: Iow -						
Comment	*						
	-						
Copy nk datasets Copy eps datasets Print tabl	e						
Fitparameters: Hide >> QK						-	
		< [۱.	

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 V	Value 1	Typ. Diff.	Min.	Max.	Reset Min.	Reset Max.	Accuracy
thickness [nm] 0 0) 2	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 \square .

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 \square . 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.

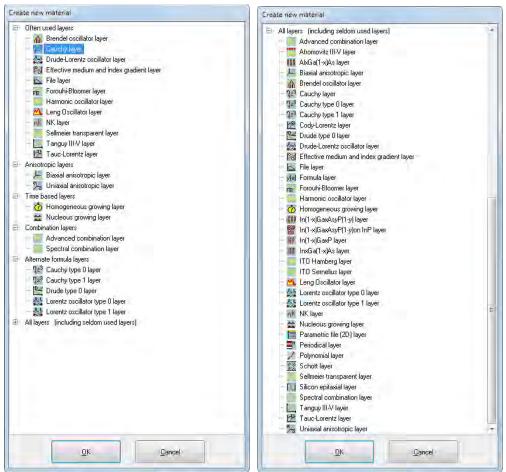


Fig. 5-112 Select a basic layer type to create a new layer

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 repeti-

tively. 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 $\overset{k}{\frown}$ 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.

Environm	ent paramet	ers						×
<u>∨</u> alues	<u>R</u> anges	<u>U</u> nits	Substrate	Inhomogeneity	<u>M</u> odel	<u>E</u> rrors		
Stand	ard values	(used if	no other val	ues are present)				
	Na∨elengt	h:	632,	,8 nm				
	Angle of incidence: 70,00 *							
	Femperatu	ire:	23,5	5°C				
F F	Process tin	ne:	0,0 :	s				
▼ [
-Data r	nodulo							51
Use	data point	s modulo	: 1					
				<u>0</u> K				

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

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).

	nt paramete					
(alues	<u>R</u> anges	<u>U</u> nits	<u>S</u> ubstrate	Inhomogeneity	<u>M</u> odel	<u>E</u> rrors
Active	ranges of v	values-				
			Minim	um:	Maximu	m:
Wavelength: 300,0 nm		nm	2500,0 r	ım		
Angle	e of inciden	nce:	0,00 *		90,00 *	
Temp	Temperature: -273,1		°C	8000,0 °	C	
Proce	ess time:	0,0 s		1,0E6 s		
			<i></i>			
				<u>0</u> K		

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

"Ranges" page

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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").



Environment parameters						
<u>Values</u> <u>R</u> anges <u>U</u> nits	<u>S</u> ubstrate <u>I</u> n	homogeneity <u>M</u> odel <u>E</u> rrors				
Standard units for value	s					
Wavelength:	nm 👻	Thickness:	nm 👻			
Angle of incidence:	* •	Growth rate vs. time:	nm/s 👻			
Temperature:	• C •	Fraction:	<mark>% •</mark>			
Process time:	s •	Diameter:	mm 👻			
		Thickness variation vs. spot:	nm/mm 👻			
<u> </u>						

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 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.



Environment parameters	X				
· · · · · · · · · · · · · · · · · · ·	homogeneity <u>M</u> odel <u>E</u> rrors				
Thick substrate with incoherent superposition of beams					
Thick layer detected:	none				
Substrate thickness:	1,000 mm				
🔲 Beam diameter:	4,000 mm				
Detector aperture diameter:	4,000 mm				
Number of backside reflections:	0				
<u> </u>					

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)

Environment parameters							
<u>V</u> alues <u>R</u> anges <u>U</u> nits <u>S</u> ubstrate	Inhomogeneity Model Errors						
-Thickness variation:							
📃 Use thickness variation within r	Use thickness variation within measurement spot						
Layer:	Ţ						
Thickness variation:	10,0 nm/mm Calculation steps: 2						
Limited wavelength resolution							
🔲 Use limited wavelength resolu	tion						
Wavelength resolution:	0,0 nm Calculation steps: 2						
Non parallel light beam							
🔲 Use non parallel light beam							
Focus angle of non parallel be	am: 3,00 * Calculation steps: 2						
	<u>Ω</u> K						
	The among the 2 of the operation operation						

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.

Environment parameters						
Values <u>R</u> anges <u>U</u> nits <u>S</u> u	ibstrate Inhomogeneity Model Errors					
Reverse stack	Reverse stack					
Reverse layer stack (turn sample upside down)						
Overlayer (partially covered s	surface)					
Number of overlayers:	1					
Fraction of overlayer:	100,0 %					
Filling material:	Edit					
	Select from existing layers					
Select from directoy						
	<u>0</u> K					

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.

Environment parameters						
Values <u>R</u> anges	<u>U</u> nits <u>S</u> ubstrate <u>I</u> nł	homogeneity <u>M</u> odel En	rors			
Error calculation						
Show result window after fit						
Enable	Enable error calculation after fit					
Calculation type f	Calculation type for derivatives: Plus/minus epsilon -					
Use precision	✓ Use precision of (\$1, \$2) to get precision of (Psi, Delta)					
Precision in measured data for error calculation						
Stokes s1 , s2:	0.0020	None:	1.0000			
Psi ["]:	0.5000	Simulation:	1.0000			
Delta ["]:	1.0000	R, T:	0.0100			
Set to default						
ŪK						

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:

(20)
$$U(\lambda) = \int_{0}^{n} \Phi(\lambda) \cdot G(\lambda - x) dx = \Phi * G$$

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

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

The half width is defined by a value of $G(\lambda)=\frac{1}{2}$. From the above equation the relation between a and the half width h follows:

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

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

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

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:

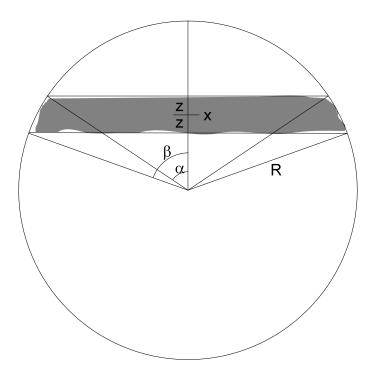


Fig. 5-120 Stripe definition for focus effect

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

The area of the stripe becomes

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

and the weight for this individual stripe will be

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

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.



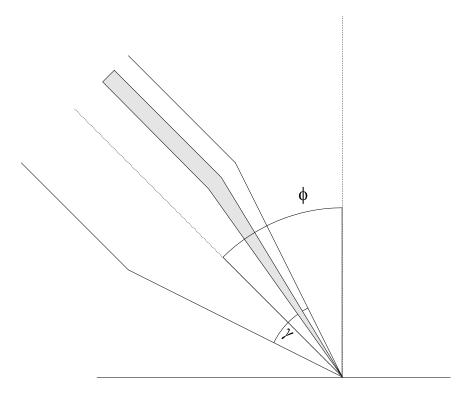


Fig. 5-121 The individual angle of a cross sectional stripe

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:

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

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:

(29)
$$\phi - \phi_0 = \arctan \frac{x}{f} \xrightarrow{f >> x} x = \frac{2(\phi - \phi_0)}{\gamma}$$

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:

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

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.

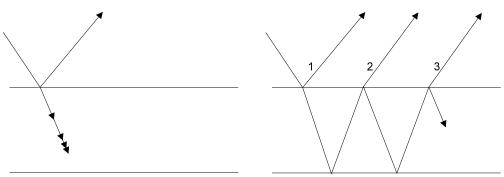


Fig. 5-122 The classical substrate model (left) and the transparent substrate (right)

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.

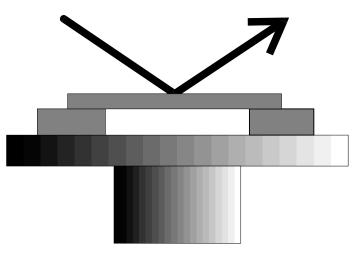


Fig. 5-123 Sample positioning for transparent substrates

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 absorbancies as well as layer thicknesses.

¹¹B. Heinze, "Optische Konstanten von Halbleiter-Mehrschichtsystemen", Diss. Aachen 1991

¹²J.A.Woollam, Doc. of VASE spectroscopic ellipsometer

idard Data Type Errors	Include error sources			-		
0.050 Delta: 0.200	Sample alignment [deg]: 0.0	20				
0.0050 T: 0.0050						1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0.0050 T: 0.0050	Wavelength calibration [nm]: 0.1	0				
rier coefficients: 0.0010	Device errors (see left)	efaults				and a second second
Ready.		Close	_		-	
yer stack at 300.0 nm wavelen Layer	ngth Thickness	Refr	active Index	Abso	rption	Comment
Air			1.0000			
Alg3 - cauchy	35.8 +/- 0.4 n	m 2.351	7 +/- 0.0089	()	
SiO2 (Silicon dioxide) - cau			1.4920			
SLG (tin side) - cauchy			1.5949	(0	
riable parameters of optical mo	del (without thicknesses)					
Name		Value	Err	or	Cor	mment
Alq3 - caud	hy: NO	1.658	0.0023	0%		
Alq3 - cauc	hy: N1	-55.2	11.58	%	Parameters is (td/2 <= a	close to zero compared with its typical difference td! $bs(x) \leq td) \rightarrow check$ the validity of the parameter yourself
Alq3 - caud	hy: N2	611.5	16.31	3%		
e: alq3_sio2.exp						

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 μ m), 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:

- $\delta \psi = 0.05^{\circ}$ (combination of sample tilt and absolute offset calibration accuracy)
- $\delta \Delta = 0.1^{\circ}$ (combines the drift caused by light source changes and temperature changes)
- $\delta R = 0.003$ (caused by positioning accuracy between reference and sample as well as noise)
- $\delta T = 0.003$ (same as R)
- $\delta s = 0.001$ (Fourier coefficients, typical noise value plus several minor sources)
- $\delta \phi = 0.02^{\circ}$ (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
- $x[0]+\delta x \dots x[N]+\delta x$ the original spectrum plus an offset
- $x[0]-\delta x \dots x[N]-\delta x$ the original spectrum minus an offset
- $x[0]-\delta x \dots x[N]+\delta x$ the original spectrum with a diagonal offset in plus direction
- $x[0]+\delta x \dots x[N]-\delta x$ 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 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 ($\delta n[i] \le 0.01$)
- check if the thickness as accurate as expected $(\delta th_k[j]/th_k[j] \le 0.01 i.e. 1 \%)$
- 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.



SpectraRay/4

b 🎽	iew Logon Collect Data Options Tools Calculate Plot Extra Window He ανεάς save REPORT NEW ENVIR SIMUL PARAM ERROR COMP PLOT SELECT APPL		
-	Experiment Explorer	Experiment Experiment No. 1 +	
Measure	Experiments [c:\sentech\spectraray4\exp] Models [c:\sentech\spectraray4\mod] Materials [c:\sentech\spectraray4\mat] [] Materials [c:\sentech\spectraray4\mat] [] [c:_experiments]	Air 1	kness 44 nm
		Sill(Sillicon)	

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	Thickness	Refrac	tive 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		
riable parameters of optical model (witho	out thicknesses)					
	out thicknesses)	3. Value		0.0158	Comment	
riable parameters of optical model (witho					Comment	

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	Thickness	Refrac	tive Index	Absorption	1	Com	ment
Air		1.	0000				
SiO2 (Silicon dioxide) - therm.	23.4 +/- 1.0 nm	1.4456	+/- 0.0413	0		lowered accu	racy: δn>0.01
Si (Silicon)		3.	8717	0.0158			
Si (Silicon) iable parameters of optical model (witho Name	out thicknesses)	3. Value		0.0158	Commen	t	
iable parameters of optical model (witho		1			Commen	t	

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:



SpectraRay/4

Layer stack at 632.8 nm wavelength

Layer	Thickness	Refra	ctive Index	Absorp	tion	C	Comment
Air			1.0000				
SiO2 (Silicon dioxide) - therm.	22.7 +/- 1.4 nm	1.472	6 +/- 0.0582	0		lowered accuracy: δn>0.01	
Si (Silicon)			3.8717	0.01	58		
	1						
ariable parameters of optical model (witho	out thicknesses)	1					
ariable parameters of optical model (witho Name	out thicknesses)	Value		rror		Comment	
		1				Comment	

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 $\pm 0.5\%$. 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

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Appendix B: Icon reference).

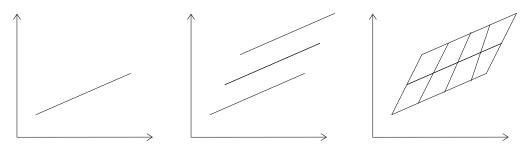


Fig. 5-125 Curve types: Curve (left), Multicurve (center), Network (right)

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.

Туре	Name	Description
beam properties	Delta(Psi)	ellipsometric angles for 2D-plots $\Delta(\Psi)$, as for measurements
		with retarder
	Delta180(Psi)	ellipsometric angles for 2D-plots $\Delta(\Psi)$, but $\Delta < 180^{\circ}$ as for
		measurements without retarder
	CosDe(TanPs)	trig. functions of ellipsometric angles for 2D-plots
		$\cos\Delta(\tan\Psi)$, 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 $\Delta < 180^{\circ}$ as for measurements with-
		out 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 inci-
		dence)
	Т	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	$\epsilon_1(\epsilon_2)$ 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 simu- lated 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 for- mat) 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 for- mat) 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 mod- ule	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 " μ m" was chosen "0.25" and "1.0" and "0.001" have to be used, respectively.

Simulation					19	
Wavelength	632.8 nm	Temperature:	23.5 °C	Devicetype,	PSCA	é
Angle of Incidence:	70.00 *	Process time.	0,0 s	Rotationtype	RAE	
Angle of Rotation	0,00 *	Environm	ent Settings	P/A angle	45,00	
Curve parameter	ē.	-				-
(0) Wavelength (nm	1					
From	10	1000,000				
	Curve step	1.000				
			Value 1:	Value 2	Туре:	
Calc unit Deltal	Psi)	1	236.016	35,983	Curve	
Add simulated d	ata to experiment					
Name at transfer file	e:	C\Sentech\SpectraRe	w/4ApplicationFra	mettemp.dat		
		2 Overwrite transfer fil	e 🔄 Add line o	colors 🗹 Mark first	t data	
i Diselau data a s	alotmodule	Name of style file: CV	Sentech/SpectraPo	ay-NApplicationFrame	Vnkd.sty	
 Disbidy data in b 						
Creete * dob file						

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 $n(\lambda)$ 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

Simulation							
Wavelength	63	3.0 nm	Temperature	23.6 °C	Devicetype	PSCA .	
Angle of Inci	gle of Incidence: 70,00 * Process		Process time:	Process time: 0.0 s		PAE .	
Angle of Rotation 0.00*		i0 ·	Environ	ment Settings	P/A angle	45,00 *	
Curve par	ameter					-	
[0] Waveler	ngth [nm]						
From 6	600,000	to:	000,000				
		Curve step:	1.000				
				Value		Туре	
Calc unit	n layer			2.115188		Curve +	
Layer:							
Add sime	lated data	to experiment					
Name of tra	inster file;		C\Sentech\SpectraF	Rey4\ApplicationFri	amelyernp.dat		
			V Overwrite transfer f	file Add line	colors @ Mark firs	t deta	
2 Display a	dats in plot	module	Name of style file C	\Sentech\SpectraP	Ray4VApplicationFrame	Vnkd.sty	
Create*	dob file						
		-	Qalc	Display	Help Ce	ancel Qua	

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.

Simulation				
Wavelength 633.0 nm	Temperature:	23.6 °C	Devicetype.	PSCA
Angle of Incidence: 70.00 *	Process time:	0,0 s	Rotationtype	RAE .
Angle of Rotation 0,00	Environm	ent Settings	P/A angle	45,00
Curve parameter:	-	Trace parameter		-
[0] Wavelength [nm]		[0] Angle [1]		1
From: 600,000 to	800,000	From: 55	10	75
Curve step:	1.000		Trace step	5
		Value:		Туре:
Calc unit Psi	16	8.453		Multi
Add simulated data to expension	C\Sentech\SpactraBr	w@ApplicationFramely	emo dat	
	Overwrite transfer file			t data
2 Display data in plot modula	Name of style file: \widetilde{CM}	Sentech/SpectraRay-N	ApplicationFrame	Unikid.sty
Create * dob file				

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 $(\varepsilon_1, \varepsilon_2)$ 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".

Simulation					lete l
Wavelength	633.0 nm	Temperature:	23.6 °C	Devicetype.	PSCA
Angle of Incidence.			0.0 s	Rotationtype	RAE
Angle of Rotation			ent Settings	P/A angle	45,00
Curve parameter	r.	-	Trace paramete	e .	
(0) Wavelength (nn	1	•	[0] Angle [1]		
From: 600,000	10	800,000	From 55	to.	75
	Curve step	1.000		Trace step:	5
	Trace step	50		Curve step:	0.1
			Value 1	Volue 2	Туре:
Calc unit	C=0.		Value 1 141.587	Volue 2: 8.453	Type: Net
Add simulated d	lata to experiment	C\Sentech\SpectraRe	141,587. syftApplicationFrame	8.453 Alemp.dat	Net
🕑 Add simulated d Name at transfer fil	lata to experiment	C\Sentech\SpectraRi g Overwrite transfer fil	141,587 sy4ApplicationFrame aAdd line colo	8.453 Ayemp.dat rs. <u>v</u> .Mark.firs	Nat •
Calc: unit	lata to experiment e: plot module	C\Sentech\SpectraRe	141,587 sy4ApplicationFrame aAdd line colo	8.453 Ayemp.dat rs. <u>v</u> .Mark.firs	Nat •

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 automat-

ed 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 least squares are the basis of the figure of merit. In the case of a set of (Ψ, Δ) -pairs it becomes:

(31)
$$MSE = \sqrt{\frac{1}{2N} \sum_{i=1}^{N} \left\{ \left(\frac{\Psi_i^{m} - \Psi_i^{th}}{\delta \Psi} \right)^2 + \left(\frac{\Delta_i^{m} - \Delta_i^{th}}{\delta \Delta} \right)^2 \right\}}$$

the "Calc unit" list. MSE is the abbreviation for Mean Square Error.

figure of merit for a single data set con-

sisting of a number of N Ψ values and the same number of Δ values.

The values $\delta \Psi$ and $\delta \Delta$ 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.

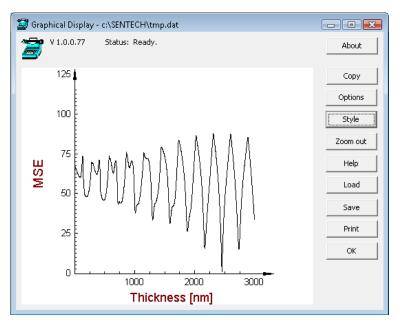


Fig. 5-130 Scanner example: 2.45 µm silicon dioxide on silicon

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^{\circ}, 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":

> 1. Environment 2. internal environment 3. x-and z-axis

stored within data set stored within data set

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	Туре	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
	Ta	ab. 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 $\cos\Delta$
"Delta180"	ellipsometric angle Δ in the range 0180°, as measured without retarder
"Psidelta"	
"Psidelta180"	
"Tanpsi cosdelta"	
"Mat. refractive index"	refractive index
"Mat_absorption"	Absorption coefficient
"TimeSec"	process time
"None"	untyped
"Epsilon1"	el 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.

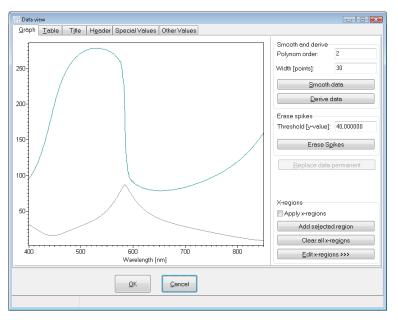


Fig. 5-132 Data editor view page

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.

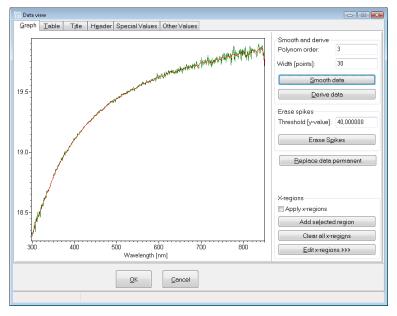


Fig. 5-133 Smoothing data

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:

(32)
$$p(x) = \sum_{i=0}^{N} C_{i} x^{i}$$

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

(33)
$$y'(x_i) = \frac{y(x_{i+1}) - y(x_i)}{x_{i+1} - x_i}$$

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:

(34)
$$y'(x_i) = \sum_{i=1}^{N} iC_i x^{i-1}$$

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.



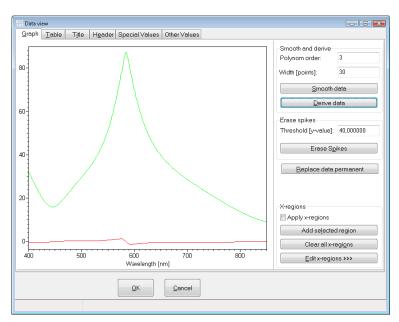


Fig. 5-134 Deriving spectra: example data set and derived spectrum (red)

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.

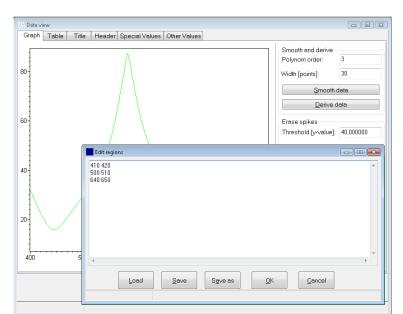


Fig. 5-135 Editing the interval list by using the ASCII editor

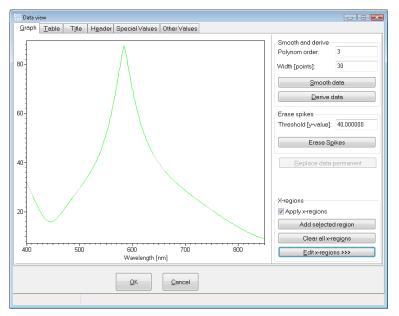


Fig. 5-136 Data points within x-regions are displayed grayed



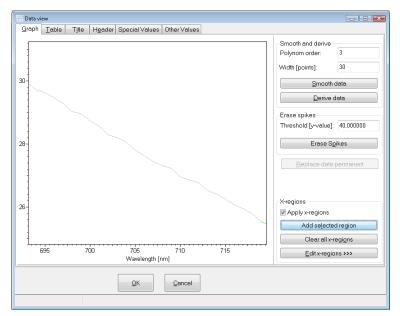


Fig. 5-137 A zoomed interval can be added to the x-region list by "Add selected region"

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.

010 101 Data	view						
Graph	n <u>T</u> able	Title	H <u>e</u> ader	Special V	alues	Other Values	
No.	Wavel	.[nm]		SI		DELTA	
				PHI:70,000		PHI:70,000	
1	400,000				95,82		
2	401,000		31,498		96,95		
3	402,000		31,030		98,22		
4	403,000		30,590		98,93		
5	404,000		30,072		100,0		
6	405,000		29,510		101,3		
7	406,000		29,105		102,2		
8	407,000		28,579		103,5		
9	408,000		28,153		105.0		
	409,000		27,652		106,3		
	410,000		27,093		107,6		
	411,000		26,738		109,1		
	412,000					41	
	413,000		25,747 112,103				
	414,000		25,354		113,4		
16	415,000		24,715		115,0		
17	416,000		24,339		116,8		
	417,000		23,884		118,6		
	418,000		23,415		120,2		
	419,000		22,916		122,1		
	420,000		22,473		123,9		
22	421,000		22,043		125,7		
23	422,000		21,615		127,8		
24	423,000		21,226		130,0		
•						III	
				<u>o</u> k		Cancel	

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.

User		Dete: 22.02.2013	Time: 095038	
		CON LE VELOTO	Timp, as as as	
Comment				
			2	
Measurementenvin				
Wavelength:	632,8 nm	Process time:	0,0 s	
Angle of incidence	70.00 '	Tempnreture:	23.5 °C	
Polarizer position	45.000	Weight	1.0000	
Device type:	PCSA	Sample rotation (theta)	0.00 *	
Change x-axis				
No. of points	750	X-axis by points:	Yes	
		Make x-toos by points	Remove x-axis by points	
New range of x-axis	380,245	970.022	Recalibrate x-axis	
			Filp x-axis direction	

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-ax	xis type and contains an exte	ensive trim
function.			

Detasare Greph Toble Title Heed	91	
x-Axis. Weivelength	Use all Use none	
t Psi + Phi		301 21,819
2 Delta + Phi		758 0,607
Current seAvja trom 388.24		

Fig. 5-140 Data editor header page

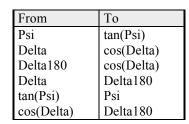
The x-axis type is selected by the first combobox. If you change this type two possible functions are executed. If the types are similar, only the label is changed. Otherwise a calculation is executed. For example for converting "eV" to "wavenumber" a multiplication is needed. If "eV" is changed to "nm" 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	Т	t	nm	cm ⁻¹
Angle of incidence (Phi)		1	1	1	1	1	1	1	1
Energy [eV]	1		1	1	1	1	1	cx	c
none	1	1		1	1	1	1	1	1
Sample Rotation (Theta)	1	1	1		1	1	1	1	1
Simulation (Sim)	1	1	1	1		1	1	1	1
Temperature (T)	1	1	1	1	1		1	1	1
Time (t)	1	1	1	1	1	1		1	1
Wavelength [nm]	1	cx	1	1	1	1	1		cx
Wavenumbers (cm-1)	1	с	1	1	1	1	1	cx	

Tab. 5-19 Conversion rules between x-units: 1 - 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. SENTECH



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:

Change d	ata 🗾
0	Do you really want to change the type of this y-axis?
	Yes No

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.

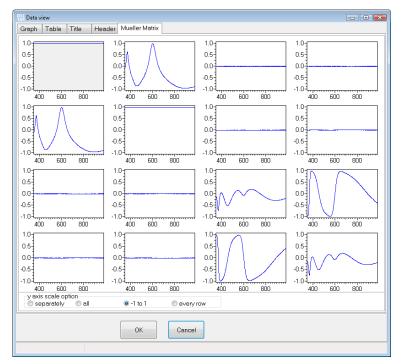


Fig. 5-142 Data editor Mueller matrix page

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 (PCSA¹³ 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).



SENTECH

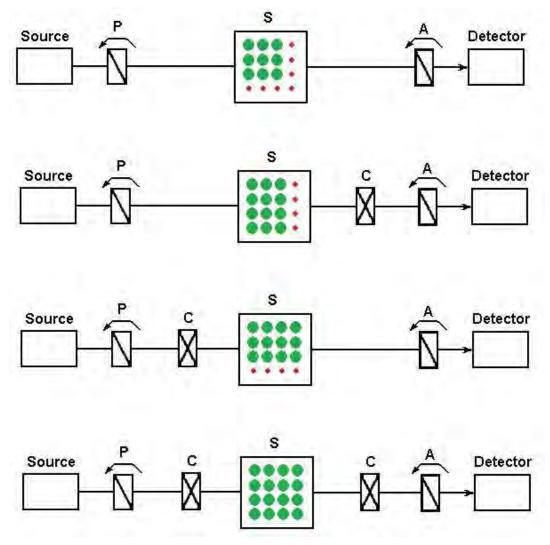


Fig. 5-143 Setups for measuring the Mueller matrix elements

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 press-

ing the icon bar button 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 \square . 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.



		All		None	
V Psi	<u>, e</u>		9. <u>1</u>		
V Delta					
Delta 180	1				
tan(Psi)					
🗆 cos(Delta)				
Reflectivit					
p-Reflecti					
s-Reflecti					
Transmis					
Refractive		1			
Absorptio					
Epsilon re Epsilon in					
Simulatio					
S1					
S2					
S1C					
S2C					
Degree o					
Mueller n					
Retarder				na	
🗌 PsiDelta p 🗌 Intensity	op ps sp	general	Ized		
S1CC 520					
3100 320	یار				

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 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 steer 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 The display shows all columns selected and uses the colors shown on the header page of each data sets editor.

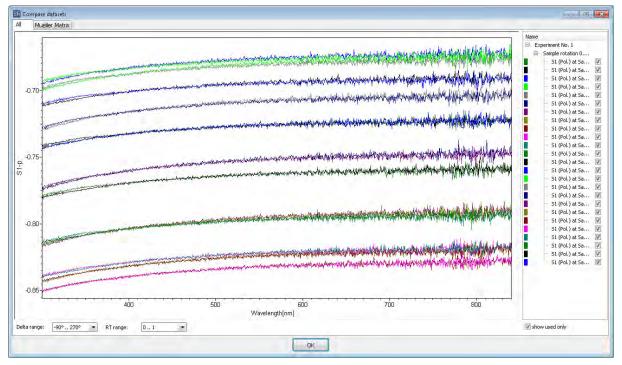


Fig. 5-145-5-146 Compare data columns viewer

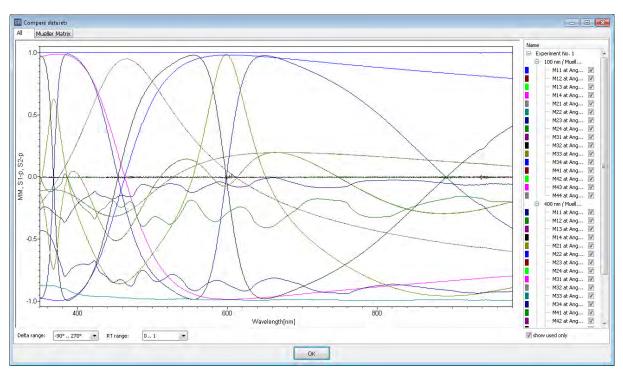


Fig. 5-147 Compare data sets containing Mueller matrices

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.

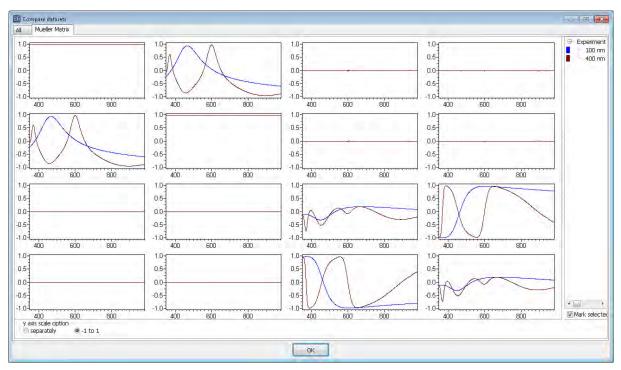


Fig. 5-148 Comparing two Mueller matrices

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	\mathbf{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
Z3	R ₁₃	R ₂₃
\mathbf{Z}_4	R ₁₄	R ₂₄

2. example: (Ψ, Δ) -measurement

_	z_1	\mathbf{z}_1	\mathbf{z}_2	Z ₂
x ₁	Ψ_{11}	Δ_{11}	ψ_{21}	Δ_{21}
\mathbf{X}_2	ψ_{12}	Δ_{12}	ψ_{22}	Δ_{22}

is swapped to

	X ₁	\mathbf{x}_1	x ₂	x ₂
z_1	ψ_{11}	Δ_{11}	Ψ_{12}	Δ_{12}
\mathbf{Z}_2	ψ_{11} 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:

$$F(\vec{p}) = \frac{\sum_{j=1}^{M} \frac{\sum_{k=1}^{C_j} \frac{\sum_{i=1}^{N_j} \left(\frac{\left(m_{ik}^j - t_{ik}^j(\vec{p})\right)}{w_k^j} \right)^2}{N_j}}{\sum_{j=1}^{M} v^j}$$

$$MSE(\vec{p}) = \sqrt{F(\vec{p})}$$

with

M N _j C _i	 = number of used data sets (measurements) = number of used rows of the k-th column in the j-th data set = number of used columns in the j-th data set
<i>.</i>	
m_{ik}^J	= measured data point in row i of the k-th column of the j-th data set
$t^{j}_{ik}(\vec{p})$	= theoretical 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.



Error calculation Show result window after fit Calculation type for derivatives: Use precision of (s1, s2) to get precision of (Psi, Delta) Precision in measured data for error calculation
Calculation type for derivatives: Plus/minus epsilon Vuse precision of (s1, s2) to get precision of (Psi, Delta)
Calculation type for derivatives: Plus/minus epsilon 👻
Use precision of (s1, s2) to get precision of (Psi, Delta)
Use precision of (s1, s2) to get precision of (Psi, Delta) Precision in measured data for error calculation
Precision in measured data for error calculation
Stokes \$1, \$2; 0.0050 None: 1.0000
Psi [']: 0.5000 Simulation: 1.0000
Delta [1: 1.0000 R, T: 0.0100
Set to defa

Fig. 5-149 Relative precision values for data types

aph Table Title	Header				
Measurement into	passes and a				
Nome Al2037	si				
Úser:		Date: Mo 05/07/2001	Time:		
Camment					
Measurement enviro	nment				
Wavelength	633 0 nm	Process time	0.001 min		
Angle at incidence	20,00 *	Temperature	296 7 K		
Polarizer position	45.00 *	Weight	1.0000		
Device type:	Unkown •	Sample rotation (theta):	0.00 +		
	Unkown				
Change x-axis					
No of points.	412	X-mos by points	Yeu		
		Make x-axis by pends	Romovo x-axis by points		
New range of x-axis	298.731	798 721	Recolibrate x-axis		
			Flip x-axis direction		
	T				
		OK Cancel			

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 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

Name	1	Fit	Value	S	croll va	alue	Minimum	Maximum	Typ. Diff.
[1] Waveleng	jth [nm]		632,8	4) *	1,0	1000000000,0	10,0
[1] Angle	e [°]		70,00	4			00,00	90,00	0,50
[1] Time	[s]	F	0,0	1		*	0,0	1000000000,0	10,0
[1] Temperat	ure [°C]	E	23,5	4		E.	-273,1	8000,0	10,0
[1] Sample ro	tation [°]	E	0,00	1		×.	-360,00	360,00	0,50
[1] Angle of	fset [°]	1 E	0,00	*			-90,00	90,00	0,10
[1] Wavelength	Offset (nm)	F	0,00	4		- + E	-10000,00	10000,00	2,00
[1] Waveleng	th Linear	E	1,00000	*	1	÷	-10,00008	10,00000	0,00300
Air: Refr.	index	E	1,000	4		×.	0,001	40,000	0,100
Air: Abso	ption	1 F	0,000	4			000,0	40,000	0,100
[1,1] SiO2: Thic	kness [nm]	F	3,00	4		- F.	0,00	40000,00	20,00
Si02: 1	NO.	E	1,452	*		E.	-100,001	100,000	0,100
Si02: 1	v1		36,0	4		- F	-40000,0	40000,0	100,0
Si02: 1	√2	E	0,0	4			-40000,0	40000,0	100,0
Si02: I	<0	1 F	0,000	4		- F	-100,000	100,000	0,100
Si02: I	<1	E.	0,000	+		÷.	-40000,000	40000,000	100,000
Si02: I			0,000	1		- F.	-40000,000	40000,000	100,000
	, în	-				_	_		
<u>Print table</u>	Fitpara	meters: 	lide >>			tore Loa /alues	ad <u>C</u>	ancel	<u>0</u> K

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 with 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.

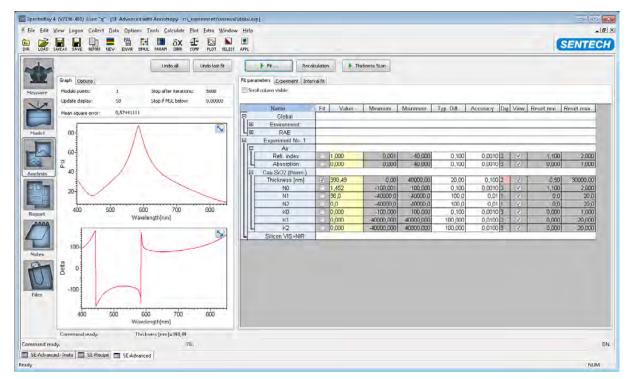


Fig. 5-152 Fitting session

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.

SR Fit Results							x
Name	Fit	Value	Minimum	Maximum	Typ. Diff.		i Vi ≜
[1,1] Cau-SiO2 (therm.): Thickness [nm]		391,33	0,00	40000,00	20,00	0,100 2	Г
Cau-SiO2 (therm.): NO	~	1,451	-100,001	100,000	0,100	0,0010 3	Г
Cau-SiO2 (therm.): N1	V	34,3	-40000,0	40000,0	100,0	0,01 1	K
4							E
			_				
Print table Fitparamet	ters: H	lide >>			<u>C</u> ancel	<u>o</u> k	

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 min- imum 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, until the interval has finally moved through the whole spectrum.

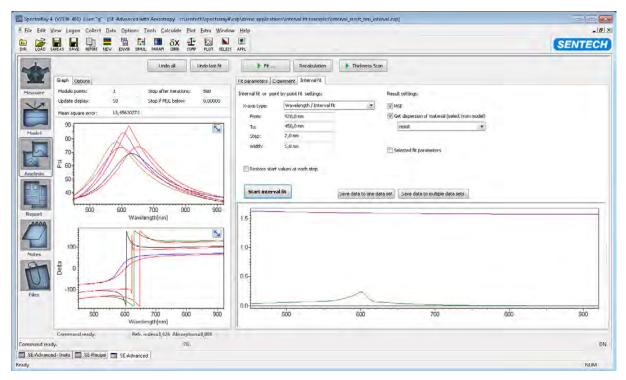


Fig. 5-154 Shifted interval fits

The settings needed to set up this interval fit are: X-axis type of X-axis select from

A-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
То	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.



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.

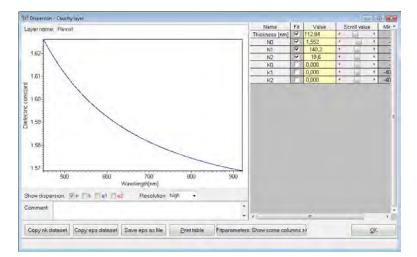


Fig. 5-155 Cauchy model of the resist film

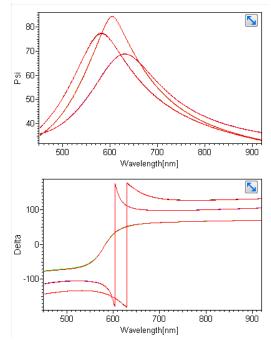


Fig. 5-156 Measured and calculated data after fit with Cauchy model

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.

Layername: Resist			Name	Fit	Value	S	croll valu	Je	Minimum	Maximu
and account of the state			Thickness [nm]		112,84	1		•	00,00	400000
			Refr. index	2	1,600	*		+	0,001	40,1
Thickness:	112,84 nm		Absorption		0,000			+	0,000	40,1
Refractive index n:	1,600									
Absorption index.k:	0,000									
Absorption index.k:	0,000									
	0,000									
Comment	0,000	÷ +	•	m						
	0,000		•	ĪĦ		-				

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:

Title	Thickness	State	Layer Type	Info [633,0 nm]
Air 📝			NK layer	n=1,0000
Resist	112,84 nm		NK layer	n=1,6000
SI DUV-UV-VIS-NIR		_	File layer	n=3,8736 k=0,01455

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.

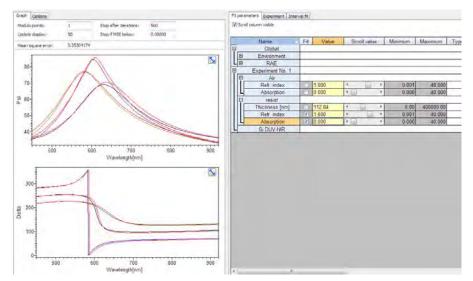


Fig. 5-159 Measurement and model with new model with "N,K layer". The model fits not exactly as a constant refractive index is used now.

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)

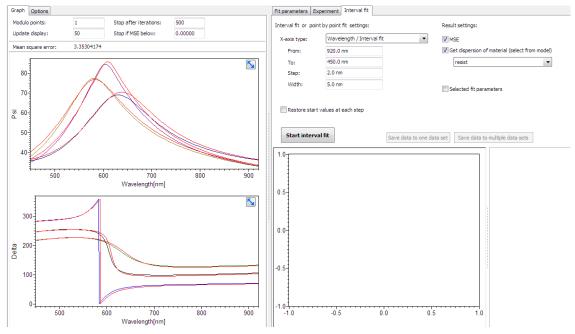


Fig. 5-160 "Shifted interval fit" window

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.

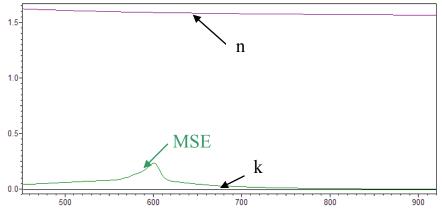


Fig. 5-161 "Shifted Interval Fit" results

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:

zeid • Simulation • 0.00000 1 1• 0.00012 0.236 iactor • None • 1 1• 1 5688 1.62
Ten Hondor RV - Use not Use none Stype - </th
Type Honodor 101 - Use all Use xione Stype y-Aviay detail 2-Aviay type 12-Vere/Mod Minimum (Maxime Ania) Stype y-Aviay detail 2-Aviay type 2-Vere/Mod Minimum (Maxime Ania) Avia - Stratation - 0.000001 - - 0.00012 2-30 Avia - Minimum (Maxime Ania) - 0.00001 - - 0.00012 -
Type Honodor 101 - Use all Use xione Stype y-Aviay detail 2-Aviay type 12-Vere/Mod Minimum (Maxime Ania) Stype y-Aviay detail 2-Aviay type 2-Vere/Mod Minimum (Maxime Ania) Avia - Stratation - 0.000001 - - 0.00012 2-30 Avia - Minimum (Maxime Ania) - 0.00001 - - 0.00012 -
tr) Use ell Use none type j-Avis detail z-Avis type z-Value Use Yeen/Mod Minimum Maximum add + Simulation - 6.0000 T = 1 0.0012 0.236 active Nene + 0.0000 T = 1 0.0012 0.236 Nene + 0.0000 T = 1 0.0012 0.236 Nene + 0.0000 T = 1 0.0012 0.236 Nene + 0.0000 T = 1 0.00000 T = 1 0.0000 T = 1 0.0000 T = 1 0.0000 T =
type ty-Axis detail z-Axis type z-Value Use View/Mod Minimum Machinum 4 Simulation 0.00000 T F 0.00312 8.238 zed + None - 0.00000 T F 1.9688 182 zed + None - 1.9688 182 1.928 1.92
type ty-Axis detail z-Axis type z-Value Use View/Mod Minimum Maximum 4 Simulation 0.00000 77 0.00312 6.2364 acdtry None 1 7.5688 1524
zeid Simulation 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 0.00000 1 1 0.00000 1
acty - None - 1 - 1 5688 1 62
south * None * - I I2 I 0.0000 0.00
from 452.000 to 320.000
from 452,000 to 920,000 each 1

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.

Da	ta
	Resist / Si Interval fit: MSE Interval fit: NK of Resist Interval fit: fit parameter: Resist: Refr. index Interval fit: fit parameter: Resist: Absorption

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

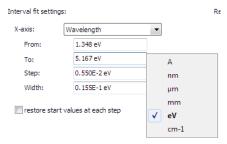


Fig. 5-164 Unit settings in edit fields

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.

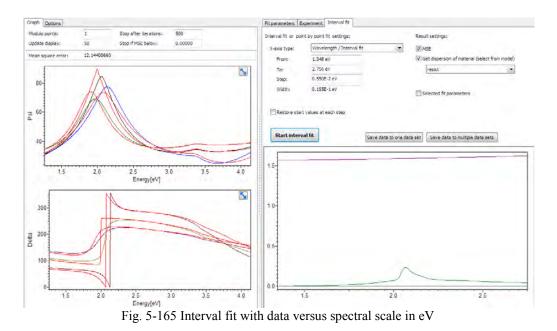


Fig. 5-165 shows the results of the interval fit with the spectral scale in eV. The data are the same as in the example in chapter 5.6.4.1.

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

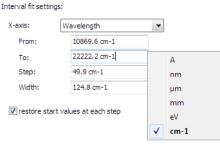


Fig. 5-166 Unit settings in edit fields

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.

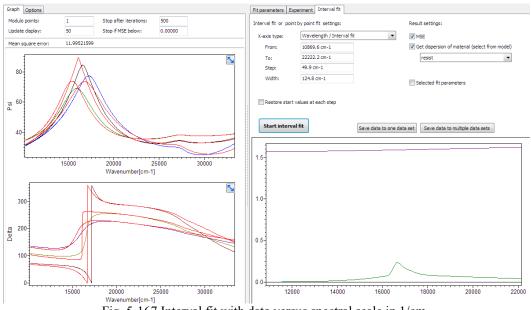
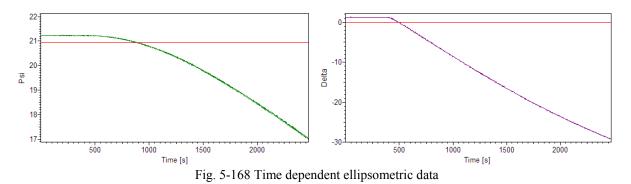


Fig. 5-167 Interval fit with data versus spectral scale in 1/cm

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.

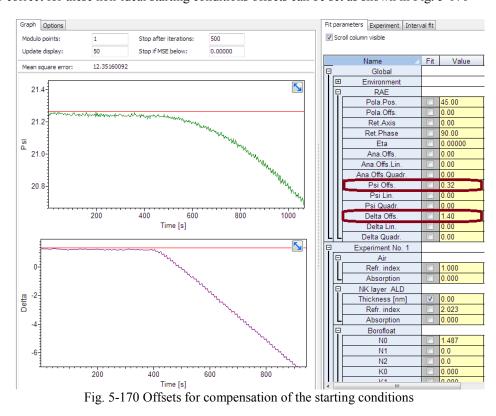


Time-dependent data from an atomic layer deposition process on glass are shown in Fig. 5-168.

Title		Thickness	State	Layer Type	Info [632.8 nm]					
er Air	\searrow			NK layer	n=1.0000					
	NoName0	0.00 nm		NK layer	n=2.0230					
L	Borofloat		_	Cauchy layer	n=1.4870					
1	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



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.

Fit parameters Ex	periment Interval fit			
Interval fit or poir	t by point fit settings:		Result settings:	
X-axis type:	Time / Interval	•	MSE	
From:	300.0 s		🔲 Get dispersion of n	naterial (select from model)
To:	2470.0 s			•
Step:	10.0 s		at wavelength:	632.8 nm
Width:	10.0 s		Selected fit param	eters
Dectore start	values at each step		Selected in paralli	
Restore start	values at each step			
Start interv	al fit	Save data to one data	set Save data to n	nultiple data sets

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-.

Layer name:	NK lavor	ALD		_	Name	Fit	Value
Edycrindine.	Nikidyei	ALD			[1,1] NK layer ALD: Thickness [nm]	V	0.00
					NK layer ALD: Refr. index		2.023
Thickness Thickness		0.00 nm			NK layer ALD: Absorption		0.000
Refractive	index n:	2.023					
Absorption	n index k:	0.000					
Comment				14			
				÷	• [m]		
Fitpar	ameters: H	lide >>	QK				

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.

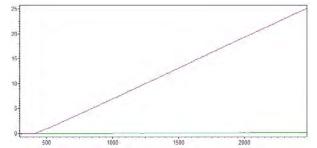


Fig. 5-173 Resulting film thickness versus time (purple) and MSE (green)

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.

see enapter 5.0.4.5 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.



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Data



Layer RTM Messung
Interval fit: MSE
Interval fit: fit parameter: [1,1] NoName0: Thickness [nm]

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.

		Layer RTM Measurement		
Interval fit or point	by point fit settings:		Result settings:	
X-axis type:	Data set - rows / Point by po	oint fit 🔹 🔻	MSE	
Use x-axis of o	data set for point by point fit (o	f experiment 1):	Get dispersion of m	aterial (select from model)
Layer RTM Me	essung	•		
Points: 1018	/ x-axis: Time [sec]		at wavelength:	632.8 nm
From: 0.109	/ To: 2473.564		Selected fit parame	ters
Use inverse	e direction of x-axis			
Restore start	values at each step			
Start interva	l fit	ave data to one data	set Save data to m	ultiple data sets

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.

_ayer name:	NK lavor	ALD.		Name	Fit	Value	
	Nicidyer			[1.1] NK layer ALD: Thickness [nm]	M	0.00	4
				NK layer ALD: Refr. index		2.023	
Thickness	5.	0.00 nm		NK layer ALD. Absorption	F	0.000	
Refractive	index n:	2.023					
Absorptio	n index k:	0.000					
Comment:			2				
			1	* m			
Fitpa	rameters: H	lide >>	<u>0</u> K				

Fig. 5-176 Starting values



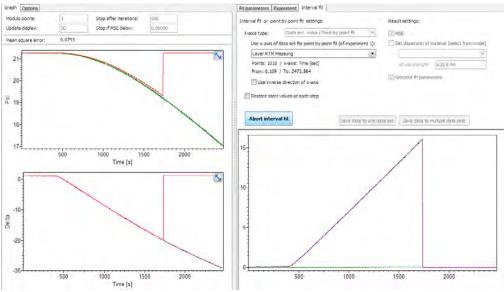


Fig. 5-177 Interval fit in progress

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.

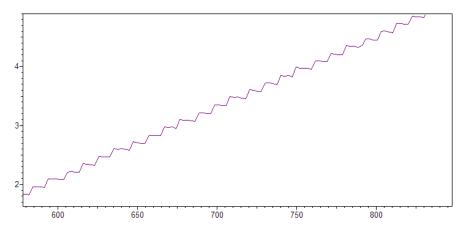
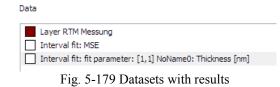


Fig. 5-178 Resulting thickness versus time showing the individual steps of an ALD deposition.

The results can be saved to files which appear in the main data box as datasets as shown in Fig. 5-179.



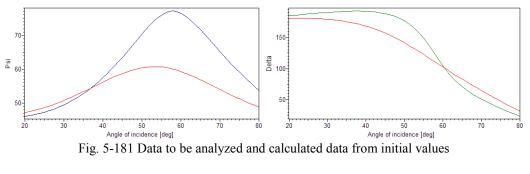
5.6.4.6 Example 4: Interval fit versus angle of incidence (phi)

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

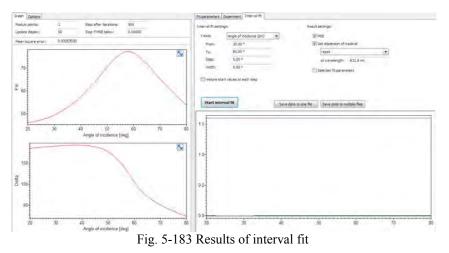
The data to be analyzed contains Ψ and Δ values versus angle of incidence. The model consists of an NK-layer with reasonable initial values. The initial data do not give a good description.



X-axis type:	Angle of incidence (phi) / Interval fit	▼ MSE
From:	20.00 °	📝 Get dispersion of material (select from model
To:	80.00 °	resist
Step:	5.00 °	at wavelength: 632.8 nm
Width:	5.00 °	Selected fit parameters

Start interval fit		Save data to one data set	Save data to multiple data sets
Eig 5 1	0) Cattinga fo	r intorvol fit vora	 a anala afinaidanaa

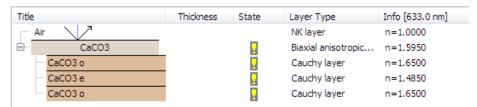
Fig. 5-182 Settings for interval fit versus angle of incidence



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 9. 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. 5-184 and Fig. 5-185.



Dispersion - Biaxia	al anisotropic layer										00	-
Lavername: CaC	203			Name	Fit	Value	Scr	oll value	Minimum	Maximum	Typ. Diff.	- A
and at the same same				CaCO3 Alpha [']	100	90.00	1	10. 1	-360.00	360.00	2 50	
	Anisotro	py option is available		CaCO3, Beta [']	101	0.00	*	<u>10</u> - K	-350.00	360.00	2,50	
			and the second	CaCO3: Gamma [']	101	0.00		12 8	350.00	360,00	2.50	
and the second second	g Z (E-vector in z-direc	son perpendicular to s	ample sunace)	Gamma N0	V	1.700	1	1. 1	-100.001	100.000	0.100	
CaCO3 o			Edit 2	Gamma N1	1.1	0.0	1.14		0.0	40000.0	100.0	
(Alphe I'l 9	00.00	From materials		Gamma N2	1.4	0.0	4	1	40000.0	40000.0	100.0	
The second is a second	be rotated around the		From layers	Gamma K0	1.5	0.000	4		-100 000	100.000	0.010	
	ale is the sum of Alpha		ieta.	Gamma K1 Gamma K2	1	0.000	1	1	-40000.000	40000.000	100.000	
Alle allegate and	The rate of a same arrithment	South Line in		Beta NO	0	1 500	2	1. 1	-100.001	100 000	0.100	
Dispersion along	gY(E-vector in sample	surface and normal to	plane of incidence):	Beta N1	1	0.0	Call	-	0.0	40000.0	100.0	-
CaCO3 e			EditY	Beta N2	6	0.0	4	10 1	40000.0	40000.0	100.0	
			Lon /	Beta K0	1	0.000	4	1. 1	-100.000	100 000	0.010	
Beta []: 0	1.00	From materials	From loyers	Beta K1	P	0.000	1.	10 1	40000 000	40000.000	100 000	
				Beta K2	11.1	0 000		12. A	-40000.000	49000.000	100.000	
Dispetsion along	gX (E-vector in sample	surface and parallel t	o plane of incidence):		-			-				
CaCO3 o			EditX									
	100	(TE)										
		From materials	From laver									
Refractive index n	nx=1.5000 ny=1.7000 nz nple rotation Theta 0.0	=1.7000		transm	issio	e geometry		flection				
@633.0 nm (sam	rx=1.5000 ny=1.7000 nz	=1.7000		e (tránsm hyfit puth	ission	geometry			085		rotation table sample rotati smission)/	
Refractive index n @ 6330 nm (sam	rx=1.5000 ny=1.7000 nz	=1.7000		transm	ission	geometry	re		085	angle of the angle of the mount (tran	rotation table sample rotati smission)/	
Refractive index n @ 633.0 nm (sam	nx=1.5000 ny=1.7000 nz pple rotation Thete: 0.00	=1.7000	700 75	transm	the E	geometry n'	re hold (nystal ont	e t	angle of the angle of the mount (tran	rotation table sample rotati smission)/	
Refractive index n @ 633 0 nm (sam 2 2 5 1 2 5 550	nx=1.5000 ny=1.7000 nz pple rotation Thete: 0.00	<1.7000 .) .) 		transm by it put by transm tra	he Ei	geometry n'	re hold (nystal ont	e t	angle of the angle of the mount (tran- tilt ξ = 0 (rot	rotation table sample rotati smission)/ ation)	on
Refractive index n @ 633 0 nm (sam 2 2 5 1 5 5 6 3 1 5 5 0 3 1 0 m 5 6 0 3 1 0 m 5 0	nx=1.5000 ny=1.7000 nz pplerotasion Theter 0.00 600 W9	<1.7000 .) .) 	700 75	transm upit put upit put upit upit put upit put upit upit put upit put upit upit put upit upit upit upit upit upit uput upit upi	he Ei	geometry n igensystem using the G	re hold (rystal ont	e t	angle of the angle of the mount (tran tilt ξ = 0 (rot Eigensys	rotation table sample rotati smission)/	on
Refractive index n 633 0 nm (sam 2 2 6 1 5 5 60 Show depension Comment	nx=1.5000 ny=1.7000 nz pplerotasion Theter 0.00 600 W9	<1.7000 .) .) 	700 75	transm 1978 perfect 2022 0 rotation of th 1aboratory sys	he Ei	geometry n igensystem using the G	re hold (rystal ont	e t	angle of the angle of the mount (tran tilt ξ = 0 (rot Eigensys	rotation table sample rotati (mission)/ ation) ation) tem of the cr (ate systems	on

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.

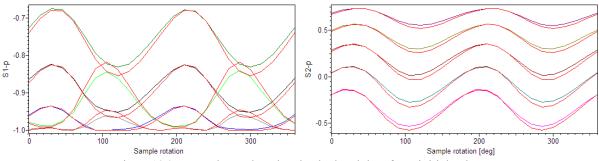
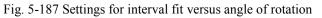


Fig. 5-186 Data to be analyzed and calculated data from initial values

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F		
From:	0.00 °	Get dispersion of material (select from mode
To:	360.00 °	
Step:	5.00 °	at wavelength: 632.8 nm
Width:	5.00 °	Selected fit parameters
Restore start	values at each step	



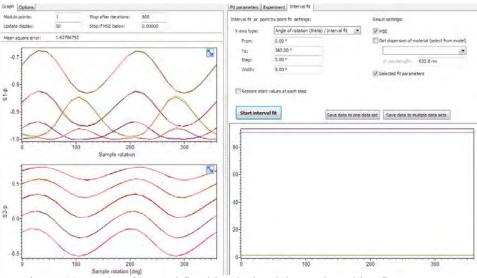


Fig. 5-188 Results of interval fit with calculated data and resulting fit parameters

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.

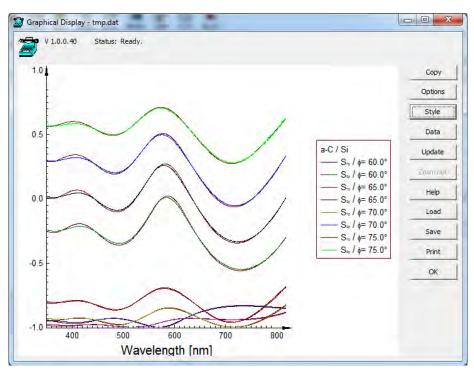


Fig. 5-189 Plot utility main screen

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:

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></file>	data file
/B: <file></file>	background file
/S: <file></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

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- 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

Options								X
Margin	5	 Fonts	;		Fran	ie – – – – – – – – – – – – – – – – – – –		
Left	10	\$ title	20	\$	Name	1 SENTE	СН	
right	10	\$ subtitle	12	\$	Name	2 Instru	ments GmbH	
top	10	\$ number	rs 12	\$	Name	3 Spectr	aRay/4	
bottom	10	\$ legend	16	\$	E 4	use frame for p	olots	
🔲 black &	white	Style C	:\SENTECH\	SPECTRA	\RAY4\APF	PLICATIONFRA	ME\NKD.STY	
						Cancel	0	<

Fig. 5-190 Option screen for selecting presets and style file

5.7.1.6 Options

Sentere

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.

SENTECH

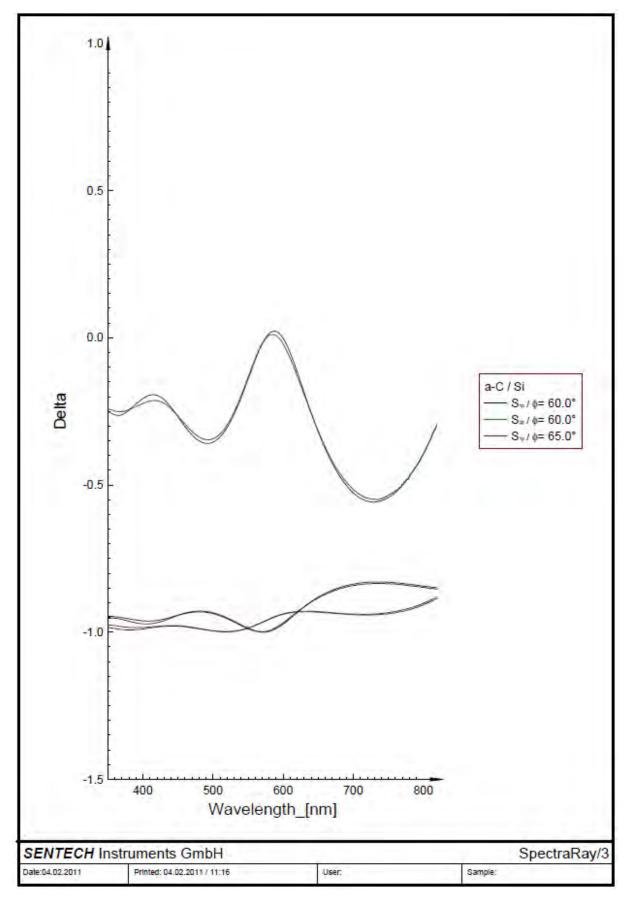


Fig. 5-191-5-192 Printout with information frame



der 1 der 2 ter 2 xis=Delta xisskip=0 nit= v=1-3 w=0 mel[1]=x aftmode=1 titern=** ad=00 background=ffffff _drawarea=c0c0c0 _number=00 _axistitel=80 Apply Load Save Save as Qu		11 ×	1	. 1
der 1 der 2 xis=vvaveiengur_[rim] xis=Delta xisskip=0 nit= nit= v=1-3 ow=0 me[1]=x aftmode=1 attern=** ad=00 background=ffffff _drawarea=c0c0c0 _axistitel=80				
der 1 der 2 xis=vvaveiengur_rimr xis=Delta xisskip=0 nit= nit= v=1-3 ow=0 me[1]=x aftmode=1 attern=** ad=00 background=ffffff _drawarea=c0c0c0 _axistitel=80	_			Save as
der 1 der 2 xis=Delta xis=Delta xisskip=0 nit= nit= v=1-3 ow=0 mel[]=x aftmode=1 attern=*** ad=00 background=ffffff _drawarea=c0c0c0 _axistitel=80	-			. F
der 1 der 2 xis=Delta xis=Delta xisskip=0 nit= nit= v=1-3 ow=0 mel[]=x aftmode=1 attern=** ad=00 background=ffffff _drawarea=c0c0c0 _axistitel=80				5ave
der 1 der 2 xis=vavelengur_int xis=belta xisskip=0 nit= nit= v=1-3 ow=0 me[1]=x aftmode=1 attern=** ad=00 background=ffffff _drawarea=c0c0c0 _axistitel=80	•			. T
der 1 der 2 xis=Vraveier xis=Delta xisskip=0 nit= nit= v=1-3 ow=0 mel[1]=x aftmode=1 attern=** ad=00 _background _drawarea= _number=00 _axistitel=80	-	l=ffffff c0c0c0		
a de dessisionit nit v m fittad d n a		r 2 ==Waveles ==Delta sskip=0 == =1-3 =0 el[1]=x mode=1 tern=** =00 ackgrounk rawarea= umber=00		a. 1

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.



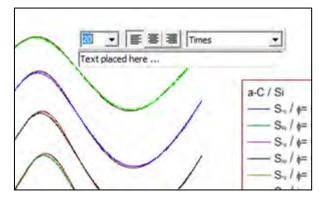


Fig. 5-194 Adding text to a plot

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).

<i>Command</i> Arial Siz Times Siz Courier Siz Symbol Siz	ize ize ize	ParameterDescriptionselects the Arial font and sets the size in points if the optional parameter is used.selects the Times font and sets the size in points if the optional parameter is used.selects the Courier font and sets the size in points if the optional parameter is used.selects the Symbol font and sets the size in points if the optional parameter is used.
Back OX W	vidth	draws an arrow of 40 pts or the length specified (optional) move to the last character position. Multiple BACK's are not allowed add an offset to the current point x-coordinate in points (for creating indices)
		add an offset to the current point y-coordinate in points (for creating indices) In 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
Сору	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

Command Reference 5.7.8

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 over-writes 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):

000000
FFFFFF
800000
FF0000
008000
00FF00
000080
0000FF
008080
OOFFFF
800080
FFOOFF
808000
FFFF00
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:

х	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:

 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):



1,1	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):

2,1
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.

2,1	2,2	2,3
1,1	1,2	1,3

;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:

2,1	
2	

;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 dl.dat
;range=0,d2.dat	Expand this range with dl.dat
;drawscale	Draw the scales
;read=d1.dat	Draw the data of dl.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 dl.dat
;range=0,d2.dat	Expand this range with dl.dat
;drawscale	Draw the scales
;read=d1.dat	Draw the data of dl.dat
;read=d2.dat	Draw the data of d2.dat
De 1 0 1 0 0	mus calls shows each other and calest the laws call
;Part= 2 1 2 2	Two cells above each other and select the lower cell
;Part= 2 1 2 2 ;range=1,d3.dat	Get the floating point range for plot no. 2 from d3.dat
,	
;range=1,d3.dat	Get the floating point range for plot no. 2 from d3.dat
;range=1,d3.dat ;range=0,d4.dat	Get the floating point range for plot no. 2 from d3.dat Expand this range with 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 xand 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 xyplane 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\0
```

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 $x>180^\circ$ 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.

SR Mapping Interface Settings
Measure methods Remote report Fit options
Select devices for remote measure
Spectroscopic elipsometer (if installed) Reflectivity R (via FTPadvanced if installed) Reflectivity Rs/Rp (via Spectroscopic ellipsometer if installed) Pass through: Measure via FTPadvanced (if installed)
Pass through device: none selected Read pass-through filename using current recipe
OK

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.



Mapping Interface Settings	- 0
Aeasure methods Remote report Fit options	
Parameter	
📝 thickness nk	
MSE	
🔲 fit parameter	
🔲 data special values from measure clients	
special values	
	?
OK	

A detailed help for the special values can be opened by clicking on the question mark.

Variable name	Replaced with content	
thickness	thickness values of all fitted layers	
thickness[1]	thickness value of surface layer	E
0	refraction index values of all fitted layers	
n[1]	refraction index value of surface layer	
n[1]:500	refraction index value of surface layer at wavelength	
refr	same as n	
k	absorption koefficient value, same syntax as n	
absk	same as k	
r.	reflectivity at observation wavelength, at angle of incidence	
r:500	reflectivity at wavelength in nm, here 500nm	
r:500-600	mean reflectivity at user spectral range in nm	
r::70	reflectivity at user defined spectral range in nm and user defined angle of incidence	
r:500:70	reflectivity at wavelength in nm and user defined angle of incidence	

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.

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Fitparam Param	eter of refle Set FitFlag	ata via SpectroElli— rt value	Param S	et FitFlag	Set s	tart value
Offset:		0,000	Damping:			1,000
CO:		1,000	Damping Linear:			0,000
C1:		0,000	Average:			0,000
C2:		0,000	Average Linear:			0,000
C3:		0,000	2.10011			
C4:		0,000				Set to default

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.

Viev	/ <u>L</u> ogon <u>C</u> ollect <u>D</u> ata <u>O</u> pti	o
\checkmark	Toolbar	
\checkmark	Status bar	
	Full screen	
	Website	
	SE-Advanced	
<	SE-Advanced - Insitu	SE-Advanced 🔜 SE-Advanced - Insitu

Fig. 6-1 Access to the in-situ view

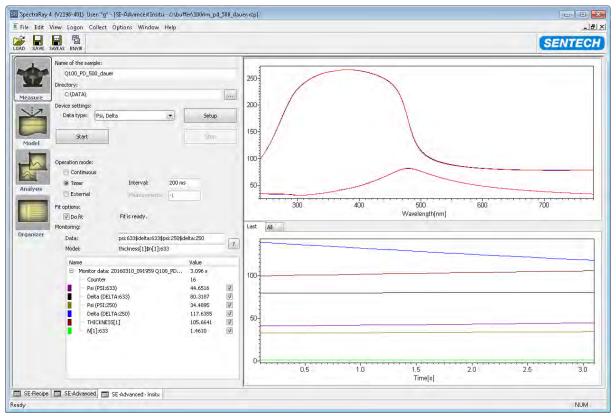
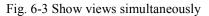


Fig. 6-2 Insitu main view

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.

<u>W</u> in	dow Help	
	Cascade	
	Tile 🕨	Horizontal
	Arrange Icons	Vertical
	Split	
\checkmark	1 SE-Advanced - c:\data\100nm_pd_500_dauer.rcp	
	2 SE-Advanced Insitu - c:\data\100nm_pd_500_dauer.rcp	



Lot Vew Logan Callect Options Window Help			SENTECH
Total Second Total Second <th>A A A A A A A A A A A A A A A A A A A</th> <th>Image: Advanced visibality Series Image: Advanced visibality Series Image: Advanced visibality Image: Advanced visibality Image: Advanced visibality Image: Advanced visibality</th> <th>Comment for 1</th>	A A A A A A A A A A A A A A A A A A A	Image: Advanced visibality Series Image: Advanced visibality Series Image: Advanced visibality Image: Advanced visibality Image: Advanced visibality Image: Advanced visibality	Comment for 1
SEPace (StAnson) (StAnson - Hu	0	Commune ready. Oc.	Ck. Dengis touris buts uncorregy.

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.



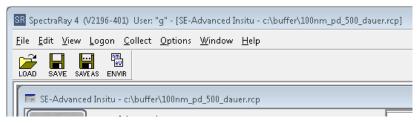


Fig. 6-5 Menu and toolbar of the insitu view

6.3 In-situ measurements

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	E			

Clicking on Measure 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:

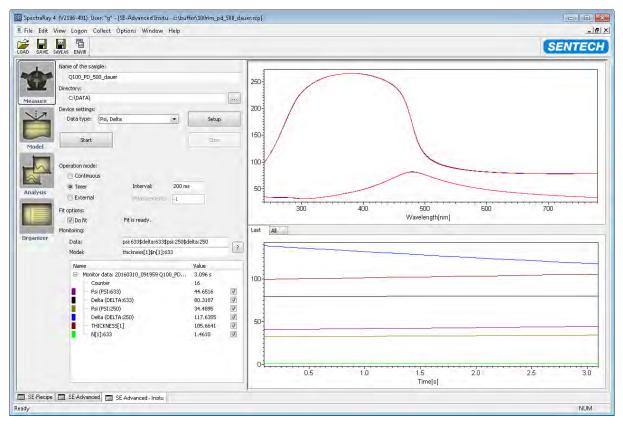


Fig. 6-6 In-situ measurement settings

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

Psi, Delta	-
Psi, Delta	
Psi, Delta and degree of p	olarisatic
Psi, Delta 180	
-S1, S2	
S1C S2C	

The desired measurement type can be selected in the list data type box S1C, S2C

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 Setup 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:

eration mode:		
Continuous		
Timer	Interval:	10000.0 ms
C External	Measurements:	-1

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

Fit options:

The option **Po** fit 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.

Monitoring:		
Data:	psi:633\$delta:633\$psi:250\$delta:250	
Model:	thickness[1]\$n[1]:633	£

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.

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ariable name	Replaced with content	
thickness	thickness values of all fitted layers	
thickness[0]	thickness values of top layer	
n	refraction index values of all fitted layers	
n[0]	refraction index value of top layer	
n[0]:500	refraction index value of top layer at wavelength	
refr	same as n	
k	absorption koefficient value, same syntax as n	
absk	same as k	
r	reflectivity at observation wavelength, at angle of incidence	
r:500	reflectivity at wavelength in nm, here 500nm	
r:500-600	mean reflectivity at user spectral range in nm	
r::70	reflectivity at user defined spectral range in nm and user defined angle of incidence	
r:500:70	reflectivity at wavelength in nm and user defined angle of incidence	
r:500-600:70	mean reflectivity at user defined spectral range in nm and user defined angle of incidence	
rs	reflectivity with s-polarization, same syntax as r	
rp	reflectivity with p-polarization, same syntax as r	
t	transmission, same syntax as r	
psi	psi, same syntax as r	
delta	delta,same syntax as r	
psipp psips psisp	generalized ellipsometry, same syntax as r	
deltapp deltaps deltapp	generalized ellipsometry, same syntax as r	
s1	s1, same syntax as r	
s2	s2,same syntax as r	
s1c	s1c, same syntax as r	
s2c	s2c,same syntax as r	
mm11 to mm44	Mueller matrix element [1,1] to [4,4], same syntax as r	
script[scriptvarname:digits]	returns a scriptvariable	
	OK	

Fig. 6-9 Monitoring special values

6.3.7 Start / stop measurement



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 (s_1,s_2) versus wavelength. If the fit option is active the fitted spectra are also displayed in red color. See for example Fig. 6-10.

SpectraRay/4

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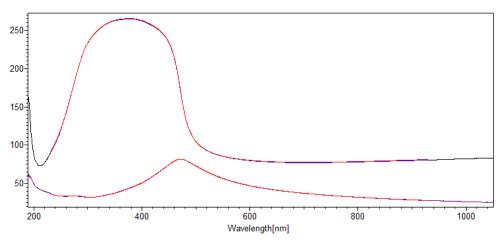


Fig. 6-10 Psi and Delta spectra with fit in online view during measurement

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.

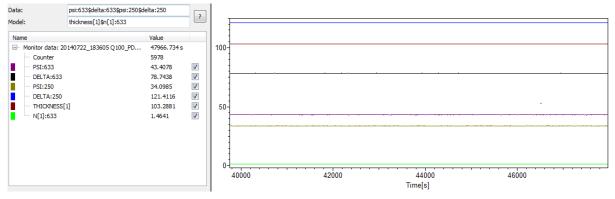


Fig. 6-11 Control lines during measurement

6.3.9 Data storing during measurement

The data are stored during the measurement procedure as shown in Fig. 6-12.

Vame	Date	Туре	Size
20140722_183605_Q100_PD_500_dauer.cont	rol.dob 22/07/2014 18:36	DOB File	336 KB
20140722_183605_Q100_PD_500_dauer.dob	22/07/2014 18:36	DOB File	292,456 KB

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.

Experiment Explorer		Experiment Experiment No. 1	+		
🛱 🖻	o 2	Model			<mark>k</mark> 🕅
⊕		Title	Thickness	State	Layer Type
🖶 🗐 Models [c:\sentech\spectraray3\mod]		Air (n=1)			NK layer
Materials [c:\sentech\spectraray3\mat] G:\data]		Cau-SiO2 (therm.)	100.00 nm		Cauchy layer
01C 20140722_183605_Q100_PD_500_dauer.control.dob		Si DUV-VIS-NIR			File layer
ic 010 20140722_183605_Q100_PD_500_dauer.dob		•		III	
□ 010 Data set count: 5980		Data			
01C 1: Q100_PD_500_dauer / 1 / 14.379 s 01C 2: Q100_PD_500_dauer / 2 / 22.380 s					
010 3: Q100_PD_500_dauer / 3 / 30.380 s		20140722_183605 Q100_P	D_500_dauer		
010 4: Q100_PD_500_dauer / 4 / 38.380 s					
01C 5: Q100_PD_500_dauer / 5 / 46.380 s					

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 subfile 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.

Experiment	Explorer					Experiment	Experiment No. 1	+		
] 👼	2		Model				
🕀 🗐 E	xperiments	[c:\sentech\spectraray3\exp]		*		Title			Thickness	State
🗎 🖶 🗐 M	odels [c:\se	ntech\spectraray3\mod]				Air (n	=ì), 🖊			
📗 🖶 🗐 M	aterials [c:\	sentech\spectraray3\mat]					Cau-SiO2 (therm.)		100.00 nm	
🖨 🧰 [c	::\data]						SI DUV-VIS-NIR			
01	c 20140722	2_183605_Q100_PD_500_dauer.control.	dob							
E 01 10	G 20140722	2_183605_Q100_PD_500_dauer.dob				•				
						·				
 =	010 Data s	set count: 5980								
	01C 101 1:	Q100_PD_500_dauer / 1 / 14.379 s				Data				
	101 2:	Q100_PD_500_dauer / 2 / 22.380 s				0100	PD 500 dauer / 4	/ 38.38	0 s	
		Q100_PD_500_dauer / 3 / 30.380 s					_PD_500_dauer / 9			
		Q100_PD_500_dauer / 4 / 38.380 s				-		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
	01C 101 5:	Q100_PD_500_dauer / 5 / 46.380 s			ł					
		Q100_PD_500_dauer / 6 / 54.380 s			i.					
		Q100_PD_500_dauer / 7 / 62.881 s								
		Q100_PD_500_dauer / 8 / 70.881 s			i					
	010 👝	0400 DD F00 J 10 170 000 -				1				

Fig. 6-14 In-situ raw data file in the data box of the standard view

6.4 In-situ model



Clicking on *model* 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.

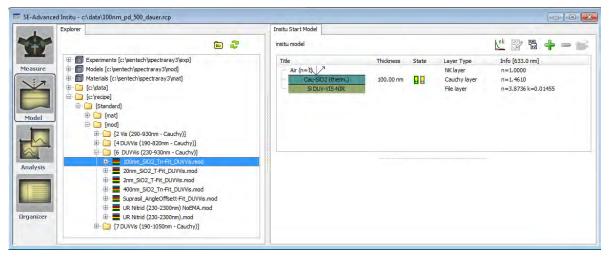


Fig. 6-15 In-situ model view

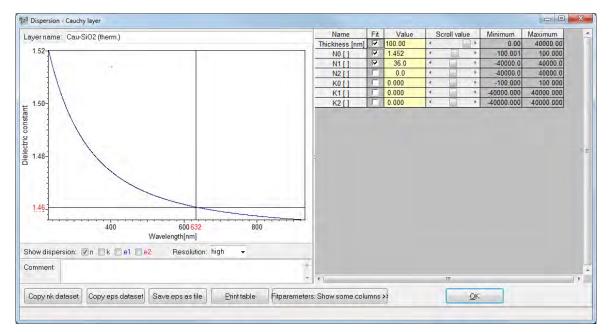


Fig. 6-16 Layer details, Cauchy layer as example

6.5 In-situ analysis

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I	5
ł	

Clicking on *Analysis* 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.

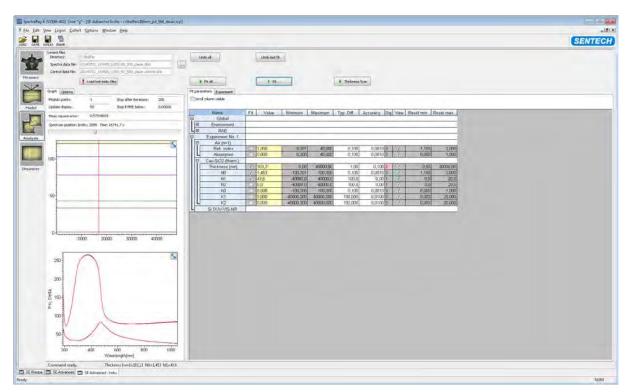


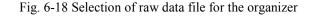
Fig. 6-17 In-situ analysis view

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.

.ook in: 🛄	DATA 👻 🧿 🥬	💌 🛄 🕈			
Name	*	Date	Туре	Size	
2014072	2_183605_Q100_PD_500_dauer.control.dob	22/07/2014 18:36	DOB File	336 KB	
2014072	2_183605_Q100_PD_500_dauer.dob	22/07/2014 18:36	DOB File	292,456 KB	
	m				
	m 20140722_183605_Q100_PD_500_dauer.dob			- Open	
 ✓ File name: Files of type: 				Open Cancel	





Current files Directory:		
Spectra data file:	C:\DATA\20140722_183605_Q100_PD_500_dauer.dob	 Load last insitu files
Control data file:	C:\DATA\20140722_183605_Q100_PD_500_dauer.control.dob	

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.

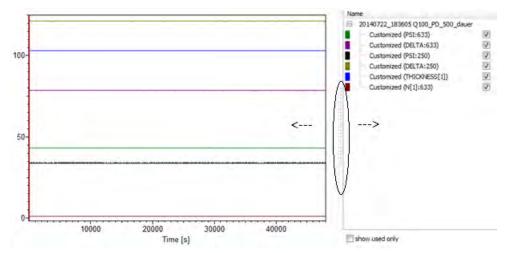


Fig. 6-20 Control data in the upper left diagram. Open legends by moving the vertical separation bar.

The diagram can be zoomed using the mouse in the usual way.

Spectrum position: Index: 2533 Time: 20335.607 s

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

SENTECH SpectraRay/4

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.

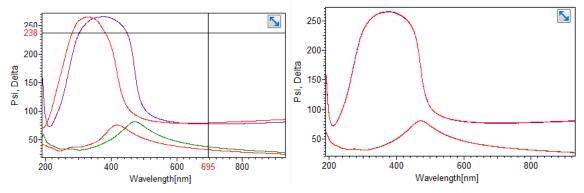


Fig. 6-22 Selected spectra with fitted (theory) spectra. Left side: before fit, Right side: after fit

As shown in Fig. 6-23 the display can be modified using the optional settings.

	Graph	Options					
	Graph o	options					
	Delt	a plot mod	e:	0° 360°	•		
	RT p	olot mode:		01	•		
	V 5	Show axis l	abel				
	V	Autoscale n	neasu	rement only			
	🔲 No update of table during fit						
I			Fig.	6-23 Optior	ıs		

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.



🕨 Fit ...

Fit par	ameters Experiment									
Scr	oll column visible									
	Name 🗸	Fit	Value	Minimum	Maximum	Typ. Diff.	Accuracy	Dig View	Reset min.	Reset max.
P	Global									
Œ	Environment									
L⊞	RAE									
민	Experiment No. 1									
II P	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
II P	Cau-SiO2 (therm.)									
	Thickness [nm]	V	103.26	0.00	40000.00	1.00	0.100	2 🗸	0.50	30000.00
	N0 []	V	1.452	-100.001	100.000	0.100	0.0010	3 🔽	1.100	2.000
	N1[]	V	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
L	Si DUV-VIS-NIR									

Ein .	6 04 E	714 - L	barameter	a attin an	- f	~~~~~		~	
F10	0-74 F	u r	barameier.	sennos	01	currrent	1n-3	SILLE	moder
	0 2 i i	10 1	Julullietel	seeings	01	carrent		orea	mouer

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.

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" n	initiates a thickness scan by searching the best agreement for thicknesses between ninimum 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.



Graph Options	
Fit options	
🔲 Do thickness scan be	fore fit
Thickness scan with	R/C0, R/C1 and/or T/C0 scan if available
Monitoring values:	
Loaded:	
Data:	
Model:	PSI:633\$DELTA:633\$PSI:250\$DELTA:250\$TH]
New:	
Data:	Psi: 500\$Delta: 500
Model:	Thickness[1]\$n[1]:500
Save options:	
Filename suffix	recalc
Autosave to file	
Copy to experiment	

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.



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		SENTED
And a space of or: Sector points (SAS) (S	Revenue Revenue	
yels	Experiment No. 1	
	Ref: index 1,000 0,001 40,000 0,000 0,000 1,000 Absorption 0,000 0,000 0,000 0,000 0,000 1,000	
607 60-	No / 102,45 0,000 40000,00 1,00 0,000 2,000 30000,00 No / (#68 100,001 0,000 10,000 0,000 10,000	
0 10 10 10 10 10 10 10 10 10 1		
20 20 20 20 20 20 20 20 20 20 20 20 20 2		

Fig. 6-26 Recalculation in progress

🔤 Spectrality 4 (V(156-41)). User "g" - [15-Advaces[a/sta-c:lba/ter.30mm.jd; 560; downcrys]	
A för Lat Vern Legen Celler Sphere Mindow Lege	_[伊]×
	SENTECH
Con Control Provided	New 314222_119665_0101_P0_301_daw Boele0 - Cultures of PTL:30 37 - Cultures of PTL:30 37 - Cultures of PTL:300 37
	Priv925200 (2) Celebral (1002)820(1) (2) Model (1002)820(1) (2) Model (1002)820(1) (2) Stateward (1002)820(1) (2) Stateward (1002)820(1) (2) Celebral (1001) (2) Celebral (1001) (2) Celebral (1001) (2)
Tme (s)	
Running Singles	
Ready	NUM

Fig. 6-27 New results from recalculation in enlarged display

6.6 In-situ organizer

100

Clicking on Organizer 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.

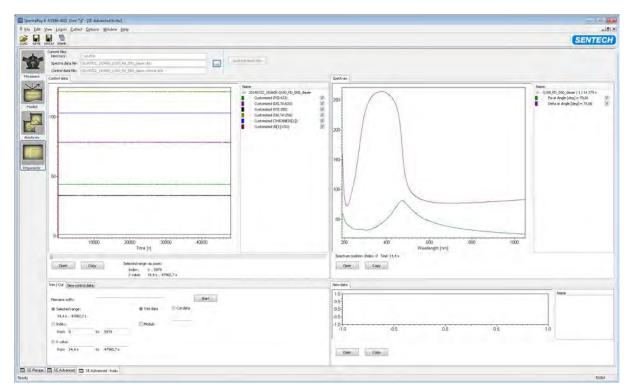


Fig. 6-28 In-situ organizer view

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.



uchen in:	🎍 buffer 🔹 🕫 🗊 🕇	
Vame	*	Änderungsdatum
201407	22_183605_Q100_PD_500_dauer.control.dob	23.07.2014 07:56
201407	22_183605_Q100_PD_500_dauer.dob	23.07.2014 07:56
	m	
e l	m 11 20140722_183605_0100_PD_500_dauer.dob	✓ Ölfnen
		Offnen Abbrechen

Fig. 6-29 Selection of raw data file for the organizer

Current files Directory:	C:\DATA	
Spectra data file:	20140722_183605_Q100_PD_500_dauer.dob	 Load last insitu files
Control data file:	20140722_183605_Q100_PD_500_dauer.control.dob	

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.

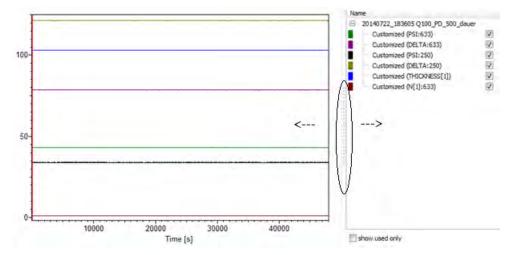


Fig. 6-31 Control data in the upper left diagram. Open legends by moving the vertical separation bar.

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.

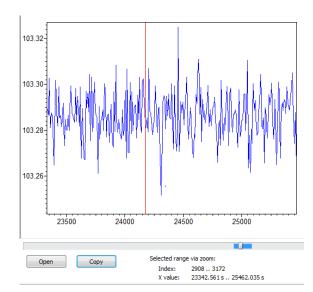


Fig. 6-32 Zoomed part of the data with slider (arrow on blue range indicator) and cursor (red line)

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.

Gra	.µn i	able Title		Header					_						_
x-A	xis: T	ïmesec		•	Use	all	Use	none							
	Color	y-Axis type	e	y-Axis detail	z-Axis type		z-Value	Use	View	Mod.	Minimum	Maximum	Device type	Rotation type	Ŀ
1		Customized	Ŧ	PSI:633	None	•		R	×		43.31212	43.49406	NONE -	RAE 🔻	4
2		Customized	•	DELTA:633	None	•		N	•		78.59212	78.86836	NONE -	RAE 🔫	-
3		Customized	•	PSI:250	None	•		K	•		34.04637	34.20603	NONE -	RAE 🔫	
4		Customized	•	DELTA:250	None	•					121.27745	121.72621	NONE -	RAE 🔫	
5		Customized	•	THICKNESS[1]	None	•		N			103.24556	103.32500	NONE -	RAE 🔫	
6		Customized	•	N[1]:633	None	•		N			1.46383	1.46442	NONE -	RAE 👻	L
Cu	rrent x-	Axis: from	1	14.379	to 47982.734										
	Trim from 14.379 to 47982.734 each 1														
	OK Cancel														

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.



Data	🖄 😑 📕 💕
Q100_PD_500_dauer / 3012 / 24170.051 s	
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.

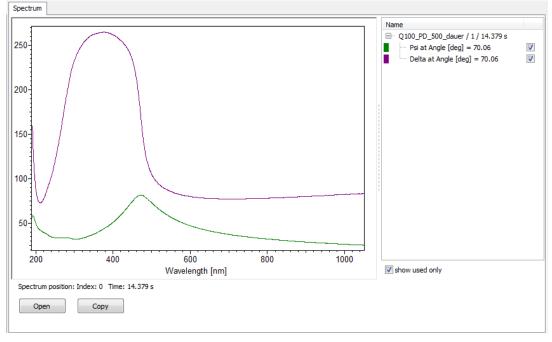


Fig. 6-36 Raw data spectra display.

The button Open 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.



raph Table Title Measurement info	e Header Spe	cial Values Other Values		
Name: COULF	0_500_dever/301	2/24170.051 6		
User:		Date: 23/07/2014	Time: 01:18:55	
Comment: Counter	: 3012		21	
Measurement enviro	onment			
Wavelength:	632.8 nm	Process time:	24170.051 s	
Angle of incidence:	70.06 *	Temperature:	23.5 C	
Polarizer position:	44.98 *	Weight:	1.0000	
Device type:	Unkown 👻	Sample rotation (theta):	0.00 *	
	Unkown 🔹			
Change x-axis				
No. of points:	1902	X-axis by points:	Yes	
		Make x-axis by points	Remove x-axis by points	
New range of x-axis	189.923	1050.001	Recalibrate x-axis	
			Flip x-axis direction	
		OK Cancel		

Fig. 6-37 Name, index, time of measurement of selected spectra

01C Tot Data view	
Graph Table Title Header Spec	cial Values Other Values
x-Axis: Wavelength 🔹	Use all Use none
Color y-Axis type y-Axis detail	
1 Psi ▼ 2 Delta ▼	Phi ▼ 70.06 ▼ Γ 25.696 82.160 NONE ▼ RAE ▼ ≜ Phi ▼ 70.06 ▼ Γ 73.324 265.218 NONE ▼ RAE ▼ ▲
	₹ ▼ ▼
Current x-Axis: from 189.923	to 1050.001
Trim from 189.923	to 1050.001 each 1
	OK Cancel

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.



Data	📐 🗕 🕌 泽
20140722_183605 Q100_PD_500_dauer	
Q100_PD_500_dauer / 3012 / 24170.051 s	

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.

rim / Cut	New control da	ata				
Filename s	uffix					Start
Selecte	d range:			🔘 Trim data	Out data	
21387	.596 s 2734	7.010 s				
Index:				Modulo		
from:	2990	to	3020			
🔘 X value						
from	14.379 s	to	47982.734 s			

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	Start .	

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

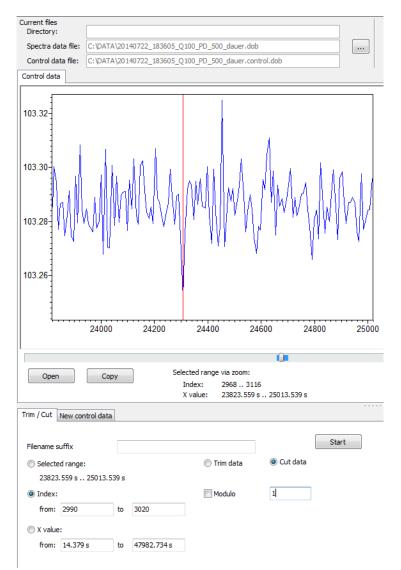
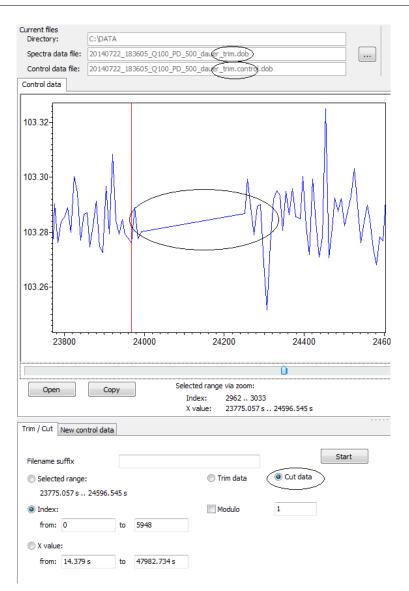
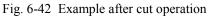


Fig. 6-41 Example before cut operation







Gover the computer to the comp	Windows (C:) > DATA		✓ 4 Search I	DATA	3
File Edit View Tools Help Organize Include in libra				i≣ • П	0
r Computer	Name *	Date modified	Туре	Size	
🏭 Windows (C:) 📃	20140722_183605_Q100_PD_500_dauer.control.dob	23/07/2014 07:55	DOB File	336 KB	
SRECYCLE.BIN 20140722_183605_Q100_PD_500_dauer.control.dob ba 20140722_183605_Q100_PD_500_dauer.dob 20140722_183605_Q100_PD_500_dauer.dob		23/07/2014 07:55	DOB File	292,456 KB	
		23/07/2014 09:51	DOB File	334 KB	
_qs	20140722_183605_Q100_PD_500_dauer_trim.dob	23/07/2014 09:51	DOB File	290,946 KB	
bata 🔶	Pormal rep	21/07/2014 16:15	PCD Ello	24 KB	

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.

Current files Directory:	C:\DATA					
Spectra data file:	C:\DATA\201	40722_183605_0	Q100_PD_5)0_dauer.dob)	
Control data file:	C:\DATA\201	40722_183605_(Q100_PD_5	0_dauer.con	trol.dob	
Control data						
			· · · · · · · · · · · · · · · · · · ·			· · · · · · · · · · · · · · · · · · ·
	10000	200	00 Time [s	30000]	40	,
Open	Сору	Se	lected range Index: X value:	05979	47982.734 s	
Trim / Cut New co	ntrol data					
Filename suffix	mo	dified				Start
Selected range	:		01	rim data	🔘 Cut data	
14.379 s 47	982.734 s		V N	1odulo	5	
from: 0	to	5979				
X value:						
from: 1200.0	00 s to	22000.000 s	_			



Current files Directory:	C:\DATA
Spectra data file:	20140722_183605_Q100_PD_500_dauex_modified.dob
Control data file:	20140722_183605_Q100_PD_500_dauer_modified.control.dob
Control data	
100-	
50-	
0-	5000 10000 15000 20000 Time [s]
Open	Copy Selected range via zoom: Index: 0 518 X value: 1200.361 s 21980.584 s
Trim / Cut New cor	ntrol data
Filename suffix	
1200.361 s	21980.584 s
from: 0	
	to 518
X value:	to 518

Fig. 6-44 Example before trim operation

Fig. 6-45 Example after trim operation

🗲 🗸 🕨 🗸 Computer 🕨	Vindows (C:) > DATA		👻 🍫 Search DAi	TA
ile Edit View Tools Help				
Organize 🔹 📄 Open 🔹	Burn New folder			🌐 🕈 📶 🧯
📲 Computer 🔷	Name	Date modified	Туре	Size
🏭 Windows (C:)	20140722_183605_Q100_PD_500_dauer.control.dob	23/07/2014 07:55	DOB File	336 KB
SRECYCLE.BIN	20140722_183605_Q100_PD_500_dauer.dob	23/07/2014 07:55	DOB File	292,456 KB
_ba	20140722_183605_Q100_PD_500_dauer_modified.control.dob	23/07/2014 10:03	DOB File	38 KB
_qs DATA +	20140722_183605_Q100_PD_500_dauer_modified.dob	23/07/2014 10:03	DOB File	26,318 KB

Fig. 6-46 New files saved on the disc

aph Io.	Time [sec]	CUSTOMIZED	CUSTOMIZED	CUSTOMIZED	CUSTOMIZED	CUSTOMIZED	CUSTOMI	
1	1200.36096	43.36751	78,71816	34,14065	121.41125	103.30365	1,46401	
2	1240.36206	43.43028	78.71469	34.11747	121.53533	103.29768	1.46407	
3	1280.86401	43.39734	78.70899	34.10592	121.57014	103.29359	1.46410	
4	1320.86499	43.37229	78.72214	34.09188	121.51944	103.30298	1.46405	
5	1360.85706	43.41149	78.70646	34.11929	121.45077	103.27677	1.46417	
6	1400.85803	43.40263	78.70745	34.10227	121.51363	103.29048	1.46409	
7	1440.85999	43.40879	78.71678	34.11192	121.48317	103.29497	1.46411	
8	1480.86096	43.43757	78.73936	34.12986	121.64115	103.27186	1.46416	
9	1520.86206	43.42577	78.73534	34.09956	121.38855	103.28327	1.46411	
10	1560.86401	43.35565	78.76516	34.11620	121.49411	103.27282	1.46420	
	4004 05400	10 11101	70 00040	01 40017	404 50500	400.00040		
 J 12	21100.00300	43.40753	78.73323	34.12070	121.57004	103.20173	1.46422	
 J 12	21740.08594	70.71122	10.17220	07.12010	121.70701	100.20110	1.70711	
513	21740.08594 21780.08789	43.40753	78.73323	34.11029	121.57004	103.27272	1.46422	
513 514	21740.08594 21780.08789 21820.08984	43.40753 43.36806	78.73323 78.74604	34.11029 34.12795	121.57004 121.52469	103.27272 103.27886	1.46422 1.46425	
512 513 514 515	21740.08594 21780.08789 21820.08984 21860.08008 21900.08203	43.40753 43.36806 43.42732 43.41845 43.38456	78.73323 78.74604 78.80419	34.11029 34.12795 34.09141	121.57004 121.52469 121.41938	103.27272 103.27886 103.29493	1.46422 1.46425 1.46409	
513 514 515 516	21740.08594 21780.08789 21820.08984 21860.08008 21900.08203	43.40753 43.36806 43.42732 43.41845 43.38456	78.73323 78.74604 78.80419 78.72044	34.11029 34.12795 34.09141 34.11989	121.57004 121.52469 121.41938 121.50877	103.27272 103.27886 103.29493 103.27350	1.46422 1.46425 1.46409 1.46423	
512 513 514 515 516 517 518	21740.08594 21780.08789 21820.08984 21860.08008 21900.08203 21940.08203	43.40753 43.36806 43.42732 43.41845 43.38456	78.73323 78.74604 78.80419 78.72044 78.75752	34.11029 34.12795 34.09141 34.11989 34.13150	121.57004 121.52469 121.41938 121.50877 121.40886	103.27272 103.27886 103.29493 103.27350 103.27702	1.46422 1.46425 1.46409 1.46409 1.46419	
512 513 514 515 516 517 518	21740.08594 21780.08789 21820.08984 21860.08008 21900.08203 21940.08203	43.40753 43.36806 43.42732 43.41845 43.38456 43.38456 43.40072	78.73323 78.74604 78.80419 78.72044 78.75752 78.68810	34.11029 34.12795 34.09141 34.11989 34.13150 34.12950	121.57004 121.52469 121.41938 121.50877 121.40886 121.44134	103.27272 103.27886 103.29493 103.27350 103.27702 103.27173	1.46422 1.46425 1.46409 1.46423 1.46419 1.46432	
512 513 514 515 516 517 518 519 (21740.08594 21780.08789 21820.08984 21860.08008 21900.08203 21940.08203	43.40753 43.36806 43.42732 43.41845 43.38456 43.38456 43.40072	78.73323 78.74604 78.80419 78.72044 78.75752 78.68810	34.11029 34.12795 34.09141 34.11989 34.13150 34.12950	121.57004 121.52469 121.41938 121.50877 121.40886 121.44134 121.47815	103.27272 103.27886 103.29493 103.27350 103.27702 103.27173	1.46422 1.46425 1.46409 1.46423 1.46419 1.46432	

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.

Trom / Club. Terre control data	New data	
Special values: so: 37554etus 275 phis60054etus 800 k Oproeni: Cardy selected	250 200 150 50 1000 2000 3000 40000	Kane Gatamaré (921:378) Custanaré (50,1%,178) Custanaré (50,1%,178) Custanaré (50,1%,178) Custanaré (50,1%,18(0))
	Time (a)	(2) show used any

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.

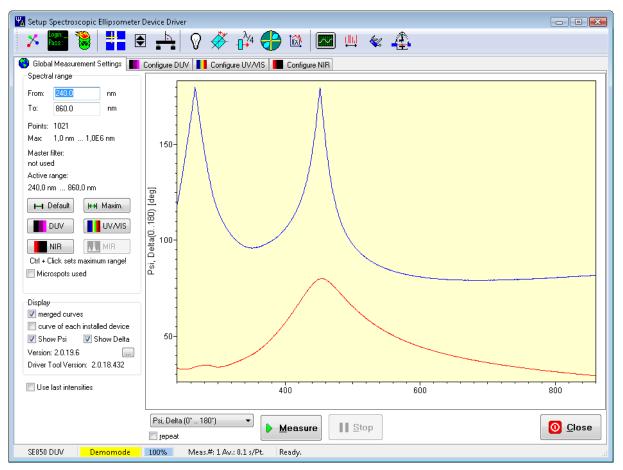


Fig. 7-1 The main window of the device driver

7.1.1 Toolbar

The toolbar gives fast access by instructive icons to the most often used functions of the device driver.



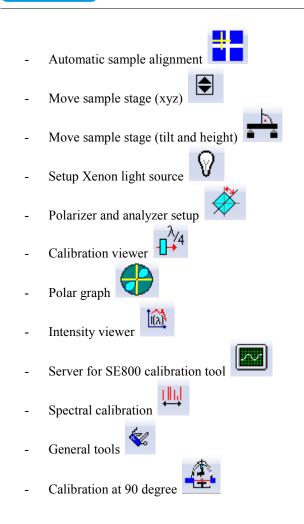
Fig. 7-2 The toolbar of the device driver window

The toolbar consists of 15 icons:

- Installed equipment
- Controller access
- Initialize the hardware again (reset all components)







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

Installed Equipment		3
🔲 General 🚺 UVVIS 📕 N	VIR 🖸 Demo mode 🗹 Behaviour 🛄, Spectrometers 🛏 Band filters	
Basic device type		
Select ellipsometer type:	SER 850 -	
General and/or optional hardwar DUV/UVVIS switch NIR/VIS switch Microspots	DUV ULVVIS VIR MIR Spectral range Enable master wavelength filter Master Maximum Default From: 240.0 nm 190.0 nm 320.0 nm	
	Tα: 930.0 nm 2500.0 nm 850.0 nm	

Fig. 7-3 Installed Equipment - General

Here you can choose the installed measurement device.

<u>S</u> elect ellipsometer type:	SER 85	i0		•
	<u>D</u> UV	<u>√</u> Uvvis	<u>√</u> <u>N</u> IR	MIR

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.

🔲 Enable master wavelength filter (nm):	190.0]	2500.0]
Enable master wavelength filter [nm]:	190.0		2500.0	

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.

General and/or optional hardware components
denotal anal of optional haranalo componente
DUV/UVVIS switch
NIR/VIS switch
INTERVED SWILCT
Microspots
- morospots





7.1.1.1.2 DUV

Installed Equipment							X
🔲 General 📕 DUV 🚺 UVVIS	📕 NIR 🚺 Demo mod	le 🔽 Behaviou	r 📙 Spectro	ometers H	Band filters		
DUV-Source switchable	-9	Spectrometer selec Spec	ction trometer Jeti		•		
DUV-retarder DUV	second retarder		Default nm 190.0 nm 450.0	with reta nm 190.0 nm 450.0	rder nm	Stray light correction enabled Type: Left based	•
		10. 1040.0	430.0	40.0			
	O <u>C</u> lose	•					

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.

	Spectra	l range	
	From:	190.0	nm
📝 DUV-retarder	To:	400.0	nm

Also you have to choose one of the installed spectrometers.

Spectrometer selection		
Spectrometer	Jeti	•

SpectraRay/4

7.1.1.1.3 UV/VIS

SENTECH

											X
uwis 📕 Nir 🔲 D	ema mode	7 Behavio	ur	III Spec	romet	ets H	Band filters	_			_
	Spect			1	i.		*				
🛄 has 3 gray filters											
	Spect	ral range						Stray light	correction		
VIS second relarder	1.0	Maximum		Default		with reta	rder	📝 enable	ed		
	From	360.0	nm	360.0	nm	360.0	nm	Type:	Left based		*
	To	1040.0	nm	1040.0	nm	1040.0	nm	Picht cho	nnals isnorad	4	1039.9 nr
										1	1039.9 nr
										30	183.0 nm
								Left chan	nels ignored:	20	169.8 nm
LOA											
	1										
	Close										
	has 3 gray filters VIS second retarder SA device I dis. new calc 435.0 nm 297 nm	has 3 gray filters Spect VIS second relarder From SA device dis. new calc To: 435.0 mm 297 mm	has 3 gray filters VIS second relarder Attion Adevice I dis. new calc Attion To: 1040.0 To: 104	Spectrometer selection Spectrometer selection Spect	 □ has 3 gray filters ○ VIS second relarder SA device dis, new calc 297 mn ○ main and the second relarder 	Spectrometer selection Spectrometer selectio	has 3 gray filters has 3 gray filters VIS second relater Xis second relate	Spectrameter Jetr has 3 gray filters VIS second relarder SA device @ dia. new calc 435.0 mm 237 mm	Spectrometer selection Spectrometer selection Spectrometer Jeti has 3 gray filters VIS second relarder SA device I dis, new calc 435.0 mm 237 mm IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	A device dis. new calc To: 1040.0 nm 1040.0 nm To: 1040.0 nm 1040.0 nm Right channels ignored. Left channels ignored.	Spectrometer selection Maximum Default with retarder Firm: 360.0 nm To 1040.0 To 1040.0 To 1040.0 To 1040.0 Spectrometer selection 1 Left channels used: 1 Left channels ignored: 20

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.

🚺 has	3 gray filters
VIS	second retarder
SA devic	e 🕡 dis. new calc
435.0	nm
297	nm
LOA	
	UIS SA device 435.0 297



7.1.1.1.4 NIR

Installed Equipme	ent										X
General 📕	DUV 📕 UVVIS	📕 NIR 🚺 De	mo mode	Behaviou	ur <mark>∣[],</mark> Spe	stromet	ers H	Band filters			
			Spectr	ometer sele Spec	ction strometer IF	_ABB		•			
			Spectr	al range							
🔽 NIR retarder	NIB :	second retarder		Maximum	Defaul		with reta	rder			
			From:	900.0	nm 900.0	nm	900.0	nm			
PSCA device	PCSA device		To:	2500.0	nm 2500.0	nm	2500.0	nm			
		0	<u>C</u> lose								

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

Installed Equipment				
General 📕 DUV 🚺 UV/VIS 📕 NIR	Demo mode	🔽 Behaviou	ur 🛄, Spectrometers	🛏 Band filters
Use demo mode Ellipsometer controller is used in demo mode set demo mode on initialization failure	Demo data simulati Model: SiO2 on S Thickness: Thickness noise: Psi noise: Delta noise: Fourier noise:		nm nm deg deg	
	Demo data storage Intensities data file			

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.

🔽 Use demo m<u>o</u>de

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).

Ellipsometer controller is used in demo mode

In demo mode the software generates simulated data based on the settings in this tab when you want to measure.

-Demo data simulatio	on (UVVIS)	
Model: SiO2 on S	i v]
Thickness:	392.00	nm
Thickness noise:	0.20	nm
Psi noise:	0.0300	deg
Delta noise:	0.0500	deg
Fourier noise:	0.001000	

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).

Demo data storage	
Intensities data file	

7.1.1.1.6 Behavior

Installed Equipment					×
🔳 General 📕 DUV	📕 UVVIS 📕 NIR 🚺	Demo mode 🗹 Behav	iour Hill, Spectrometers	 Band filters 	
	Iways (override the current rec ment laser off before measurin asure to Custom		 Use wavelengt Use wavenumb 		
Auto align system avail Alignment system type:		m available	Ÿ]	
Stage:	Automatic mapping xy-stage	(200 mm Travel, 200 mm (diameter samples) 🔹 🔻		
	motorized height mot	orized tilt 📃 Sensor for H	Height and tilt		
Goniometer:	Automatic goniometer (40°	. 90*)	•]	
	Additional offset).00	🔲 Offsets visible		
	Additional microspot offset).00			
	0	<u>C</u> lose			

Fig. 7-8 Installed Equipment - Behavior

In this tab you can set the behavior of some hardware components.

🔲 use polarizer tracking always (override the current recipe setting for this purpose)

If this option is checked the polarizer tracking will be activated, also the option is not set in the recipe.

always switch the alignment laser off before measuring (S1, S2, Psi, Delta, ...)

If this option is checked the alignment laser (if available) is always switched off before a measurement.

set light path after measure to none

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.

• 0



Here you

	Unit options © Use wavelength © Use wavenumber
can choose the unit for the wavelength	
Alignment system type: Video based	d height system 👻

These settings display the installed alignment system.

Stage:	Fixed sample stage (150 mm diameter samples)	
	Fixed sample stage (150 mm diameter samples) Automatic mapping xy-stage (50 mm Travel, 150 mm diameter samples) Automatic mapping xy-stage (150 mm Travel, 150 mm diameter samples) Automatic mapping xy-stage (200 mm Travel, 200 mm diameter samples) Automatic mapping xy-stage (300 mm Travel, 300 mm diameter samples)	
] motorized height 📃 motorized tilt 📃 Sensor for Height and tilt	
Goniometer:	Manual goniometer (40° 90° in 5° steps)	-
	Fixed angle of incidence Manual goniometer (40° 90° in 5° steps) Automatic goniometer (40° 90°)	

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.

Additional offset	0.00	🔲 Offsets visible
Additional microspot offset	0.00	

7.1.1.1.7 Spectrometers

Installed Equipment					×
General DUV	Demo mo	ide 🔽 Behaviou	III, Spectrometers	H Band filters	
Spectrometer definition				· · · · · · · · · · · · · · · · · · ·	
Spectrometers (ID)					
Add 0	Name	DUWis			
Remove 2	Туре	Tec5	•		
Configure					
<u>р</u>	_				
	0 <u>C</u> lose	•			

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:

Туре	Tec5 🔹
	Controller
	Tec5
	Varian Scimitar/Excalibur
	Avantes_USB1
	Avantes_USB2
	External server
	Hamamatsu NIR
	OceanOptics_USB



7.1.1.1.8 Band Filters

Installed Equipm	ient								X
General 📕	DUV 📕	UV/VIS	NIR 🚺 Demo ma	de 🔽 Beh	aviour 🛄, Spe	ctrometers	н	Band filters	
Filter definition									
	Filter (ID)								
Add	0		Name	Lamp					
Remove			From:	653.0	nm				
			To:	659.0	nm				
				General		•			
						•			
				Filter activ	e				
	O Close								

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.

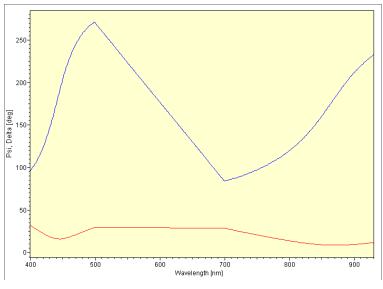


Fig. 7-11 Example for activated filter (500nm-700nm)

7.1.1.2 Controller access

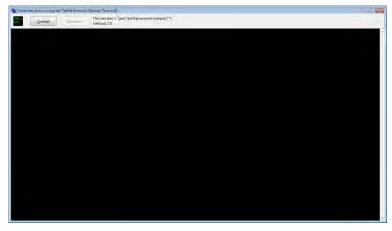


Fig. 7-12 The controller access window

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



SpectraRay/4

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

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Setup Xenon Light Source	
O Life time:	134 hours of 1000 hours in use (13.38 %) 🚥
V Intensity:	no intensity sensor available 🚥
Power On Settings	
Minimum required intensity [%] :	0.0
Maximum allowed noise [%]:	100.00
Maximum wait time for OK [sec]:	10
Switch ON !	Switch OEF !

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 "Life-Time.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.



Polarizer
Measurement Position [deg]: 45.00 Offset [deg]: 0.24
Additional align offset [deg]: 0.00
Goto reference Goto (p) Goto (s) Goto (M)
Analyzer
Use angle of incidence dependent offsets
Offset [deg]: -0.25
Additional align offset [deg]: 0.00
Use velocity dependent additional offsets
Fast mode addtional offset: -0.25
Goto reference Goto (p) Goto (s)
Load offsets from SpectraRay settings
O <u>C</u> lose

Fig. 7-14 Polarizer and analyzer setup

The position of the analyzer for measurements is set in the field

ol	lar	ize	er		

Measurement Position [deg]: 45.00

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

Goto reference	Goto (p)	Goto (s)	Goto (M)

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

Goto reference	Goto (p)	Goto (s)
----------------	----------	----------

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.

Delecters

The offsets for the analyzer and polarizer are given in the fields

	Offset [deg]:	0.24
and		
Analyzer Image: Constraint of the second s	sets	
	Offset [deg]:	-0.25

These entries are used to define the offset between the mechanical reference and the optical coordinate system.

In certain cases calibration values for 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.

Analyzer							
Use angle of incidence dependent offsets							
Angle of incidence	Offset						
Angle of incluence	Oliset						
20	-0.2000						
45	-0.2500		Add				
70	-0.3000		Remove				

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.

Use velocity dependent additional offsets

Velocity [ms/round]	Offset		
195	-0.3500		
208	-0.2500		Add
250	-0.3000	-	Remove
200	0.0000	*	

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 Load offsets from SpectraRay settings and selecting the correct file 'spelli.ini' in a file selection box. SENTECH SpectraRay/4

7.1.1.9 Calibration viewer

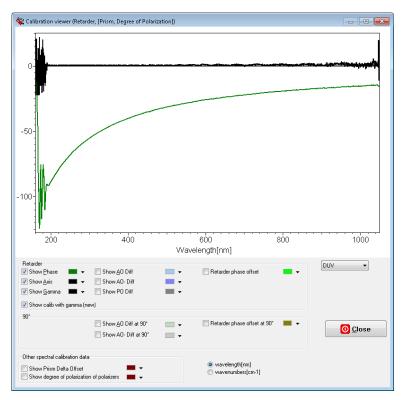
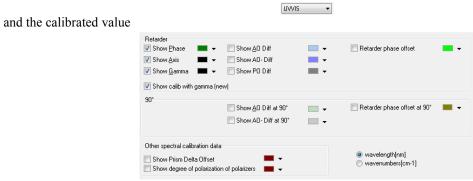


Fig. 7-15 Calibration viewer window

In the calibration viewer window all calibrated values (like retarder phase and axis,...) are displayed. You can choose the spectral range



which should be displayed in the graph. You cannot change the calibration in this dialog.



7.1.1.10 Polar graph

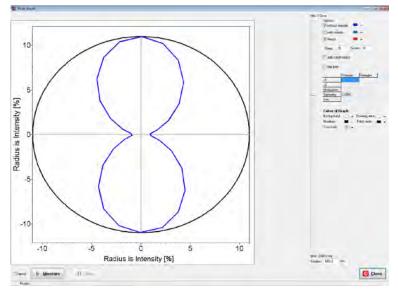


Fig. 7-16 Polar graph window

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.



The slider on the right side allows setting the wavelength for which the polar diagram should be displayed.

Position: 655.0 nm

7.1.1.11 Intensity viewer

Intensity Viewer		
- 19		UVMS •
		Hidonsky Sedings Overtax: 30 % Terget: 70 % Underhow: 50 % Int. Time(m): 100 Scens: 1 Analyzer last mode Ø Seg-Scens: intensities Privilegrabon time Orak constrainties Frivilegrabon time Orak constrainties Frivilegrabon time Orak constrainties Orak constrainti
	Wavelength[nm]	

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).

Speichern unter	uter 🕨 141si0508 (C:) 🕨	temp 🔹 🆅 Suchen	کی م
🋂 Organisieren 👻 🏢	Ansichten 👻 📑 Nei	uer Ordner	0
Linkfavoriten Dokumente Weitere » Ordner	Name	Änderungsdatum Typ Dieser Ordner ist leer.	Größ
	ensity files (*.intensity.xn		•
Ordner ausblende.	ensity files (*.intensity.xm 211 files (*.dat;*.txt)	Sherment 1)	Annieculeu

Fig. 7-18 "Save"-dialog

Just above the spectrum the maximum and average intensity in percent as well as "underflow" (or "overflow") is displayed.

Maximum: 17.00 % Average: 8.75 UNDERFLOW



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.

Overflow:	49	%	
Target:	46	%	
Underflow:	31	%	
		. 4	

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.

📃 StepScan intensities
Fix integration time
📃 Use last intensities
Dark correction

It also possible to switch between wavelength and wavenumbers.

wavelength[nm]
 wavenumbers[cm-1]

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.

🔲 No light path activation

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.

Gray Filter:	0.50000	

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.

Cycle [ms]:	500 🗸	

Clicking on will start a single measurement or if repeat is checked will measure the whole time until "repeat" is unchecked again.

7.1.1.12 Server for SE800 calibration tool

SENTECH

<u>S</u> tart	Stop 8093	
Time	Info	
	Server started.	

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

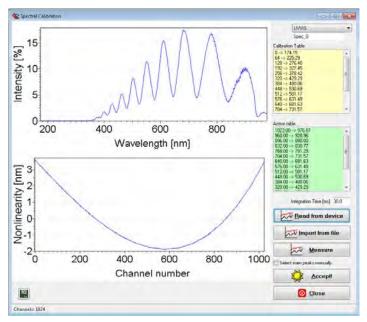


Fig. 7-20 Spectral calibration window

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".

SENTECH SpectraRay/4

7.1.1.14 General tools

General Tool	s	X
-Controller Ac	Cess	
	r can be directly operated via the TelNet comman nected. By means of the FTP connection it is ansfer files.	nd
IP address :	192.168.90.246 Pinged successfully.	
Port:	12349	
Login:_ Pass: ⊥∈	elnet	
	Comm	
Automatic go	niometer goniometer	
	O Close	

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

SENTECH

ctral range Current range: 790.0 2500.0	nm	UVVIS
eral Analyzer Detector correction Retarder / Degr	ee of Polarization	
(1) Analyzer Analyzer offset [']: Calibrate with prism	0.750000	Accept AD
(2) Polarizer Polarizer type:		A
Mot. polarizer offset (at reference) (*):	-4.480000	Measure PO at ref.
Mot. polarizer angle used at ref. (incl. cal. tab.) (*): Mot. polarizer angle destination (usually 45*) (*):	45.00	Coto polarizer meas pos.
Mot. polarizer angle used at dest. (incl. cal. tab.) [*]:		C Measure PO at meas pos.
		Accept P0
Retarder		
Retarder available + enabled: Calibrate retarder	yes	Accept retarder axis + phase

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

	Spectral range	400.0	700.0	nm		UVVIS	•
and click on	Calibr	ate with prism	The Analyz	er-tab will be	opened.		



Spectral range Current range 790.0 nm Seneral Analyzer Detector correction Retarder / Degree of Polarization Calibrate analyzer offset with prism Measure the current polarization asis at 30° angle of incidence with an additional polarizer that is set in two directions as shown: Left axis ['] Flight axis ['] Left axis ['] Flight axis ['] Keasure difference ['] 0.750000 Measure difference ['] New analyzer offset would be [']	UWI5 -
Analyzer Detector correction Retarder / Degree of Polarization Calibrate analyzer offset with prism Measure the current polarization axis at 90° angle of incidence with an additional polarizer that is set in two directions as shown: Image: Constraint of the current polarization Image: Constraint of the current polarization axis at 90° angle of incidence with an additional polarizer that is set in two directions as shown: Image: Constraint of the current polarization Image: Constraint of the current polarization Image: Constraint of the current polarization Image: Constraint of the current polarization Current analyzer offset would be [1] Image: Constraint of the current polarization New analyzer offset would be [1] Image: Constraint of the current polarization	UWIS
Calibrate analyzer offset with prism Measure the current polarization axis at 30° angle of incidence with an additional polarizer that is set in two directions as shown: Image: Comparison of the compar	
Measure the current polarization axis at 90° angle of incidence with an additional polarizer that is set in two directions as shown: Image: Comparison of the compa	
with an additional polarizer that is set in two directions as shown: Image: Constraint of the state of the st	
Left axis ['] Current analyzer offset ['] 0.750000 Measured difference ['] New analyzer offset would be [']	
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Left axis [']: ··· Flight axis [']: ··· Current analyzer offset [']: 0.750000 Measured difference [']: ··· New analyzer offset would be [']: ···	
Left axis [']: ··· Flight axis [']: ··· Current analyzer offset [']: 0.750000 Measured difference [']: ··· New analyzer offset would be [']: ···	
Left axis [']: ··· Flight axis [']: ··· Current analyzer offset [']: 0.750000 Measured difference [']: ··· New analyzer offset would be [']: ···	
Left axis [']: ··· Flight axis [']: ··· Current analyzer offset [']: 0.750000 Measured difference [']: ··· New analyzer offset would be [']: ···	
Left axis [']: ··· Flight axis [']: ··· Current analyzer offset [']: 0.750000 Measured difference [']: ··· New analyzer offset would be [']: ···	
Current analyzer offset ['}: 0.750000 Measured difference ['}: New analyzer offset would be [']:	
Measured difference [']: ···· New analyzer offset would be [']: ····	
Measured difference ["]: New analyzer offset would be ["]:	
New analyzer offset would be [*]:	
Accept the new analyzer offset and set to config	
	(market)
Alignment Alignment	
nmand ready. OK	0 <u>C</u> lose

Fig. 7-23 Calibration at 90 degree - Analyzer

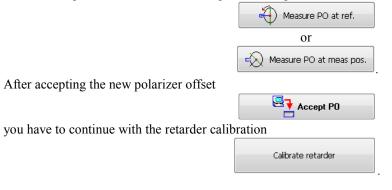
For the analyzer calibration you need a special prism, which has to be aligned on the sample stage in two positions as can be seen on the buttons.



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

Accept the new analyzer offset and set to config	

In second step return to the first tab and perform the polarizer calibration (without additional prism) by clicking





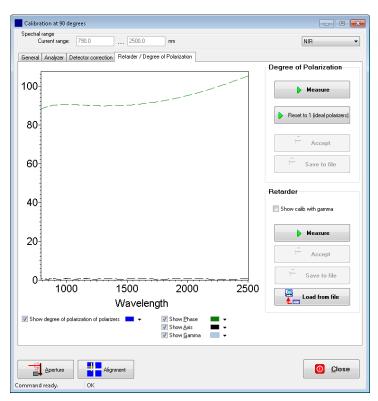


Fig. 7-24 Calibration at 90 degree - Retarder/Degree of Polarization

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

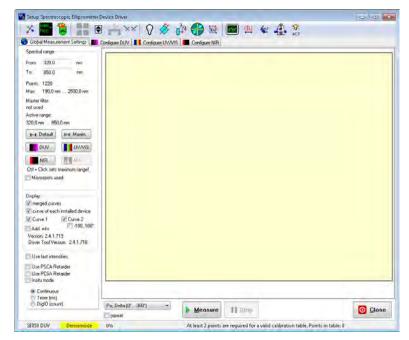


Fig. 7-25 Global measurement settings



The "Global measurement settings"-tab allows performing ellipsometry measurements by clicking on



Similar to the intensity viewer (see sec. 0) I repeat allows repeated measurements until unchecked. You can select different measurement tasks:



If $\square Use last intensities$ is checked the last measured spectra will be used to perform the actual measurement task without measuring new spectra.

In the "Spectral range"-frame

Constant					
Spectral	range				
From:	400.0		nm		
To:	930.0		nm		
Points:	531				
Max	190,0 nn	n 25	00,0 nm		
Master filter: not used Active range:					
400,0 nm 930,0 nm					
H Default H→ Maxim.					
	VUV		UV/VIS		
NIR MIR					
Ctrl + Click sets maximum range!					
Micro	ospots use	ed			

The spectral range for the measurement can be set. Clicking UP Detault will set a default spectral range, clicki	ng
WH Maxim. will set the maximum spectral range. Clicking UV, or WIR will set the co	r-
responding 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!**

Microspots used

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).

Uisplay
Dispidy
🔽 merged curves
👿 curve of each installed device
🗹 Curve 1 🛛 📝 Curve 2
🔲 Add. info 👘 -180180°
Version: 2.4.1.719
Driver Tool Version: 2.4.1.718

7.1.3 Configure DUV

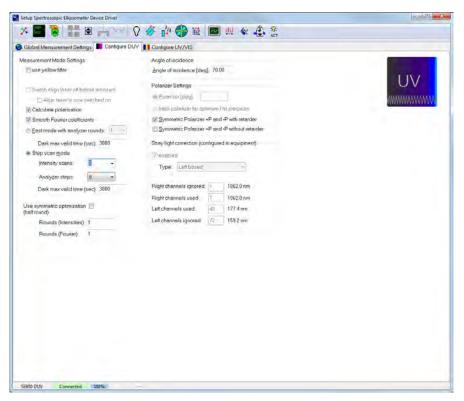


Fig. 7-26 Configure DUV settings

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.	Explanation
Setting	settings	Explanation
Use yellow filter	Off	The optional yellow filter may be switched in to protect certain sam- ples from short wavelength radition.
Calculate Polarization	On	Depolarization effects due to non-idealities of the sample (e.g. inho- mogeneities, backside reflections or nano particles) will falsify the (Ψ , Δ) spectra. In combination with the compensator/retarder measure- ment 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 con- tinuously. 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 Step scan dark valid time (sec)	8-16 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 optimi- zation	Off	It should be switched on only when a high measurement speed is nec- essary (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 $P \neq 45$ 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 re- tarder	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

	•
2	975.3 nm
6	971.5 nm
6	179.7 nm
2	175 7 nm
	6

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

tessurement Mode Settings Angle of incidence Lue pollow filter Angle of incidence Lue pollow filter Angle of incidence Lue pollow filter Angle of incidence Switch align laser in now switched on Polanzer Settings Angle rounds: Polanzer (deg) Simooth Fourier coefficients Polanzer i for optimum Par precision Dark max valid time (sec) 3000 Stray light correction (configured in aquipment) Site scan gode Internet valid time (sec) 3000 Dark max valid time (sec) 3000 Right channels ignored Dark max valid time (sec) 3000 Right channels ignored Dark max valid time (sec) 3000 Right channels ignored User symmetric optimization Left channels ignored Rounds (Fourier) T Polanzer before measure 10620 nm Dark max valid time (sec) 3000 Right channels ignored Polands (fremalies) 1 Left channels ignored Rounds (Fourier) T	Use yellow filter Angle of incodence (deg) Use yellow filter Folanzer Settings Data in lower of before measure # Dolanzer Settings Colculate polersation # botak dona er for opfinum Pis precision Z Colculate polersation # botak dona er for opfinum Pis precision Z Smooth Fourier coefficients # Symmetric Polanzer +P and +P without retarder Dark max valid time (sec): 3000 Stray light correction (configured in equipment) # Step scan gode Immetrial Internsity scans Imperative Dark max valid time (sec): 3000 Flight channels ignored Dark max valid time (sec): 3000 Flight channels ignored Use symmetric optimization Left channels used Rounds (internation) Left channels ignored Polanzer Start Step zerometric start	Global Measurement Settings 📘 Configure DU	V Configure UV/VIS	
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Switch align laser of before measure Polarizer Settings Align laser is now switched on Explorizer (deg) Calculate polarizer sounds Explorizer (deg) Smooth Fourier coefficients Symmetric Polarizer +P and -P with raterider Eastmode with analyzer rounds: 1 Dak max valid time (sec): Stay light correction (configured in equipment) Step scan mode Expendence Dak max valid time (sec): 3000 Mannalyzer roles: Image: Last based Dak max valid time (sec): 3000 Pight channels ignored 1 Dak max valid time (sec): 3000 Pight channels used 1 Dak max valid time (sec): 3000 Pight channels used 1 Dak max valid time (sec): 3000 Pight channels used 1 Dak max valid time (sec): 3000 Pight channels used 1 Dak max valid time (sec): 1 Last channels used 1 Pight channels used 1 Pight channels used 1 Pight channels used 1 Pight channels used	Switch align laser of before measure Polarizer (deg) 45.00 Align laser is now switched on In tock polarizer for optimum Pair precision Image laser is now switched on		Angle of incidence [deg]:	1 100
Adam tesen is now switched on Polanzer (deg) 45 00 Polanzer (deg) 40 - Polanzer (deg) Polanzer (deg) 40 - Polanzer (deg) Polanzer (deg) 40 - Polanzer (deg) 40 - Polanzer (deg) 40 Polanzer (deg) 40 - Polanzer (deg) 40 - Polanzer (deg) 40 Polanzer (deg) 40 -	Alagn Testamis now switched on Polonzer (deg) 45 00 Polonzer (deg) 40 - Polonzer (deg) Polonzer (deg) 40 - Polonzer (deg) Polonzer (deg) Polonzer (deg) 40 - Polonzer (deg) 40 - Polonzer (deg) Polonzer (deg) 40 - Polonzer (deg) 40 - Polonzer (deg) Polonzer (deg) 40 - Polonzer (deg) 40 - Polonzer (deg) Polonzer (deg) 40 -		Polarizer Settings	
Calculate polensehon Calculate polensehon Calculate polensehon Cancel Part of polenser for optimum Pis precision Cancel Part of Part Part Pend P with rotarder Cast max valid inter (sec) 3000 Stray light correction (configured in equipment) Step scen gode Interview			e Epilanzer [deg] 45.00	http://www.com
Image: Smooth Fourier coefficients Image: Symmetric Polarizer +P and -P with rotarder Image: Smooth Fourier coefficients Image: Symmetric Polarizer +P and -P with rotarder Image: Smooth Fourier coefficients Image: Symmetric Polarizer +P and -P with rotarder Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equipment) Image: Stray Sight correction (configured in equi	Smooth Fourier coefficients If Symmetric Polarizer +P and -P with ratarder East mode with analyzer rounds: 1 Dark max valid time (Lec): 3000 Stray light correction (configured in equipment) Internsity scene: 1 Internsity scene: 1 Dark max valid time (Lec): 3000 Bitay light correction (configured in equipment) Internsity scene: 1 Dark max valid time (Lec): 3000 Dark max valid time (Lec): 3000 Pilph Channels (gnored) 1 Dark max valid time (Lec): 3000 Pilph Channels (gnored) 1 Dark max valid time (Lec): 3000 Pilph Channels used 1 1 1062.0 nm Use symmetric optimization Left channels used 1 Rounds (Internation) Left channels used 1 Rounds (Fourier) T Left channels used 1 Rounds (Fourier) T 1 1		Track polarizer for optimum Psi precision	000000
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Use symmetric optimization Pight chennels used 1 1062 0 nm Use symmetric optimization Left chennels used 40 1727 4 nm Rounds (Intensities): 1 Left chennels ignored. 72 159.2 nm	Dark max valid time (sec): 3000 Plight chemiels used: 1 1062.0 nm Use symmetric optimization Left chemiels used: 40 172.4 nm Rounds (Intensities): 1 Left chemiels ignored: 72 Rounds (Fourier): T 1 159.2 nm	Analyzer steps. 8 +	All Transferrer	
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(hell round) Leff chemiele ignored. 20 177 mm Rounds (Intensities) 1 Leff chemiele ignored. 72 159.2 mm Rounds (Fourier): T T 1<	(half round) Child calaminis using Column Calaminis using Column Calaminis using Column Calaminis Colu		Right chennels used 1 1062.0 nm	
Rounds (Intensities): 1 Left chemiels ignored. 72 159.2 mm Rounds (Fourier): 1	Rounds (Internations) 1 Left channels ignored. 72 159.2 mm Rounds (Fourier): 1		Left channels used. 40 177 4 nm	
			Left channels ignored. 72 159.2 nm	
Check lamp befole measure	Check lamp before measure	Rounds (Fourier) 1		
The provide and the provide and the provided and the prov	The second manufactory of the second s	Check lamp bolous strugging		
		Check lamp before interesue		

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 $(1-32 \text{ cm}^{-1})$ and the sensitivity (1-16).

Resolution [cm-1]: 16.00 -Sensitivity: 1.00 -

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

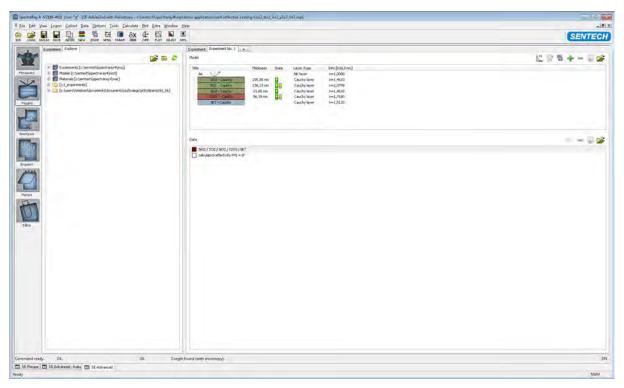


Fig. 8-1 SE-Advanced client

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.

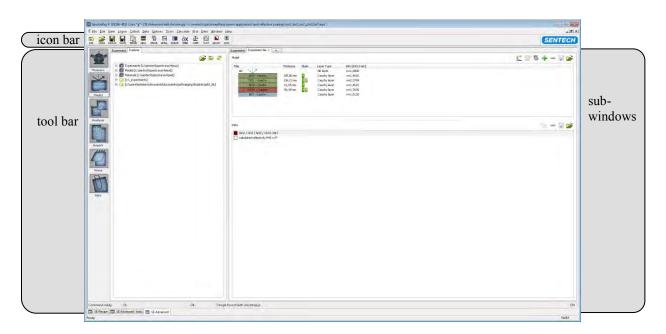


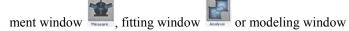
Fig. 8-2 Main window

Icon bar:

The icon bar contains buttons for loading, saving and windows for important settings like the environmental parameters and fitting parameters and fitting parameters.

Tool bar:

The most important functions of SE-Advanced are represented in the icon bar for fast access like the measure-



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.

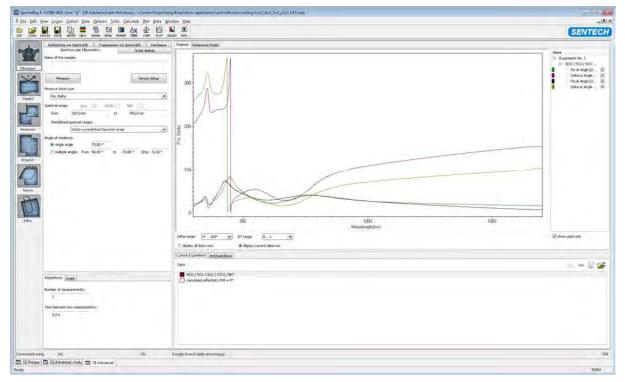


Fig. 8-3 Measurement window

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.

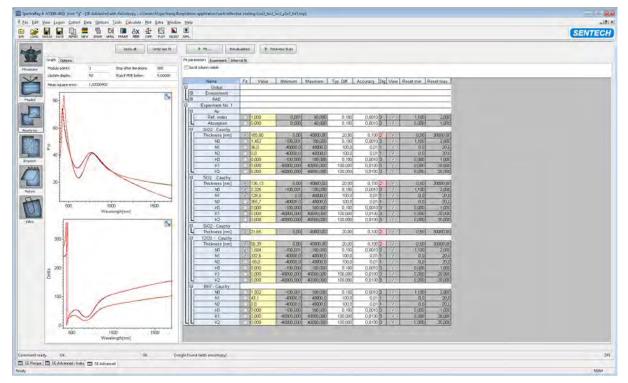


Fig. 8-4 Analysis window



Report:

Here you can report your results and export them into a WORDTM-file.

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					<u>الا الا ا</u>
P PLOT VALACE APP					SENTECH
Aktuelles Experim c:sentechispedra	erfolg durch Leistr	Applications\anti			Img Stay Img I
Number 0 1 2 3 4	Layer Name Air SiO2 - Cauchy TiO2 - Cauchy SiO2 - Cauchy Y2O3 - Cauchy	105.80 136.13 21.65 56.39	Refr. Index [632.8 nm] 1.000 1.461 2.380 1.461 1.763 1.513	Fitted no yes yes yes no	
[1,2] TIO2 - Cauc	hy: Thickness [ni	m) 105,80			
	Aktuelles Experim C'SENTEC SENTEC Aktuelles Experim c'sentechlapectric coatings/sio2_tio/ Modelbeschreibu Number 0 1 2 3 4 5 Fit parameter [1,1] SiO2 - Cauc [1,2] TiO2 - Cauc	Aktuelles Experiment c.'seritechispectraray4\exp\Demo coatings\sio2_tio2_sio2_y2o3_bk7 Modelbeschreibung Number Layer Name 0 Air 1 SiO2 - Cauchy 3 SiO2 - Cauchy 4 Y2O3 - Cauchy 5 BK7 - Cauchy Fit parameter Fit parameter [1,1]SiO2 - Cauchy: Thickness [n	Aktuelles Experiment. c:sentechispectraray4kexplDemo Applicationstanti coatingstsio2_tio2_sio2_y2o3_bk7.exp Modellbeschreibung Number Layer Name 1 SiO2 - Cauchy 2 TiO2 - Cauchy 1 SiO2 - Cauchy 2 TiO2 - Cauchy 3 SiO2 - Cauchy 5 BK7 - Cauchy 6 Fit parameter [1,1] SiO2 - Cauchy Thickness [nm] 105,80 105,80 2 TiO2 - Cauchy 5 BK7 - Cauchy 6 Sio2 - Cauchy 6 Sio2 - Cauchy 7 Sio3 - Sio3 7 BK7 - Cauchy	Attuelles Experiment C'sentechiepectraray4explDemo Applications\anti reflective coatings\sio2_tio2_sio2_y2o3_bk7.exp Modelbeschreibung Number Layer Name Thickness [nm] Refr. Index [632.8 nm] 0 Air 1022 - Cauchy 105.80 1.461 2 TiO2 - Cauchy 136.13 2.380 3 SiO2 - Cauchy 21.65 1.461 4 Y2O3 - Cauchy 56.39 1.763 5 BK7 - Cauchy 5.151 Fit parameter [1,1] SiO2 - Cauchy: Thickness [nm] 105,80 [1,2] TiO2 - Cauch	Aktuelles Experiment: c: Vertex big durch Leistung Berlin, 10.03.2016 Aktuelles Experiment: c: Vertex big durch Leistung Modellbeschreibung Number Layer Name Thickness [nm] Refr. Index Fitted 0 Air 1 SIO2 - Cauchy 105.80 1 SIO2 - Cauchy 105.80 3 SIO2 - Cauchy 105.80 3 SIO2 - Cauchy 56.39 5 BK7 - Cauchy 56.39 Fit parameter Fit result [1,1] SIO2 - Cauchy: Thickness [nm] 105.80 [1,1] SIO2 - Cauchy: Thickness [nm] 105.80 [1,2] IO2 - Cauchy: Thickness [nm] 105.13

Fig. 8-5 Reporting

Notes:

Here you can write down notes for the current experiment. These notes are saved within the experiment.

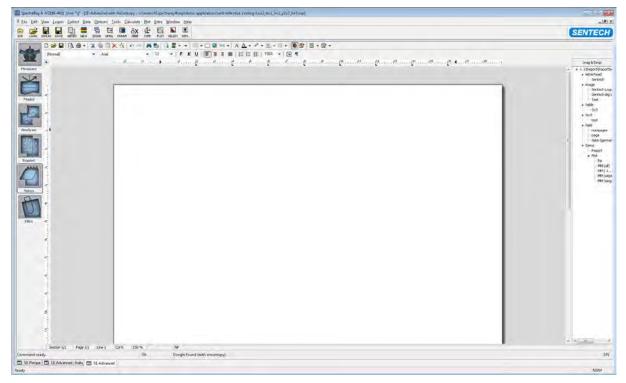


Fig. 8-6 Notes windows



Files:

It is also possible to save external files within your current experiment. You can ad files up to 260 MB.

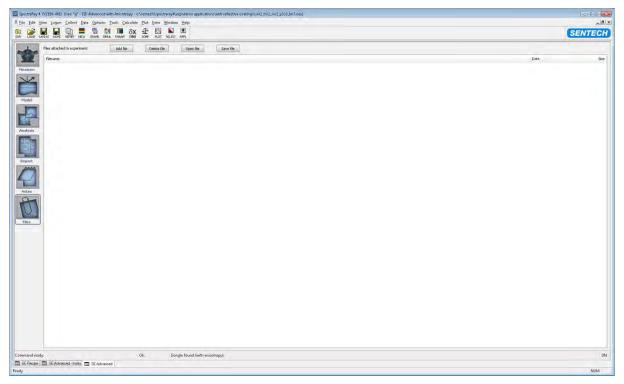


Fig. 8-7 Files window

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

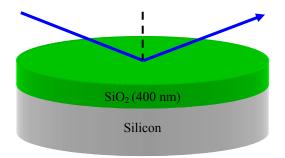
- 3.1. Creating a model
- 3.2. Selecting fit parameters
- 4. Fitting

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

SENTECH

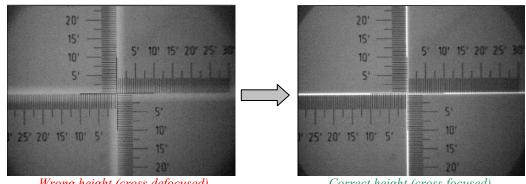
The Auto collimating telescope (ACT) in combination with the objective lens is used for the alignment.

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 _

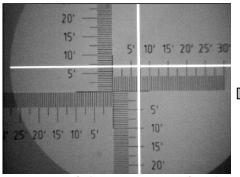


Wrong height (cross defocused)

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

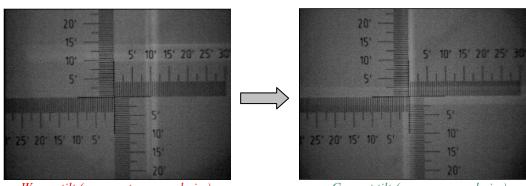
In case the sample is specular but not perfectly flat the cross in the tilt-mode is blurred. The "**dark-tilt**" position is recommended because it will show the sharper cross compared to the "**light tilt**" position.

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)



- Alignment of non-ideal samples, not specular

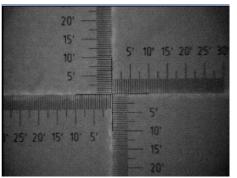
In case the sample is not-specular or very rough the tilt alignment can't be done, because the white cross isn't visible anymore. Then e.g. a specular Si wafer can be used first to align the tilt of the stage which won't be changed then anymore. Then the rough sample is placed on the stage and the height 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

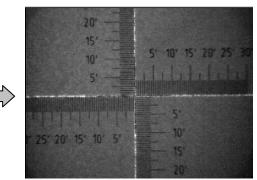
- Place a Si wafer on the stage. Move objective lens out to "light tilt" or "dark tilt" position
- Use the two tilt screws to align the tilt by aligning the white cross to the crosshairs

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 **Fine** 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

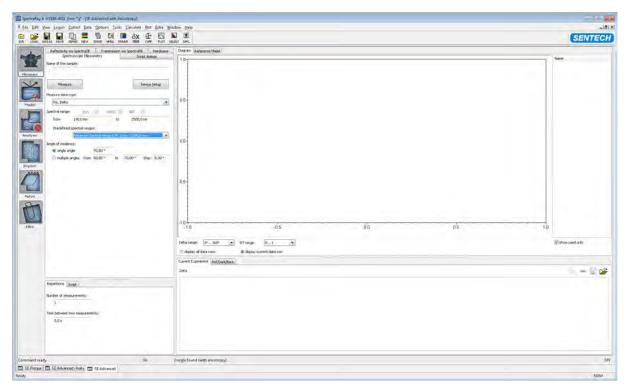


Fig. 8-8 Measurement settings

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.

SENTECH SpectraRay/4

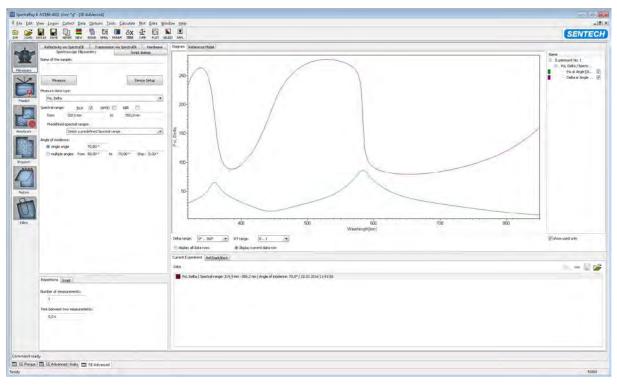


Fig. 8-9 Measurement results

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.

Name 400nm 2	SIO2 on Si/Por	, Delta / Speciral range: 408.0 to 85	0,0 nm/Angle of madeno	ar: 20.1	
User	_	Date: 08/03/2011	Time: 11 58.23		
Comment.				~	
				- X	
Measurement enviro	onment				
Wavelength:	632.8 nm	Process time:	0.0 s		
Angle of incidence:	70.00 '	Temperature:	23,5 10		
Polenzer position	45,000	Weight	1,0000		
		Sample rotation (theta)	0,000.*		
Change x axis					
No of points	451	Xeous by praints	Yos		
		Maku seens by points	Remove x-axis by	ahnoq	
New range of x-axis	400,000	850,000	Recalibrate x-a	ón -	
			Flip x-exis direct	ion	

Fig. 8-10 Data view "Title"-tab



New name:

Measurem	ent info			
Name:	400nm SiO2 / Si - SENTECH ret	erence sample		
User:	Date	We 10/30/2002	Time:	

Beneath the "Title" tab, there are other tabs. Important is the "**Graph**" tab. It shows the (Ψ, Δ) -spectra versus wavelength in nm.

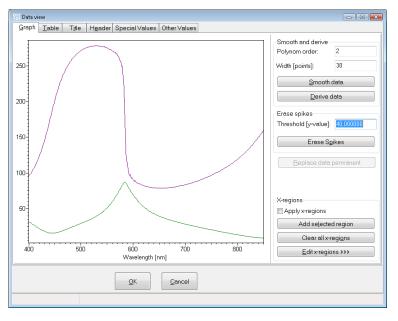


Fig. 8.-8-11 "Graph"-tab of data view

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.

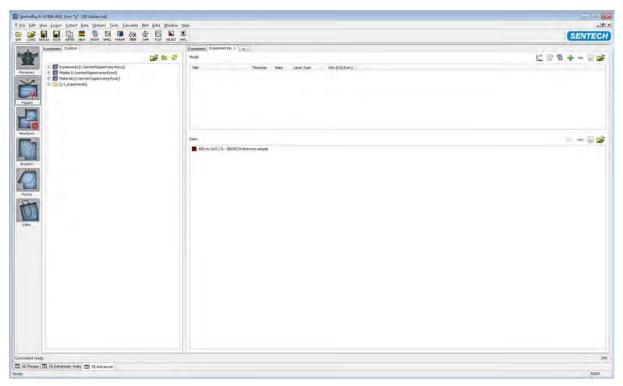


Fig. 8-12 Model window

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:

■ SpecinaRay & M7136-413 User "q" - [35: Addacted]		
A Die Lat View Logan Callest Data Ontoni Isali Lavades Bet Data Window Die Sei La Callest Data Callest Data Dieter Isali Sei Sei La Callest Data United A Die Lata Callest Callest Data Dieter New Dieter Hause Theor Theory Wildow		sentech
Piccaster Hosaite: Book (- Literatoliscotte et fac)	Hoad Hoad The Decrees Ske Lave Type Mo(202,0m) The Ske Type Mo(202,0m) The Ske Type Mo(202,0	년 양 정 수 - 달 64
Image: Solution of the soluti	Guin. I 493 ms 502 / 530400 Straformer sample	n - 9 a
Notes Solars		
Command ready.		DN .
E SE Respe SE Advanced Inata SE Advanced Residy		NUM

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".

^a Dispersion - Cauchy layer								00
avername: Cau-SiO2 (therm.)	Name	Fit	Value	Scroll vi	lue	Minimum	Maximum	
	Thickness [nm]			1		0,00		
1.49	ND		1,452	1		-100,001	100,000	
	N1	~	36,0	1		-40000,0	40000.0	
	N2		0,0	4		-40000,0 -100,000		
4	K0 K1	H	0,000	1	-	-40000,000		
1.48-	K2	H	0,000	4	-	-40000,000		
1.47 1.46 500 1000 1500 2000 2500 Wavelength[rm] show dispersion: Win K of Resolution: high •								
Comment								
Comment -	4				-mr			

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.

Model					<u>nk</u>	2	+	-	8
Title	Thickness	State	Layer Type	Info [632,8 nm]					
Air 📝			NK layer	n=1,0000					
Cau-SiO2 (therm.)	400,00 nm		Cauchy layer	n=1,4610					
Silicon VIS+NIR			File layer	n=3,8717 k=0,01576					

8.1.3.4 Fitting



The fitting window is opened by pressing the fitting button: Analysis . The "fitting" window is opened as you can see in Fig. 8-15.

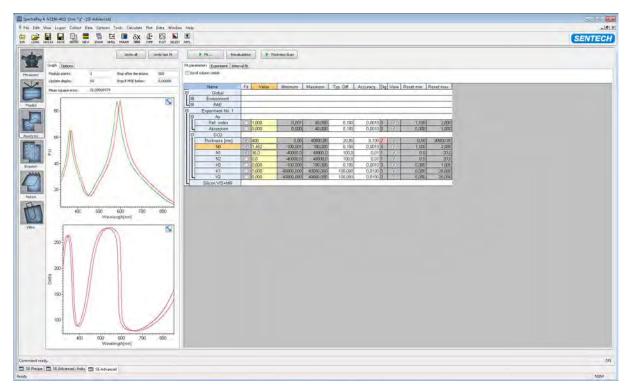


Fig. 8-15 Analysis-window

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.

		`
# 110: 36.546506717016 (31.0)	Thickness [nm]=684,42 N0=1,50	15 N1=-251,5

When the fitting procedure stops the results window is shown:



Fit Results						- • •
Name	Fit	Value	Minimum	Maximum	Typ. Diff.	Accuracy Dig Vi
[1,1] Cau-SiO2 (therm.): Thickness [nm]		391,86	0,00	40000,00	20,00	
Cau-SiO2 (therm.): ND		1,455	-100,001	100,000	0,100	
Cau-SiO2 (therm.): N1		35,3	-40000,0	40000,0	100,0	0,01 1 🛛 📕
•		n.				
•		11				•
Print table Fitparame	ters: H	lide >>			<u>C</u> ancel	<u>o</u> k

Fig. 8-16 Fit results

It can be closed with "OK" to return to the fitting screen.

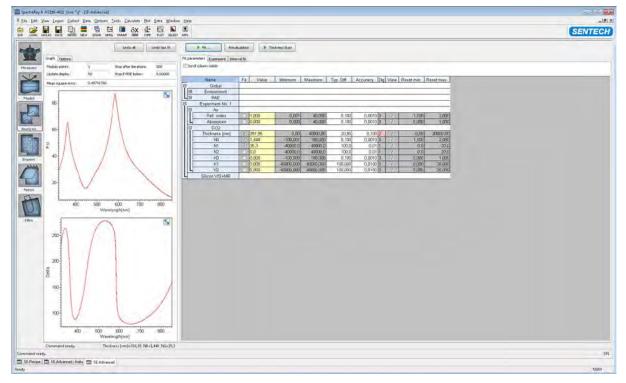


Fig. 8-17 Resulting fit parameters

Now a decision is necessary:

Fit quality is good	\rightarrow ready	\rightarrow	proceed with "Reporting"
Fit quality is below expectation	is \rightarrow not ready	\rightarrow	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.

Model				🗠 🔀
Title	Thickness	State	Layer Type	Info [633,0 nm]
Air 🖊			NK layer	n=1,0000
Cau-SiO2 (therm.)	391,86 nm		Cauchy layer	n=1,4638
Silicon VIS+NIR			File layer	n=3,8714 k=0,01577

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.

Environment parameters: Global En	vironment 🔤
<u>V</u> alues <u>R</u> anges <u>U</u> nits <u>S</u> u	bstrate Inhomogeneity Model Errors
Standard values (used if no c	ther values are present)
Wavelength:	632,8 nm
Angle of incidence:	70,00 *
Temperature:	23,5 °C
Process time:	0,0 s
Additional fit paramaters Display environment pa Display RAE paramete	rameters in list of fit paramaters 's in list of fit parameters
Data modulo Use data points modulo:	4
	٥K

Fig. 8-18 Environment parameters - Values

8.1.3.5.2 Measurement report

An automatic report can be created and displayed as WORDTM-document in the "Report"-window. After click-

ing on **u** in the tool bar the following window appears.

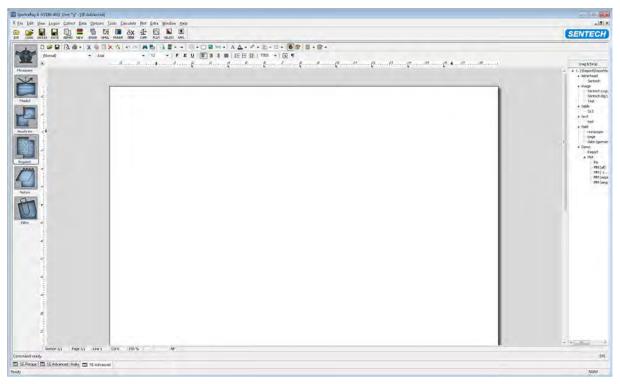


Fig. 8-19 Reporting window

Here you can create an automatic report and save it as WORDTM-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 WORDTM-document will create a standard report of your measured data. You can simply modify your report or built your report.

SpectroRay & N7256-#US User "g" - [SE-Addisoced]						- E ki
* tie Idt Yew Logan Callest Data Bottom Lach Calculate Ber-	Extra Window Male					_ (伊) ×1
	PLOT HELACT APPL					SENTECH
	6,138++ 0+1 10 + €×010 1 + €×010	ECH trialy durch Leist		la - 144 - la	Berlin, 10.03.2016	Service S
AUTO:	Number	Layer Name	Thickness [nm]		Fitted	
They are a second secon	0	Air		[632.8 nm] 1.000	no	
	1	SiO2	391.95	1.457	yes	
	2	Silicon VIS+NIR		3.872	no	
	Fit parameter	Gilcon Horivin		0.072		
	Fit parameter [1,1] SiO2: TH SiO2: N0 SiO2: N1		Fit resu 391,95 1,448 35,3			
Second () Page Sto Lane 2 Col 1 150 %	All parameter					- 14
SE Respect SE Advanced - Insta						Dav
Ready						PADM

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-SiO₂ (therm.)" layer versus wavelength will be calculated.

The "Simulation" is started by clicking on [nm]". Set the wavelength range from 300nm to 850nm (step: 1). The "Calc unit" is the y-axis \rightarrow Select "[0] wavelength range r". Select the "Layer": SiO2.

Press "Calc". The data is now calculated, displayed and saved into the "Data" window.

SR Simulation	1									
Wavelength	1:	632,8 nm		Temperature:		23,5 °C		Devicetyp	e: PSCA	•
Angle of Inc	idence:	70,00 *		Process time:		0,0 s		Rotationty	pe RAE	•
Angle of Ro	tation:	0,00 *		Enviro	nmer	nt Settings		P/A angle	45,00	•
Curve par	ameter	:								
[0] Wavele	ngth [nm]			•					
From:	300	t	o:	850						
		Curve step	c F	1,000						
						Value:			Туре	
Calc. unit:	n laye	r			•	1,487222			Curv	
Layer:	SiO2				•					
🔽 Add sim	ulated d	ata to experimer	it							
Name of tra	ansfer file	e:	C.1	Sentech\Spectri	aRay	4\ApplicationFra	me\ter	np.dat		
			V	Overwrite transfe	rfile	🔽 Add line c	olors	Mark	first data	
📝 Display	data in p	olot module	Na	me of style file:	C:\Se	entech\SpectraRe	ay4\Ap	plicationFre	ame\nkd.sty	
🔲 Create *	.dob file									
		Ē	lit laye	r <u>C</u> alc		Display	H	elp	Cancel	Quit

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":

lata serie	100.000	Intere		1.10.10	Intere	
non Javin Title Hander Species/Values Other	Values	Grach Tattle Title repaider Spo	cisiValues Other Verson		Greak Tattle, Tito Pipecial Spr	erini Velave Other Veroes
9	Dirocoh and derive Polynonioritat 2 Widh (points) 33	Commont (0)Wavelengih +632.8 mm	Cere (5.02.23/1	True, 144338	Provis (Conscience) - Cable grave school C - Mar jefacto - Itane	Usergi Usergare > Value User Valettiad Mineran Maamans
\backslash	Synooth data Derive data Erose spikes Thisphold Swelves 40,080000	(0) Angle-72.00 (0) Time 4.8 is (1) Templetare -22.5 C (1) Sample action -2.6 C (1) Sample action -2.6 C (1) Angle office -0.01 (1) Angle office -0.01		9		
	Grove Spikes	Vesuelangte 5/2.8 km Angle of incidence: 70,19 Politiker parkaar 45,000	Process lone Temperature Weight Schuld (Setter (Setter)	104 (141) 1.090 3.03*		
	Hreigises Apply wegione Add solocted region	Change k data No. of points 551	Shavis by points Make make by points	No Percovery colin by power		
0 40 60 100 70 800 Waqturgh jun	Clear al amagine	Monerango of source: 128,600	610.000	Fincultrative size	Content to Average Trainer 3002,3000 Trainer Trainer 3002,3000	tu 650.000 No 950.000 anuli 1 Avintage
Wastlergh [sm]			Ok Sancal			

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.

Data
400nm SiO2 / Si - SENTECH reference sample
[0] Wave.=300,0 nm850,0 nm [1,000]

Select from the menu: "File" \rightarrow "Save as ..."

Speichern	DATA	•	G 🗊 🕫 🛄 🕇	
Name	*		Änderungsdatum	Тур
≧ n_SiO2.	bxt		10.03.2016 11:49	Notepad + + Docu
•		m		
e latei <u>n</u> ame:	1	III		✓ Speichern

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 EXCELTM or OriginTM.

	ad++ - C1\Sentech\SpectraRay\Exp\Diemo Applications\oti		0.0
	earbeiten Sychen Ansicht Format Sprachen Einst		
	「日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日	: (QQ) (QQ) (QQ)	
n_S0	214		
-	WAVELENGTH MAT. REFRACTIVE INDEX		
1	300.00000 1.49456		
1.2	301.00000 1.49431		
A.	302,00000 1,49406		
	303,00000 1,49382		
-	304.00000 1.49357		
2	305.00000 1.19333		
8.	306.00000 1.49310		
5.	307.00000 1.49286		
10-	308,00000 1,49263		
	309.00000 1.49240		
78	310.00000 1.49217		
35	311.00000 1.49195		
19	312.00000 1.49172		
35	313.00000 1.49150		
14	314,00000 1,49128		
87	315.00000 1.49106		
10	316.00000 1.49085		
19	317.00000 1.49064		
110	318.00000 1.49042		
21	319.00000 1.49022		
2.2	320.00000 1.49001		
23	321.00000 1.48980		
-	7		
-	at file nb char : 19505	Ln:1 Col:1 Sel:0 Do:\Window	ANSI INS

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: PARAM
- 2. from the analysis window

Name	i la contra de l	Fit	Value	Scro	l value	Minimum	Maximum	Typ. Diff.
[1] Waveleng	h [nm]		632,8	4	1.	1,0	1000000000,0	10,0
[1] Angle	[*]	E	70,00	*	1.	00,00	90,00	0,50
[1] Time	s	T T	0,0			0,0	1000000000,0	10,0
[1] Temperatu	ire [°C]	L.	23,5	*	1 E	-273,1	8000,0	10,0
[1] Sample rot	ation [°]	F	0,00	4	1 1	-360,00	360,00	0,50
[1] Angle off	set [°]	I C	0,00	X	1.00	-90,00	90,00	0,10
[1] Wavelength ()ffset (nm)	T	0,00	•	ŧ	-10000,00	10000,00	2,00
[1] Wavelengt	n Linear	. 0	1,00000	*	÷	-10,00000	10,00000	0,00300
Air: Refr. ir	ndex	- F	1,000	4	1 +	0,001	40,000	0,100
Air: Absorp	ition	10	0,000	*	*	0,000	40,000	0,100
[1,1] SiO2: Thick	ness [nm]	N.	391,95	1	+ ·	0,00	40000,00	20,00
SiO2: N	0	V	1,448	4	11 F	-100,001	100,000	0,100
Si02: N	1	V	35,3	4	1 1	-40000,0	40000,0	100,0
Si02: N	2	F	0,0	a 1	1.00	-40000,0	40000,0	100,0
Si02: K	0	F	0,000		1 +	-100,000	100,000	0,100
Si02: K	1	10	0,000	4	- F	-40000,000	40000,000	100,000
Si02: K		5	0,000	*	E	-40000,000	40000,000	100,000
	, îŭ							
Printtable	Fitpara	meters: H	Hide >>	B	estore Lo Values	ad C	ancel	<u>o</u> k

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

SENTECH

Environment parameters: Global &	Environment 💽
<u>V</u> alues <u>R</u> anges <u>U</u> nits <u>S</u>	<u>S</u> ubstrate Inhomogeneity <u>M</u> odel <u>E</u> rrors
-Standard values (used if no) other values are present)
🔲 Wavelength:	632,8 nm
Angle of incidence:	70,00 *
Temperature:	23,5 °C
Process time:	0.0 s
Display RAE parame	parameters in list of fit paramaters ters in list of fit parameters
Data modulo Use data points modulo:	1
	<u>ш</u> к

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

<u>V</u> alues	<u>R</u> anges		l Environmen <u>S</u> ubstrate	Inhomogeneity	<u>M</u> odel	Errors
	L	_		Internegenera	<u></u> 0001	<u>E</u> 11010
Active	ranges of	values				
			Minim	um:	Maximu	m:
Wave	elength:		190,0 nm		2500,0 r	nm
Angle	e of incider	nce:	0,00 *		90,00 *	
Temp	oerature:		21,0 *0	0	1000,0 °C	
Proce	ess time:		0,0 s		3600,0 s	3
				<u>o</u> k		

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

Environment parameters: Glob	al Environment			X
<u>V</u> alues <u>R</u> anges <u>U</u> nits	<u>S</u> ubstrate <u>I</u> nho	mogeneity <u>M</u> odel <u>E</u> rrors		
Standard units for values	;			
Wavelength:	nm 🗸	Thickness:	nm	•
Angle of incidence:	• •	Growth rate vs. time:	nm/s	•
Temperature:	°C 🗸	Fraction:	%	•
Process time:	s 🔻	Diameter:	mm	•
		Thickness variation vs. spot:	nm/mm	•
		<u>o</u> k		

Fig. 8-27 Environment parameters: units

- **"Wavelength"** defines whether the wavelength scale is defined in "nm", photon energy "eV" or wavenumber "1/cm"

Tab: Substrate

Environment parameters: Global Environment		—
Values Ranges Units Substrate Inf	omogeneity <u>M</u> odel	Errors
Thick substrate with incoherent superpos	tion of beams	
Thick layer detected:	none	
Substrate thickness:	1,000 mm	
Number of backside reflections:	0	
=0 coherent and >0 incoherent		
🔲 Beam diameter:	4,000 mm	Calc mode
Detector aperture diameter:	4,000 mm	Calc with diameters
Backside factor:	1,000	Calc with factor
	Resetvalues	
Thicklayer thickness for detection (Minim	um value)	
Thickness:	0,100 mm	
Depolarization		
Remove degree of polarization from	measurement	
	<u>0</u> K	

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



Values Banges Units Substrate Inhomogeneity Model Errors Thickness variation:
Use thickness variation within measurement spot
Limited wavelength resolution Use limited wavelength resolution Wavelength resolution: 0,0 nm Calculation steps: 5
Non parallel light beam Use non parallel light beam Focus angle of non parallel beam: 3,00 * Calculation steps:
OK

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.

<u>V</u> alues <u>R</u> anges	<u>U</u> nits <u>S</u> ubstrate	Inhomogeneity Model	Errors
Error calculation			
	i		
Show result v			
Enabl	e error calculation af	terfit	
Calculation type	for derivatives:	Plus/minus epsil	lon 👻
🛛 🖾 Use precisio	n of (s1, s2) to get pre	ecision of (Psi, Delta)	
Duration in march			
	sured data for error o		
Stokes s1, s2:	0,0020	None:	1 0000
	-,	None:	1,0000
Psi ["]:	0,5000	Simulation:	1,0000
Psi ["]:	0,5000	Simulation:	1,0000
Psi ["]:	0,5000	Simulation:	1,0000 0,0100
Psi ["]:	0,5000	Simulation:	1,0000
Psi ["]:	0,5000	Simulation:	1,0000 0,0100
Psi ["]:	0,5000	Simulation:	1,0000 0,0100
Psi ["]:	0,5000	Simulation:	1,0000 0,0100

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

Tab: Errors

SENTECH SpectraRay/4

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 SiO₂ / Si for different film thicknesses of th = 0 ... 20 nm with a 5 nm step size?

Stack:

Air- n and k are fixedSiO2- CauchySi- File layer

Simulation:

Ψ, Δ versus wavelength and film thickness of SiO₂ Spectral range: **300 ... 850** nm Angle of incidence: **70** deg SiO₂ 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 SiO₂ 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

SR Simulation			
Wavelength: 632,8 nm Angle of Incidence: 70,00 * Angle of Rotation: 0,00 *	Temperature: Process time: Environme	23,5 °C 0,0 s ent Settings	Devicetype: PSCA Rotationtype RAE P/A angle 45,00 *
Curve parameter: 1		Trace parameter:	3
From: 300,000	to: 850,000	From: 0	to: 20
Curve	step: 1,000		Hate step. 5
4 Calc. unit: Delta(Psi)	•		alue 2: 2 Type: 9.022 Multi •
Add simulated data to experi Name of transfer file: Display data in plot module	C:\Sentech\SpectraRa	y4\ApplicationFrame\ter	🗖 Mark first data
Create *.dob file	6 <u>C</u> alc	Display H	elp Cancel Quit

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)

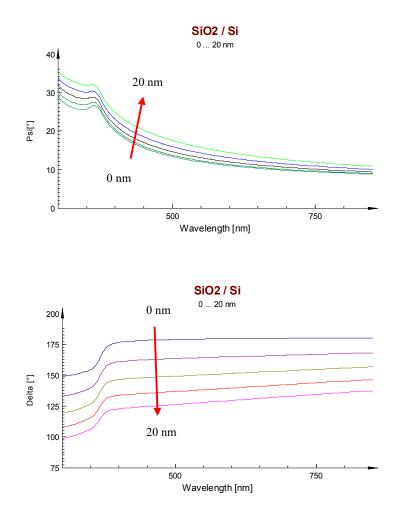
5) "Add simulated data to experiment" is switched on to store the calculated data to the Data subwindow.

6) "Calc" is pressed to do the calculation; the results are stored in the "Data" section.



SpectraRay/4

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:



Air NK layer	n=1,0000
Cau-SiO2 (therm.) 391,97 nm Cauchy layer	n=1,4644
Silicon VIS+NIR File layer	n=3,8714 k=0,01577

The "Simulation" window is opened and the following settings are selected:

SR Simulation					
Wavelength:	632,8 nm	Temperature:	23,5 °C	Devicetype:	PSCA -
Angle of Incidence:	70,00 *	Process time:	0,0 s	Rotationtype	RAE
Angle of Rotation:	0,00 *	Environme	ent Settings	P/A angle	45,00 *
Curve parameter	:				
[0] Wavelength [nm]	•			
From: 300,000	to:	850,000			
	Curve step:	1,000			
			Value 1:	Value 2:	Туре:
Calc. unit: n(k) la	ver	•	1,487222	0,00000000	Curve -
Layer: SiO2					
☑ Add simulated d	ata to experiment				
Name of transfer file		C:\Sentech\SpectraRa	v4\ApplicationFram	e\temp.dat	
		☑ Overwrite transfer file			data.
📝 Display data in p	lot module	Name of style file: C:\S	entech\SpectraRay	4\ApplicationFrame ⁴	hkd.sty
Create *.dob file					
	Edit	layer <u>C</u> alc	Display	Help Ca	ncel Quit

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 subwindow.

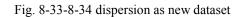
6) "Calc" is pressed to do the calculation; the results are stored in the "Data" section.



The data is saved into the Data section as a new dataset:

Data





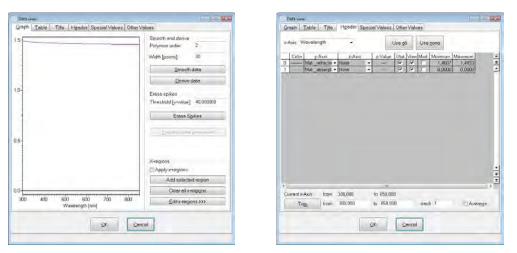


Fig. 8-35 Dispersion of n and k of SiO_2 and header tab

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 \leftrightarrow photon energy (nm \leftrightarrow eV)

$$\frac{1239.85}{nm} \hat{-} eV$$
, $\frac{1239.85}{eV} \hat{-} nm$

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 \leftrightarrow wavenumber (nm \leftrightarrow cm⁻¹)

$$\frac{10^7}{nm} \hat{-} cm^{-1}$$

Examples:

 $200 \text{ nm} = 50000 \text{ cm}^{-1}$ $500 \text{ nm} = 20000 \text{ cm}^{-1}$ $1000 \text{ nm} = 10000 \text{ cm}^{-1}$ $2000 \text{ nm} = 5000 \text{ cm}^{-1}$

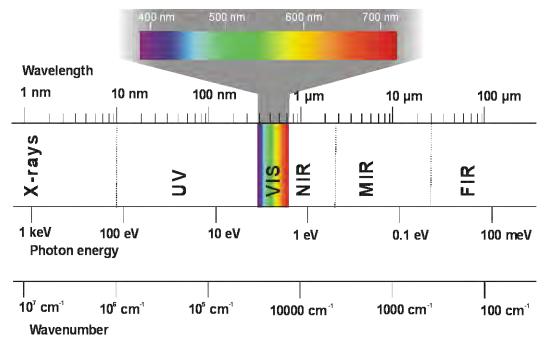


Fig. 8-36 Spectral ranges

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 /°
- $\tan \Psi, \cos \Delta$
- 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:

🔲 Transmissi	on.txt - Editor		- • •
<u>D</u> atei <u>B</u> earb	eiten F <u>o</u> rmat	<u>A</u> nsicht	2
300.37640 301.18359 301.99081 302.79800 303.60519 304.41241 305.21960 306.83401 306.83401 307.64120 308.44839 309.25562 310.06281 310.87000 311.67719 312.48441 313.29160 314.09879 314.90601 315.71320 316.52039	0.41700 0.41954 0.42052 0.42218 0.42343 0.42499 0.42707 0.42790 0.42790 0.42790 0.42926 0.43027 0.43231 0.43231 0.43231 0.432489 0.43562 0.43562 0.43799		
			P

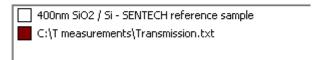
Fig. 8-37 Example for transmission data

The file is imported into the data section of the SE-Advanced client by Menu \rightarrow File \rightarrow Load ...

Euchen in:	bata 💧			- 🕒 🗊 💌 🖽 -		
Name		-		Änderungsdatum	Тур	
	ission.txt			10.03.2016 11:49	Notep	ad++Docu
			m			
-	Transmiss	sine by	m			ňífner,
e lateiname:	Transmis	sion, txt	m		•	Ŭffnen Abbrechen

Fig. 8-38 Importing data

Data



The units of the imported files must be set. The transmission measurement is double clicked and the "header" tab is selected.

010 101 Data view								
Graph Table Ti	tle H	Header Spe	ecial V	alues	Other	Valu	es	
x-Axis: None		•		U	lse <u>a</u> ll		Use <u>r</u>	one
Color y-Axis		z-Axis	z-\	/alue	Use		Mod.	<u>Minin</u> ≖
1 None	- N	lone	-					<u>0,≜</u>
<		III						,
Current x-Axis: fro	m 30	00,376	to !	920,350				
Tri <u>m</u> fro	m 31	00,376	to	920,350)		each	1
			<u>0</u> K		<u>C</u> t	ancel		

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"
- z-Value: "0.00"

(unit of the angle of incidence of T measurement)

(the value of the angle of incidence)



010 Tot Data view		<
Graph Table Title	Header Straylight Special Values Other Values	s
x-Axis: Wavelength	✓ Use <u>a</u> ll Use <u>n</u> one	
Color y-Axis	z-Axis z-Value Use View Mod. Mi	E
1 Transmission	▼ Phi ▼ 0,00 ▼ ▼ □ (≜∥
Current x-Axis: from	Ⅲ ► 300,376 to 920,350	
	300,376 to 920,350 each 1	
Tri <u>m</u> from		
	<u>Q</u> K <u>C</u> ancel	

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.



400nm SiO2 / Si - SENTECH reference sample
 dispersion n, k of SiO2



Important: Only "used" data will be exported.

010 Tot Data view			
Graph Table Title	Header Speci	al Values Other Va	lues
x-Axis: Wavelength	•	Use <u>a</u> ll	Use <u>n</u> one
Color y-Axis	z-Axis	z-Value Use Vie	w Mod. Minin 💻
		🔽 🔽	
1 Matabsorpt 🔫	None 🔻	🔽 🔽	
•			× ⊕ ×
Current x-Axis: from	300,000	to 850,000	
Tri <u>m</u> from	300,000	to 850,000	each 1
		<u>D</u> K <u>C</u> anc	el

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 \rightarrow "Save As..." menu entry is selected. The file extension "ASCII (*.txt) and a filename are selected and saved.

Speichern	💧 Temp	+ Ġ 🗊 💷 +		
Name	*	Änderungsdatum	Тур	
	Es wurden	keine Suchergebnisse gefunden.		
-		m		
∢ [Dateiname:	nk_Si02	III	-	Speichern
	nk_SiO2 ASCII (*.txt)	m	•	Speichern Abbrechen

Fig. 8-43 Filename and extension ASCII (*.txt) are selected

nk_SiO2.txt - Editor	x
<u>D</u> atei <u>B</u> earbeiten F <u>o</u> rmat <u>A</u> nsicht <u>?</u>	
<pre>; WAVELENGTH MATREFRACTIVE_INDEX MATABSORPTION 300.00000 1.49333 0.00000 301.00000 1.49309 0.00000 302.00000 1.49284 0.00000 303.00000 1.49286 0.00000 305.00000 1.49212 0.00000 305.00000 1.49188 0.00000 307.00000 1.49165 0.00000 307.00000 1.49165 0.00000 309.00000 1.49119 0.00000 311.00000 1.49096 0.00000 311.00000 1.49074 0.00000 312.00000 1.49030 0.00000 314.00000 1.49088 0.00000 315.00000 1.48965 0.00000 315.00000 1.48965 0.00000 316.00000 1.48964 0.00000 317.00000 1.48944 0.00000 318.00000 1.48923 0.00000 319.00000 1.48881 0.00000</pre>	•

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: $n(\lambda)$ and $k(\lambda)$. Different types of materials show different types of dispersions. Four different kinds of materials illustrate the variety of different dispersion relations:

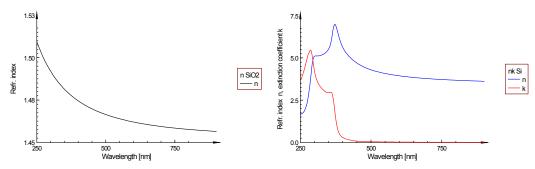


Fig. 8-45 Typical dispersions of a dielectric (SiO₂, left) and a crystalline semiconductor (Si, right)

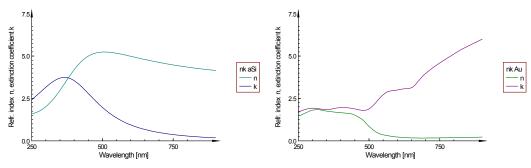


Fig. 8-46 Typical dispersions of an amorphous semiconductor (aSi, left) and a metal (Au, right)

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
Н	Fixed n and k	Constant dispersion	Only air
Η	Cauchy	transparent dielectric materials Photoresist Glass	SiO ₂ , Al ₂ O ₃ , Si ₃ N ₄ , TiO ₂ PMMA BK7, quartz
Н	Tauc-Lorentz	Absorbing dielectric materials amorphous materials	Si ₃ N ₄ , TiO ₂ a-Si, a-C
Н	Drude-Lorentz	Metals TCO (transparent conductive oxide)	Au, Ag, Cu, Cr, Ni ITO, ZnO:Al
Н	File-Layer	Table of wavelength, n, k,	Good for all
		no fit parameters substrates	Si, Ge, GaAs, quartz
Μ	Leng-Lorentz	Crystalline indirect semiconductors polycrystalline indirect semiconduct. conjugated polymers (OLED, OFET)	c-Si, c-Ge, c-SiGe poly-Si MEH-PPV, P3HT
Μ	Brendel	Absorption (vibration) bands in the \ensuremath{MIR}	SiO2, SiN, CH-bonds
Μ	Sellmeier	Like Cauchy but for broader spectral range (VIS + NIR)	SiO ₂
Μ	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
Η	EMA (effective medium approximation)	Mixture of two materials Roughness Interface Gradient	mixture: Air / layer mixture: layer1 / layer2
М	Biaxial anisotropic	Direction dependent dispersion	Crystalline quartz
М	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 _x Ge _{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.

🚑 Dispersion - Drude-Lorentz oscillator la	yer				- • ×
Layername: NoName0		Name		alue Scroll value	
		Thickness [nm]	0,0		•
Thickness: 0,00 nm		Epsilon-infinity-real	1,00		•
		Epsilon-infinity-imag	0,000		•
e1 infinity: 1.00	📄 omega_p (1/cm): 0.00	w-p-free-carriers-(1/cm)	0,00		•
B 8999		w-tau-free-carriers-(1/cm)	0,00		+
e2 inf imag.: 0.000	🔲 omega_tau (1/cm): 0.00	(1)Omega-O-(1/cm)	0,0		•
No. Use Fit Omega-0 Fit	Omega-p Fit Omega-tau 🏼	(1)Omega-p-(1/cm)	0,0		+
1 yes - 0,00		(1)Omega-tau-(1/cm)	0,0	0 <	·
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6 no 🕶	· · ·				
7 no 🕶	· · ·				
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E					
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Dielectric constant 90 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0					
2					
忘 0.4-					
lei l					
0.2-					
0.04					
1.5 2.0 2.5	3.0 3.5 4.0				
	Energy[e∨]				
Show dispersion: 🔽 n 🔽 k 🔳 e1 [e2 Resolution: low -				
Comment:	۸ ۳				
Copy nk dataset Copy eps datas	et Save eps as file Print table				
Fitparameters: Hide >>	QK				*
		< III			P.

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

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The Lorentz-oscillator consists of three parameters for the spectral position, strength and damping. Its contribution to the dielectric function ε is:

$$\varepsilon = 1 + \frac{\Omega_P^2}{\Omega_0^2 - v^2 - i\Omega_\tau v}$$

Its parameters are summarized in the following table.

Lorentz-Oscillator				
Parameter	Description			
Ω_0	Center frequency of the oscillator in cm ⁻¹			
$\Omega_{ m P}$	Strength of the oscillator (amplitude)			
$\Omega_{ au}$	Damping of the oscillator			

Tab. 8-3 Parameters of the Lorentz oscillator

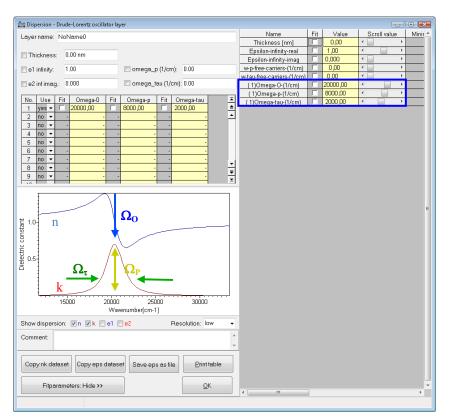


Fig. 8-48 Example for a Lorentz oscillator

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 $\omega_0=0$. Its contribution to the dielectric function ϵ is:

$$\varepsilon = 1 + \frac{\omega_P^2}{-v^2 - i\omega_\tau v}$$

	Drude-oscillator
Parameter	Description
ω _P	is dependant from the concentration N and the effective mass m* of the free carriers:
	$\omega_P = \sqrt{\frac{N e^2}{\varepsilon_0 m^*}}$
ωτ	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

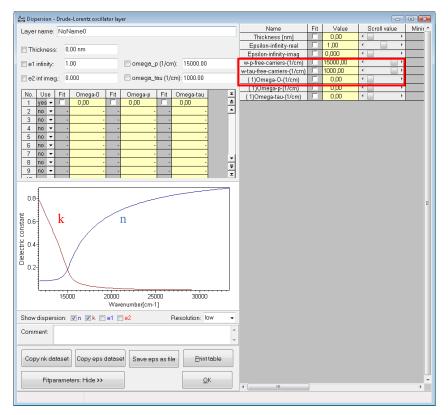


Fig. 8-49 Example for a Drude oscillator

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).

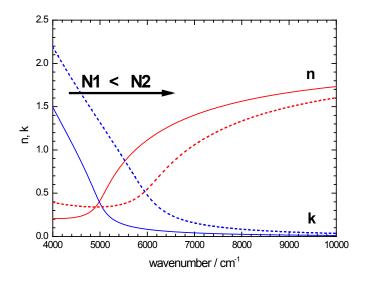


Fig. 8-50 Influence of carrier concentration N to the dispersion on n and k

→ With increasing carrier concentration the onset of the absorption is shifting to higher wavenumbers (shorter wavelength).

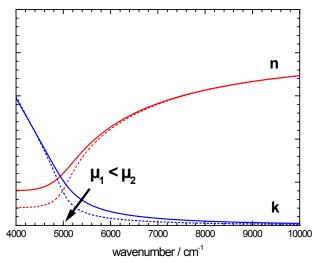


Fig. 8-51 Influence of carrier mobility $\boldsymbol{\mu}$ to the dispersion on n and k

 \rightarrow 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.

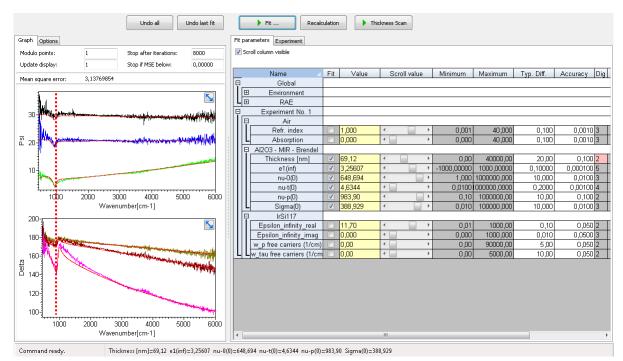


Fig. 8-52 Modeling of the AlO absorption band at around 700 cm^{-1}

The screenshot of the Brendel dispersion window for Al_2O_3 shows the dispersion of n and k using a single Brendel oscillator.



Dopersion - B	endel oscillator	layer									
Lavername: H	1203 - MIR - B	rendel			_	Name	Fit	Value		Scroll value	Minimum
						Thickness [nm]	¥.	76,00			0,00
Thickness	75.00 nm					e1(inf)		2,49100	•		-1000,00000
						nu-0(0)	80	691,363		100	1,000
2 pl infraty;	2,49100					nu-t(0)		46,9911	4	1	0.0100 1
						nu-p(0)	2	800,87		- Inf A	0,10
						Sigma(0)	2	332,879	1	- Int - 2	0,010
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	691,363	45,991	1 💌 800,87	332,079							
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2 10 +		-									
3 no -	4 <u>+</u>	-	+	-							
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5 110 -	A 7	-									
6 no -		-		1 10	•						
7 h0 -	-	-			-						
8 no -	a a	-									
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2.0-											
1.5					-						
	(
1.0- N											
1.8											
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		Waven	umber[cm-1]								
how dispersio	n En Ek	Del De	e P	esolution low	•						
Comment					1						
				1.2							
Copy nk data	copy e	s dataset	Save eps as file	Enint tak	le						
				1							
Fitpere	meters: Hide	>>		QK	-	41-0					

Fig. 8-53 Brendel dispersion for Al₂O₃

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.

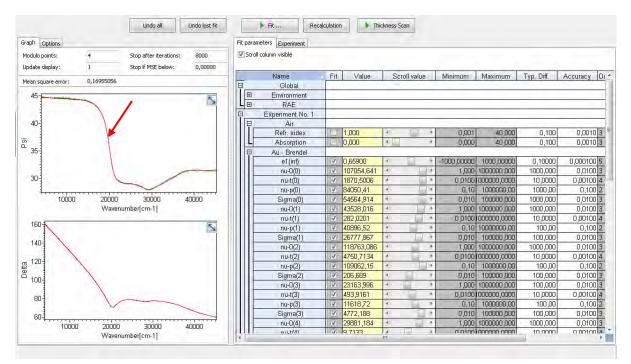


Fig. 8-54 Modeling of an Au film on glass

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.

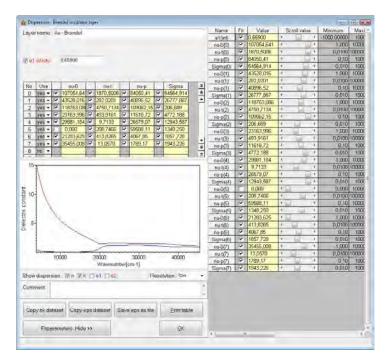


Fig. 8-55 Dispersion of Au

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.

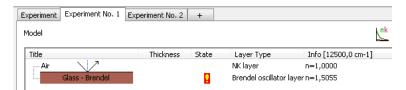


Fig. 8-56 Ellipsometric model without backside reflections

Experiment Experiment No. 1	Experiment No. 2	+		
Model				L ^{nk}
Title	Thickness	State	Layer Type	Info [12500,0 cm-1]
Air			NK layer	n=1,0000
Glass - Brendel	4000000,00 nm		Brendel oscillator	layer n=1,5055
Air		_	NK layer	n=1,0000

Fig. 8-57 Transmission model without backside reflections

Graph Options				Fit parame	eters Experiment								
Modulo points: Update display:	2	Stop after iterations: Stop if MSE below:	500		olumn visible		_						
		stop in the contri			Name	Fit	Value	S	croll value	Minimum	Maximum	Typ. Diff.	Accuracy [
Mean square error:	0,34193332			⊑ L⊕	Global			r_ =	1 - F			1.	
1			5	L	RAE								
and milling				E	Experiment No. 1	1							
21.0-				Đ	Local Environment								
				Ð	Air								
20.5	the second				Refr. index		1,000	4		0,001	40,000	0,100	0,0010
	THE REAL PROPERTY OF	The second s			Absorption		0,000			0,000	40,000	0,100	0,0010
1 1 2	a fitte	LAN HA CARE TO A	2	Ę.	Glass - Brendel							1.120.00	
20.0		And the hash			e1(inf)		1,00000			-1000,00000	1000,00000	0,10000	0,000100
		and the	Ser.		nu-0(0)	1	12377,297	4	· · ·	1,000	1000000,000	1000,000	0,0100
19.5-			Can.		nu-t(0)	2	9,4606	4		0,0100	0000,000000	5,2000	0,00100
19.97					nu-p(0)	~	12,84	4		0,10	1000000,00	1,00	0,100
1.000		20000 25000	30000		Sigma(0)	J	6057,426			0,010	100000,000	100,000	0,0100
	Waven	umber[cm-1]	1		nu-0(1)	1	8764,686	4	11 +	1,000	1000000,000	1000,000	0,0100
<i>i</i> -					nu-t(1)	1	3,9274	4	1	0,0100	0000,000000	5,2000	0,00100
1 August					nu-p(1)	~	17,86	*		0,10	1000000,00	1,00	0,100
0.8	and the second se				Sigma(1)	1	5694,963			0,010	100000,000	100,000	0,0100
			1		nu-0(2)	5	22818,119	4	- III +	1,000	1000000,000	1000,000	0,0100
0.6			1		nu-t(2)	2	4,1995	4	+	0,0100	0000,000000	5,2000	0,00100
					nu-p(2)	V	9,69	*		0,10	1000000,00	1,00	0,100
0.4					Sigma(2)	J	10897,659		1.15	0,010	100000,000	100,000	0,0100
0.6			1		nu-0(3)	1	26130,586	4		1,000	1000000,000	100,000	0,0100
0.2			1		nu-t(3)	X	44,7675	4		0,0100	0000,000000	0,2000	0,00100
			A A		nu-p(3)	V	3,40	*		0,10	1000000,00	4,00	0,100
0.0					Sigma(3)	1	781,750			0,010	100000,000	100,000	0,0100
1000	15000	20000 25000	30000		nu-0(4)	7	33537,200	1	U +		1000000,000	10,000	0,0100
TUQUU		umber[cm-1]	00000		nut(A)	D	105 2000			0.0100	מחחה ההההה	ก วอออไ	0.00100

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.

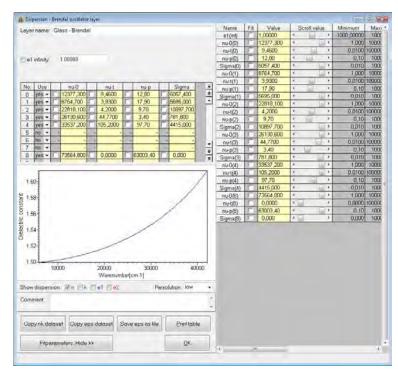
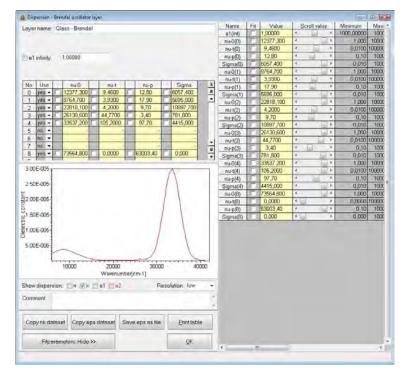


Fig. 8-59 Brendel oscillator for glass - n



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 \rightarrow Extra \rightarrow Applications
- Single mouse click on the application icon:

The "Application runner" is started which might already show existing scripts:

Applications		
Directory:	c:\sentech\spectraray\applications\	
Group:	Applications:	
Examples	Example 1: 10 consecutive fits	Run
		Edit
		Lait
		Quit

Fig. 8-61 Application runner

The existing applications are located in the folder Directory: c:\sentech\spectraray\applications\ . If you want to change the directory of the applications you have to click on DIR in the main window:

Directories	E	- 0 🔀
Materials:	c:\sentech\spectraray/mat	
Measurements:	c:\sentech\spectraray/data	
Models:	c:\sentech\spectraray\mod	
Experiments:	c:\sentech\spectraray\exp	
Applications:	c:\sentech\spectraray/applications	
Custom Directories:	c:\experiments	
		-
	🖌 ок	

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.

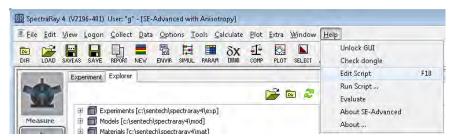


Fig. 8-63-8-64 Starting the script editor

Script Editor - Version 2.2.0.16/1	
Edit Start Icols Help	
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1	
	+

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.

😵 Script Editor - Version 2.2.0.1071	
File Edit Start Tools Help	
D B 🕼 B B 🖆 / 🖻 🖉 M A 🖧 🦸 Bur., Bill Debug hre for SN 🐨 💋 🙂	
1]:title-Examples\Example 1: 10 consecutive fits	
3 SpectraRay.autofit fit U	
4 SpectraRay.autofit Fit 0 5 SpectraRay.autofit Fit 0	
6 SpectraRay.autofit Fit 0	
7 SpectraRay.autofit Fit U	
A SpectraRey.autofit Fit D	
9 SpectraRay.autofit fit 0	
10 SpectraRay.sutofit Fit. 0	
11 SpectraRay.autofit fit 0	
12 SpectraRay.autofit Fit 0	
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	+^

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.

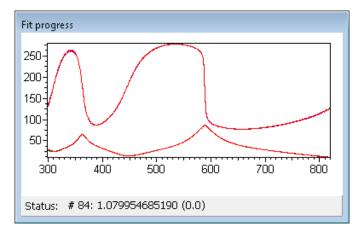


Fig. 8-67 Fit progress

SENTECH SpectraRay/4

The script can be cancelled before it automatically ends by holding the "CTRL" key. Then a window appears asking to confirm the cancelling.

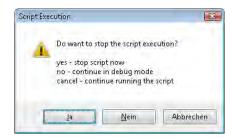


Fig. 8-68 Cancelling the script execution

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:

Script Editor - Version 2.2.0.1671	
Elle Edit Start Tools Help	
🗅 🗟 📽 🖬 🖆 / 👘 🛍 🗠 🗰 옮 🕼 🦸 Bur 🗟 Debug hre for 80 😇 💋 💟.	
example2	
1 [:1116-Examples\Example 2: 10 consecutive fits using a loop 2 sinteger 1, j 4 sinteger 1, j	*
6 j=10 7	
0 Label1: 9	
<pre>30 SpentraRay.autofit Fit 0 11 12 i=i+1 13 14 if i<j 15="" 16="" end<="" gott="" labell="" pre=""></j></pre>	
* 2	.*

Fig. 8-69 Non-trivial script example

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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 Label
if i \le 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.

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.

🛠 Skript Editor - Version 2.2,0,1671	
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D 월 🖉 월 월 월 1 🔞 🗠 🗛 옮 🌾 🖗 월un. 🗒 Debug hor fan SN 🖶 💋 번.	
exampled	
1 (title-Examples\Example 3: Sum of all layer thickness in a stack	
a present the second se	
3 integer Lavers.i	
4 double th, thtotal	
5 string sthtotal	
6	
7 1=0	
n th=0	
9 thtotal=0	
10	
11 SpectraRay.CountRodelLayers U Layers	
12 Layers=Layers=1	
13	
14 Label1:	
15 16 1=1+1	
17 SpectraRay.GetHodelLayerThickness 0 : th	
is thotal-thotal+th	
19	
20 if i <layers< td=""><td></td></layers<>	
21 goto Labeli	
22 end	
23	
24 Dbl2str thtotal achtotal 2	
25 message "Total stack thickness: {statotal; nm"	
	-
•	
2	

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:

Information 🔀
Total stack thickness: 317.21 nm
QK

Fig. 8-71 Resulting message

SE-Advanced tutorial

This is the script with comments:

SENTECH

```
;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 $\Phi = 8^{\circ}$.

	C	Data		
		SiO2 / TiO2 / SiO2		
The important informat x-Axis: None – (this wi y-Axis: None – (this wi z-Axis: None – (this wi z-Value: – (this wi	ill become: wavele ill become: reflecti ill become: angle o	ngth / nm) vity) f incidence)	-	
	H Data view			
	Graph Table Title	Header Special Valı	ues Other Val	lues
	x-Axis: None	•	Use <u>a</u> ll	Use <u>n</u> one

1 None ▼ None ▼ ▼ ▼ □ 0,4150 0,7000

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:

SENTECH

;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.

101	Data viev	v							
	Graph	Table Title	Header	Speci	al Values	Other	Values		
>	x-Axis: Wavelength Use <u>a</u> ll Use <u>n</u> one								
	Color	y-Axis	z-A×	is	z-Value	Use	View Mod.	Minimum	Maximum
1		Reflectivity -	Phi	•	8,00			0,41495	0,70000

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.

SpectraRay & W236-400 User "g" - (SE-Ad-Roced with Associatory - c/_operim	ent/imanual/disu3 exp[
* Lie Ldt Yow Logon Collect Data Dotarii Looli Calculate Bet Ex		×(市)。
DIR LOAD DELLA DIRA ADAL MAN DIRA SHEL MAAN THE CAR	CALINA AND	SENTECH
Expenses Expenses Expenses	Experience Experiment Vin () * Hode Tool Tool Autory Type Indiana Autory Trin 1000	にゅきょうしゅ
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Among an	tate	
Image: A standard	I forene ⊇ too ⊇ too Start Starten	
Command ready. Oil:	CADATAW, SOZAL	DN
SE Recipe SE Advanced Indu SE Advanced		
Ready		NUM

Fig. 8-73 dataset of five different positions

The following figure shows the resulting file of the script shown below.

🧾 resul	lt.txt - Editor	,				x
<u>D</u> atei	<u>B</u> earbeiten	F <u>o</u> rmat	<u>A</u> nsicht <u>?</u>			
Point	Thickne	ss n(400) (n633)	MSE		*
0 1 2 3 4	391.97	1.4768 1.4768 1.4768 1.4768 1.4768 1.4768	1.4641 1.4641 1.4641	1.080 1.080 1.080 1.080 1.080 1.080		
						Ŧ
)	•

Fig. 8-74 Resulting file

SE-Advanced tutorial

SpectraRay/4

This is the script file with comments:

SENTECH

```
;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 \le 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

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 + l
if i<number
 goto jumphere
 end
; loop ends here
. *****
```

Command running... Current measurement number: 5 ellapsed_time: 5 s

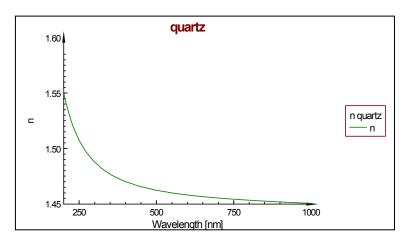
Fig. 8-75 Status bar

8.7 Application examples

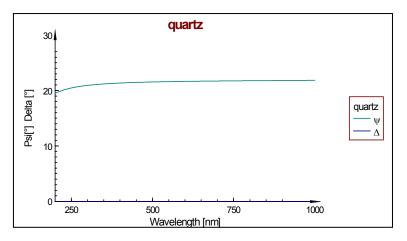
8.7.1 Measurement of substrates

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.

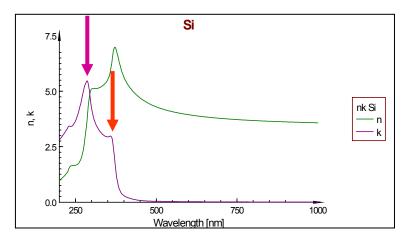


This results also in monotone spectra (here at $\Phi=70^\circ$). Ψ shows no particular structures. Δ is constant at 0° . It can also be constant at 180° when the angle of incidence is lower than the Brewster angle.

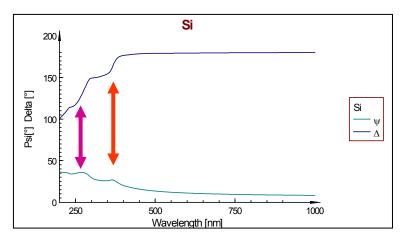


8.7.1.2 Absorbing substrates

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.

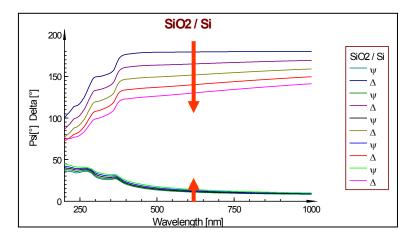


These characteristic structures appear also as structures in the ellipsometric spectra Ψ and Δ .



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 SiO₂ 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: (Combined Ellipsometry and Transmission) 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.

Title							Thi	ickr	ness	State	Laye	r Ty	/pe		Info [62	200,8 cm-	1]
A	ir			7							NK lay	/er		n=1,0000			
-			P200	0		_	40						: !!!				_
_		_				_	40	, IU	Inm	88			oscillator la			· ·	э
I			Supra	sil							File la	yer		1	n=1,443	3	
Dispe	rsion -	Brene	fel oscillato	se lave			_									100	1
-				and a	~						Name	Fil	Value	Se	roll value	Minimum	ľ
layer n	ome:	P20	00								Thickness (nm)	10	46,10	*	1	0,00	t
The			6.10 nm								e1(inf)	-	2,08500	*	1	-1000,00000	
Thick	KITESS	4	0.19.00								nu-0(0)	12	39300,100	+	L F	1,000	T
/initial	Entry	2	00260								nu-t(0)	4	2195,0400	4	- Jul P	0,0100	
-											nu-p(0)	×	21582,80		- U.	8,10	
											Sigma(0)	2	1506,100	•	10.2	0,010	
the I		-	7.0.7	-		-	1	-	1	1	nu-0(1)	4	25588,200	4	he ?	1,000	
	Uşe	100	D-Un	177	nu-t	-	nu-p	-	Sigma	-	nu-t(1)	1	3456,4500			0,0100	
	ng -		100,100		2195,040		21582,80	2			nu-p(1)	17	7601,20	10	1.1.1	0,10	
	09.7		5588,200 12056,700		3456,450 3148,890		7601,20	Ť	6299,900		Sigma(1)	1	6299,900	1	1.1	0,010	
	05 =		9411,700		3146,890		19346,00	1	3595,300	-	nu-0(2)	9	32056,700			1,000	
	#99 + #95 +		6590,900		100,0000		1500,00	F	900,000		nu-t(2)	1	3148,8900	•	1.0	0,0100	
	85 -		22013,700		27,2600		7738.60	17			nu-p(2)		19345.00	1	100	8,10	
	0. *		2013,700		27 2000	1	1130.00	1	4540,100		Sigma(2)	P	10876,900	*	<u></u>	0,010	
	0 -				_			-		-	nu-0(3)	*	19411,700		100	1,000	
	0 -				-			1			nu-t(3)		227,3800		10	0,0100	
- 1			-	1		-		1	-	=	NU-p(3)	2	8387,80	-		0,10	
	_	_		-		_	_	_			Sigma(3)	2	3595,300			0,010	
2.0-				1	-	1					nu-0(4)	~	16590,900			1,000	
	_					1	~				nu-t(4)	2	100,0000		10.1	0,0100	
							-	-		-	nu-p(4)	1	900,000			0,10	
1.5											Sigma(4)	2	22013,700			1,000	
											nu-0(5)	-	27,2600	-	10.1	0,0100	
											nu-t(5)	2	7738.60		-	0,10	
1.0											nu-p(5) Sigma(5)	7	4346,100	4		0,10	
1.5		100	00	15000	Wavenu	zabar		00	3000	0							
	-	sión	i₹in i₹ik		el 🗍 ez		P	Reso	dution low	•							
Comme	ent		_		_												
Сору	nk da	laset	Copy	eps d	ataset	Sav	e eps as file		Print tai	ble							
	Eiters		kurs: Hidu					1	QK.								

Fig. 8-76 Dispersion of P2000 describe using Brendel oscillator model

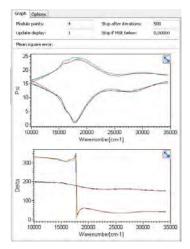


Fig. 8-77 Measurement and model at $\varphi = 50^{\circ}$ and 70°



8.7.2.3 Second experiment for transmission

8.7.2.3.1 Creating the second experiment

The second experiment is created by: Menu \rightarrow Edit \rightarrow Model + Data sets \rightarrow Add

DIR	Copy parameters to clipboard Data		MUL PARAM COMP PLO	
	Create interface		-	
	Model + data sets	(F	Add empty	🎽 🖮 🧯
	Fit script		Delete	
	Contraction and the second sec		\mod]	
Meas	Delete fit script		ay\mat]	

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.

Experiment	Experiment No. 1	Experiment No. 2	+		
Model					
Title		Thickness	State	Layer Type	Info [6200,8 cm-1]
; Air	\backslash	mentoss	Stato	NK layer	n=1,0000
	P2000	46,10 nm		Brendel oscillator la	ayer n=1,8109 k=0,00951
	Suprasil			File layer	n=1,4433

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 \rightarrow Tools \rightarrow 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 \rightarrow Options \rightarrow General Options...". The checkbox "Use global environment" has to be unchecked in the "Experiment options" tab.

SR General options				
Color calc options	Hardware / Re	emoteinterface	Unit precision	Messages
Experiment options	Display options	File version options	Display colors	Data options
Environment	ame environment for al	l experiments in the multi-e	xperiment)	
Default		QK		

Fig. 8-80 Uncheck "Use global environment"

Now at least on backside reflection can be activated for the second experiment.

Environment parameters: Local Enviro	onment for B	Experiment No.	2		×
Values Ranges Units Sub	ostrate <u>I</u> nh	omogeneity	<u>M</u> odel	<u>E</u> rrors	
Thick substrate with incoherent	tsuperposi	ition of beams			
Thick layer detected:		Suprasil			
Substrate thickness:		1,000 mm			
🔲 Beam diameter:		4,000 mm			
Detector aperture diamet	er:	4,000 mm			
Number of backside reflectio =0 coherent and >0 inc		1			
Thicklayer thickness for detect	ion (Minimu	um value)			
Thickness:		0,100 mm			
Depolarization					
Remove degree of polariz	ation from r	measurement			
		<u>0</u> K			

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 \rightarrow File \rightarrow Load (*.spc extension is selected).



The two experiments appear as shown in the screenshot:

eriment Experiment No.	1 Experiment No. 2	+		
del				
Title	Thickness	State	Layer Type	Info [6200.8 cm-1]
- Air Z			NK layer	n=1,0000
00000	46,10 nm		Brendel oscillator	layer n=1,8109 k=0,00951
P2000				

Experiment	Experiment No. 1	Experiment No. 2	1.0		
Model					
Title		Thickness	State	Loyer Type	Info [6200,8 cm-1]
Air	NA			NK layer	n=1,0000
- 31	P2060	-16,10 mb	60	Brendel usuilator	layer n=1,8109 k=0,0095
1.000	Supresi	1000000,00 rm	-	rile layer	n=1,4433
- 100	40	-		NK layer	m=1.0000

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:

Name	Fit	Value	Scroll value	Minimum	Maximum	Typ. Diff.
[1] Wavelength [cm-1]	100	6200,8	8 E F	0,0	10000000,0	0,1
[1] Angle [°]	5	70,00	+ E F	00,0	90,00	0,50
[1] Time [min]	E	0,00	4 F	0,00	16666666,67	0,17
[1] Temperature [K]	E	296,7	*	0,0	8273,1	10,0
[1] Sample rotation [°]	F	0,00	4 🗍 i	-360,00	360,00	0,50
[1] Angle offset [°]	1	0,00	4 🗌 E	-90,00	90,00	0,10
[1] Wavelength Offset (nm)	E	0,00	1 F	-10000,00	10000,00	2,00
[1] Wavelength Linear	E.	1,00000	4 F	-10,00000	10,00000	0,00300
Air: Refr. index	The second se	1,000	< +	0,001	40,000	0,100
All Absorption		0,000	4 🔄 🕴 F	0,000	40,000	0,100
[1,1] P2000: Thickness [nm]	M	46,10	* F	00,0	40000,00	20,00
P2000 4(%)	V	2,08500	a 🔲 0.	-1000,00000	1000,00000	0,10000
P2000: nu-0(0)	V	39300,100	10 10	1.000	1000000.000	10,000

Print table Fitparar		neters:	Hide >>	B	estore Load Values	d <u>C</u> ancel		QK
Delta Li	n. Itti	- Dr.	0,00	*		-3000,00)	3000,00	5,00
Delta Offs.			0,00	+		-3000,00	3000,00	5,00
Psi Quadr.		E	0,00	*	1 1	-3000,000	3000,00	5,00
Psi Lin.		Г	0,00	4	+	-3000,000	3000,00	5,00
Psi Offs.		E	0,00	4		-3000,000	3000,00	5,00
Ana. Offs. Quadr.		F	0,00	1	1	-3000,000	3000,00	5,00
Ana.Offs.Lin.		E.	0,00	*	1 E	-3000,000	3000,00	5,00
Ana.Offs.		T.	0,00	*		-360,00	360,00	5,00
Eta		F	1,00000	*		0,00000	1,30000	0,00100
Ret.Phase			90,00	4	- +	-360,00	360,00	5,00
Ret.Axis		E	0,00	*	1 6	-360,00	360,00	5,00
Pola Offs.		T	0,00	•	1 1	-360,00	360,00	5,00
Pola Pos.		F	45,00	4	- P.	-360,00	360,00	5,00
			1000000,00	*		00,0	4000000,00	20,00
[2,1] P2000: Thickness [nm]		V	46,10	*	E F	0,00	40000,00	20,00

Fig. 8-82 Parameter list of both experiments

The fit script is now created by: Menu \rightarrow Edit \rightarrow Fit script ...



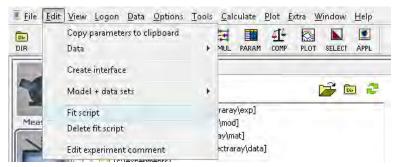


Fig. 8-83 Starting the script editor

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 "*SpectraR-ay*. *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.

Name		Fit	Value	S	croll v	alue	Minimum	Maximum	Typ. Diff.
[1] Wavelength [cm	i-1]		6200,8	4		1.1	0,0	10000000,0	0,1
[1] Angle [°]			70,00	*		E F	0,00	90,00	0,5
[1] Time [min]			0,00	4			0,00	16666666,67	0,17
[1] Temperature [K]		296,7	4			0,0	8273,1	10,0
[1] Sample rotation [°]			0,00				-360,00	360,00	0,50
[1] Angle offset [*]			0,00	+		÷	-90,00	90,00	0,10
[1] Wavelength Offset (nm)			0,00	4			-10000,00	10000,00	2,00
[1] Wavelength Linear		E.	1,00000	4		*	-10,00000	10,00000	0,00300
Air: Refr. index			1,000	4		+	0,001	40,000	0,100
Air: Absorption			0,000	41		- F	.0,000	40,000	0,100
[1,1] P2000: Thickness [nm]		2	14,22	4			0,00	40000,00	20,00
P2000: e1(inf)		2	14,20170	4		111	-1000,00000	1000,00000	0,10000
P2000: nu-0(0)		V	39548,844	4			1,000	1000000,000	10,000
P2000: nu-t(0)		1	2194,9414	4		TH	0,0100	100000,00000	0,2000
P2000: nu-p(0)		2	21634,07	4			0,10	1000000,00	10,00
P2000: Sigma(0)		2	1878,081	*		114	0,010	100000,000	10,000
P2000: nu-0(1)		4	25539,701	1			1,000	1000000,000	10,000
	m		-			_			
Print table	ble Fitparameters: Hide >>			<u>R</u> estore Los Values		ad D	ancel	<u>0</u> K.	

Fig. 8-84 Parameter list of the experiments

SE-Advanced tutorial

The fit script appears as follows:

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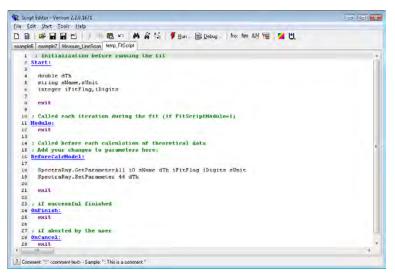


Fig. 8-85 Fit script

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 $0 \dots 90^{\circ}$ and $0 \dots 360^{\circ}$ while transmission is only between $0 \dots 1$. 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.



Measureme							
Name:	P2000/						
User:			Date:		Time:		
	UV/VIS Mode: Motor s	SE 850 (190.000 Settings: Standard stops=8 cycles=1	nm 2500.00	0 nm)		A III	
Measureme	nt envirc	onment					
Wavelengt	h:	1,000E30 eV	Process	time:	0,0 s		
Angle of inc	idence:	0,00 *	Temper	ature:	0,0 °C		
Polarizer p	osition:	45.000	Weight	Weight			
			Sample	rotation (theta):	0,00 *		
Change x-a:							
No. of point	S:	1382	X-axis b		Yes		
			Mak	e x-axis by points	Remove x-axi	s by points	
New range	of x-axis	189.719	2502.62	5	Recalibrat	e x-axis	
					Flip x-axis o	lirection	

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.

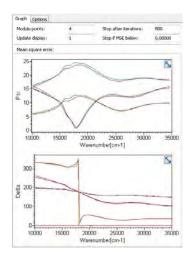


Fig. 8-87 (Ψ , Δ) and transmission measurement

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.



seAxis. Wavel	Title			Use pll	1	1	
				1.000	Use none]	
1 Pei 2 Delts		7-Axis Pho Pho			2 1 Z	num Maximum 1830 60,145 1,216 222,470	
	from	169.719	to 2	502.625	н		
Current x-Axis:		189.719	10 2	502 625	each 1	Average	

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.

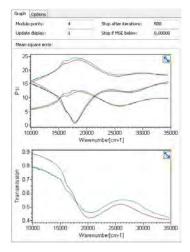


Fig. 8-89-8-90 Ψ and transmission measurement

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.



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.

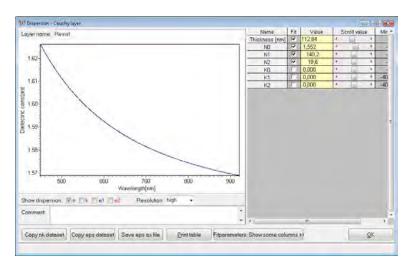


Fig. 8-91 Cauchy model of the resist film

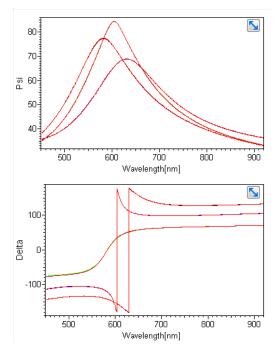


Fig. 8-92 The measurement and model after fitting

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".

Create new material	
Afromovitz III-V layer	^
III AlxGa(1-x)As layer	
📙 Biaxial anisotropic layer	
🔐 Brendel oscillator layer	
12 ³ Cauchy layer	
😹 Drude-Lorentz oscillator layer	
🔀 Effective medium and index gradient layer	
ka File layer	
y 🗷 Formula layer	
🚯 Forouhi-Bloomer layer	
Harmonic oscillator layer	
🙆 Homogeneous growing layer	
IIII In(1-x)GaxAsyP(1-y) layer	=
📅 ln(1-x)GaxAsyP(1-y)on lnP layer	-
🕼 In(1-x)GaxP layer	
🔢 InxGa(1-x)As layer	
ITO Hamberg layer	
ITO Semelius layer	
🔼 Leng Oscillator layer	
nk NK layer	
🗮 Nucleous growing layer	
Parametric file (2D) layer	
📑 Periodical layer	
🔀 Polynomial layer	
🐹 Schott layer	
Sellmeier transparent layer	
N Silicon epitaxial layer	
Spectral combination layer	
Tanduv III-V laver	*
	_
OK Cancel	

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.

Layer name:	Desist			_	Name	Fit	Value	:5	Scroll val	ue	Minimum	Maximu
Loyer norne.	riesisi				Thickness [nm]		112,84			P.	0,00	400000
			_		Refr. index		1,600			+	0,001	40,
Thickness	š:	112,84 nm			Absorption	2	0,000	1		+	0,000	40,1
Refractive	index n.	1,600										
Contractives	anteres in	1,000										
		0.000	-									
Absorption	n index.k:	0,000										
Absorption	n index.k:	0,000										
	n index k:	0,000		×.								
Absorption Comment	n index.k:	0,000		4.4	* 1	m						
	n index k:	0,000		1	* [III		1				

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:

Title	Thickness	State	Layer Type	Info [633,0 nm]
Air 📝			NK layer	n=1,0000
Resist	112,84 nm		NK layer	n=1,6000
Si DUV-UV-VIS-NIR			File layer	n=3,8736 k=0,01455

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.

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Reidy	14054

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)

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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.

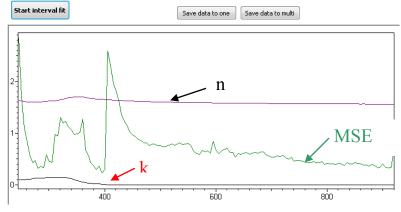


Fig. 8-97 "Shifted Interval Fit" results

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:

			Data									
			📕 Resist / Si									
			🔲 Interval fit									
Data view		Part of the			Data view							E
araph Table T Measurement into	tte Header Spe	cial Values Other Values			Graph Table Ti	le Mgadar Spec	ial Values Other Va	lues	_			
Nome Interval	10				x-Axip Waxdoreth	1	Use gli	Use pone				
User	1	lete	Time		Color	V-Axis	2 Axis	z-Vatue L	te View Mod	Minimum IA	daximum]	
Comment Result of MSE NK of R Interval from 92		6.1			1 None 2 Mat_refract 3 Mat_absorp		None - None -			0,2410 1,5691 0,0000	2,8676 1,7132 0,1497	- (clear
Measurement envin	anment											
Wavelength:	632.8 nm	Process time:	0,00 min									
Angle of incidence	70,00 '	Temperature	296.7 K									
Polanzer position:	45.000	Weight	1.0000									
		Sample rotation (theta)	0.00 *									
hange x-axis												
No. of points:	136	X-axis by points	Yes									-
		Make x-axis by points	Remove x-axis by points	4								Tute Is
New range of x-axis	245.000	920.000	Recalibrate x-axis	1	 Current x-Axis: from 	m 245.000	to 520.000				-	1
			Flip x-exis direction	1		m 245.000	15 920.000	each 1	-	verage		
		QK. Qancel					QK. Canc					

In case you click on "Save data to multiple data sets" each fitting result is saved into one data set:

Data	
Resist / Si Interval fit: MSE Interval fit: MK of Resist Interval fit: fit parameter: Resist: Refr. index Interval fit: fit parameter: Resist: Absorption	

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).

Environment parameters: Global Environment								
<u>V</u> alues <u>R</u> anges	<u>U</u> nits	<u>S</u> ubstrate	lnł					
Standard units fo	or values-							
Wavelength: 🗾 🗸								

Select the NK data set "Interval fit: NK of Resist" and convert the x-Axis from wavelength scale to "eV" (photon energy).

115 D	Hi Data view										
Gr	Graph Table Title Header Special Values Other Values										
x-4	xis:	ν.	•			Jse <u>a</u> l		Use	none		
	Color	y-Axis	z-Axis		z-Value	Use	View	Mod.	Minimum	Maximum	
1	1 Matrefractiv - None 🔲 🗹 🔲 1,5687 1,7132										
2	2 Matabsorpt ▼ None ▼										

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.

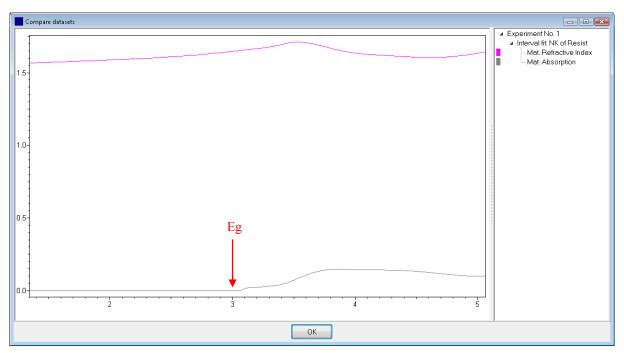


Fig. 8-98 Resulting n and k

The following two oscillators are build up using the Tauc/Lorentz oscillator model:

LM Dispersion - Taue-Loverta layer		14 Dispension - Tauc-Loventz layer	100.000
Layer name Perch TL et intrady: 1.0000	ma Fit Value Scrott-value Minimum Massi * (mg 1 20000 * * 1000 00000 1000 0,0 ♥ 3,0000 * 1000 0000 1000 0,0 ♥ 30,000 * 100000 1000 0,0 ♥ 30,000 * 100000 1000	Leger mene Result TL al vinde, 10000	Name Fr Value Stork view Normann Mass * eited 1 0.000 * 0.000 1.000 + 0.00000 1000 c, t) 1.0000 0.0000 1000 1000 1.0000 1.0000 1.0000 10000 1000 1000 1

Fig. 8-99 Tauc/Lorentz Oscillators

The combination of both oscillators is already quite similar to the "shifted interval fit" results:

Dispersion - Tauc-Lorentz layer					Lieu	0
avername. Resist-TL	Name	Fit		Scroll value		Max
	e1(inf)	DC.	1,00000	4	+ -1000,00000	1000
More	Eg(0)	15	3,0000		• 0,0000	
	A(0)	10	30,00	1	• -1000,00	10
e1 infinity: 1,00000	E0(0)	10	8,0000	1 W	0,0000	1D
when I retrain I man I retrain I other I al	C(0)	10	4,0000	*	• 0,0000	10
No. Esteril Aleril Esteril Slovil X 0 V. T 30.000 T 8,0000 T 4,0000 1	Eg(1)	2	3,0000	4 bal	+ 0,0000	10
1 yes 3,0000 20,00 3,5000 1,0000	A(1)	11	20,00	1	-1000,00	10
2 00 -	E0(1)	10	3,5000	1	0,000	10
3 10 +	Ć(1)	18-1	1,0000	ALC: N	• 0,0000	10
4 80 *						
5 m +						
8 m2 +						
7 no +						
8 m -						
10 00 0						
Oscillator 1+2						
how dispersion ligin ligit i e1 ⊡e2 Resolution low •						
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Copy nk dotaset Copy ops dotaset Save ops as file Print table Fitperameters: Hide >> DK						

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:

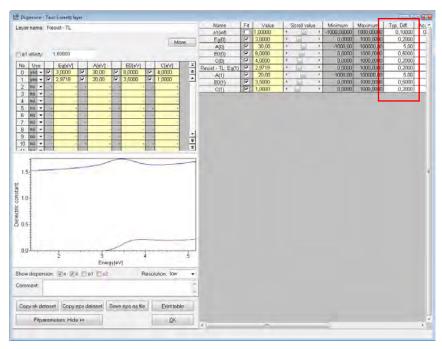


Fig. 8-101 "Typical Differences"

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.

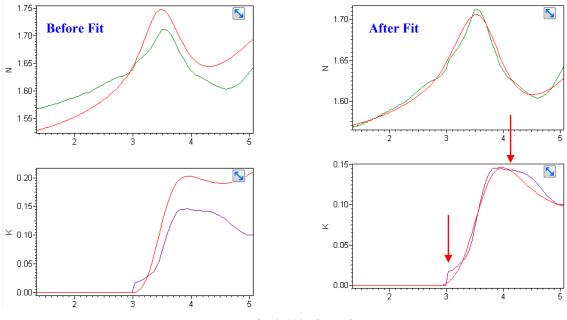


Fig. 8-102 Fit result

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

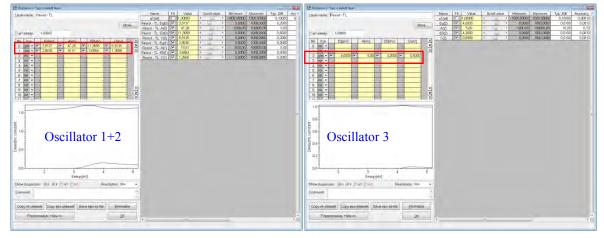


Fig. 8-103-8-104 Another Tauc/Lorentz Oscillator



Dispension - Tauc-Lorentz layer								9	
Layer name: Resist-TL	Name	Fit	Value		where then	Minimum	Maximum	Typ. Diff.	Ac
	e1(inf)	171	1,00000	0	100	1000,00000		0,10000	0
More		1	3,9137	1		0,0000		0,2000	
- Control -		4	47,26	1	and the second	1000,00		5.00	-
e1 infinity: 1,00000	Resist - TL: E0(0)		11,3658		1000	0,0000		0,5000	
No Line Estan Later Friend Chan -		3	6,9135	- K.		0,0000		0,2000	
	Resist TL Eg(1)	3	2,8636			0,000,0	1000,0000	0,2000	
0 yes	Resist - TL A(1)	19	10,51		1.	1000,00	100000.00	5,00	
	Resist - TL: E0(1)	4	3,6564	4	100	9,0000	1000,0000	0,5000	
2 yes - 2 4,0000 2 5,00 2 4,2000 2 0,5000	Resist - TL C(1)	2	1,2656	4		0,0000		0,2000	
	Eg(2)	2	4,0000	4	- Lat	0,0000		0,0100	
4 10 -	A(2)	1	5,00	e	- Just - 1	-1000,00	100000,00	10,00	
5 00 *	E0(2)	4	4,2000		had to re-	0,0000	1000,0000	0,0100	
	C(2)	4	0,5000		And in the	0,0000	1000,0000	0,0100	
1.5									
Oscillator 1+2+3									
Oscillator 1+2+3									
Oscillator 1+2+3									
Oscillator 1+2+3	- / / / / / / / / / / /								
Oscillator 1+2+3	- / / / / / / / / / / /								
Oscillator 1+2+3	- / / / / / / / / / / /								

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:

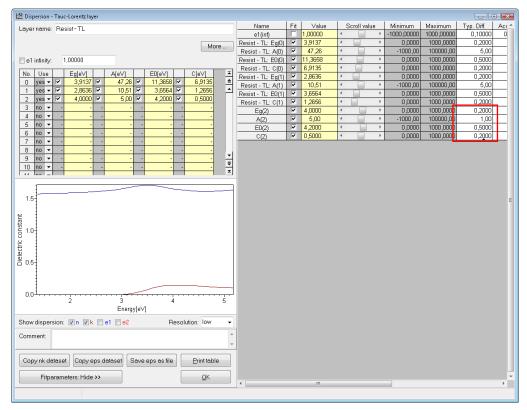
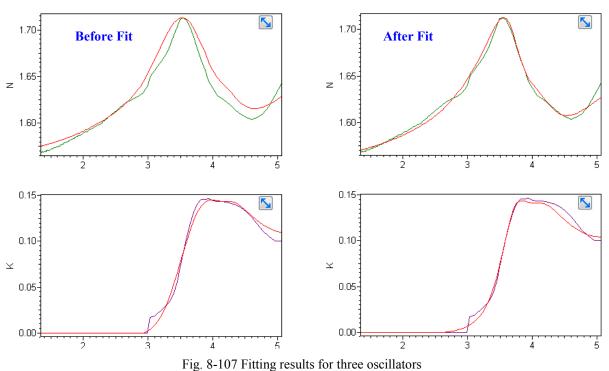


Fig. 8-106 "Typical Differences" for the third oscillator





The structure at 4.2 eV is now described well by the model.

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.

Experiment	Experiment No. 1	+				
Model					🗠 📝 🚽	- 🗌 🛩
Title		Thickness	State	Layer Type	Info [1,959 eV]	
; Air	\checkmark			NK layer	n=1,0000	
	Resist - TL			Tauc-Lorentz layer	n=1,5858	

Save as			
Speichern	other 📃	- 🧿 🥩 🛤 -	
Name	Änderungs Typ	Größe	
ac_s		aginsbte .	
air		aist.	
🔊 alsi_s		🛃 alsiti_sopra	
dlc_fb		🔁 h2o_aspnes	
H2O_w	ater	🛃 linbo_ap.	
a oscill		🔁 relorenz	
🔊 sellmei		🔁 thf4_pa	
aurban0	1	void_a	
ZnGa20	04_TL1_300_850nm		
ateiname:	Resist		Speichern
ateityp:	Materials (*.mat)		Abbrechen
elected: Oth	her		

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.

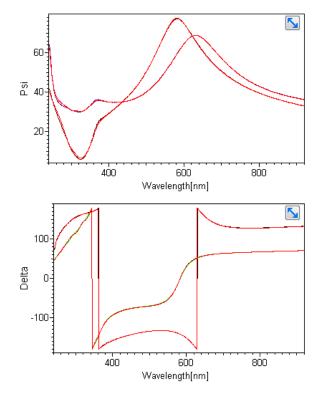


Fig. 8-108 Fitting result for the (Ψ, Δ) -spectrum

The model fits the measurement well. The final dispersion of the Resist film is shown in the following screenshot:



Lowram Pour-	11								Mairie	TI	Value	Selder	Mairman	Measure	(T)
roka casar sasar.	14								11.11 Report To: Thickness Inert	P	112,00	4	10,00	40000,00	-
Printees 1124							1.0	LIN	#10#10	111	1,00000	0 E 4			
							1.0		Wathing . HL Eggl3	10	3,3209	8. Lin 14			
Calabaly. 280	60								Rest TL AD	2	63.72	P			
No Use Ld	and a	I. al	15.1		Elevi	1	C(ev)	1001-11	Report TL EURS	R	11,3809	A			
	0E 10		72	01	1,3008		7,230		Party - TL COL	12	7,2983	4			L
	3. 1		14	51	1 /7021	10	0.7309		HINDIE-TH. EXET	5	2(035	1. 1			-
2 100 - 19 - 10			DI I		60510	12	0.5304		Pero T Art	4	104	4 11 19		MOTHIZ/F	-
1 10 1	-		-	litti -		1	0,000		Papet 1L: EQU	4	37701	4			1
1 10 1		-	-	10	-	- 10	-	100.6	Finuel - 11, C(1)	4	07270	1 10 1			-
5 00 -	-	-	-	88		-100			HORER - HL EIKA	5	1,1259				-
5 20		-			-	- 55	-	200 I	Repsile TL AC	ě.	42619	1 1			-
7 88 *	-	-	-	56		15			Ratid TL 00(2) Return TL C(2)	÷.		4		1000.0000	
3		-	_		_	1			Secure-TL-CO	124.1	0,5304	1	11100	300,000	_
13	-	1	1					1							
13		1		国				1							
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13 10 10 10	1 4.10					-	iden ov								
	9.4.1					-		5							
1.5		Int I	*	Inel		Ł		1 × 1							

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.

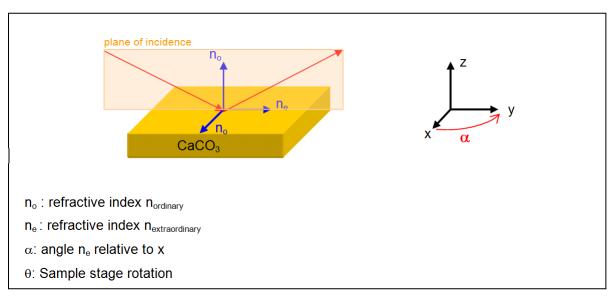


Fig. 8-110 Anisotropic sample and coordinate system

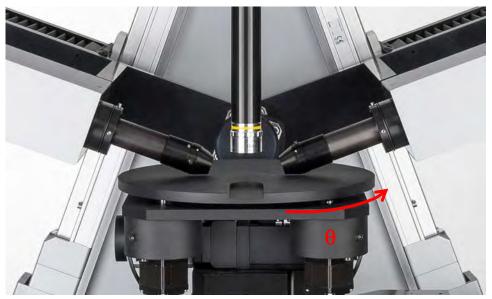


Fig. 8-111 Sample on rotatable sample stage

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 $\theta = 0^{\circ}$ to 360° every 15°. These results in a set of measurements are added as a single dataset to the data section of SpectraRay.

Data	
Sample rotation 0.00 360.00 [15.00] deg at angle = 70.00 deg / Th 03/2	5/2010 at 15:13:02

The tab "Header" shows the individual spectra for each angle θ .

115 Data vie	w									
Graph	Table Title	Header Sp	seci	al Values	Othe	r Valu	ies			
y-Avis:	Wavelength	•			se a		l leo	none		
					00 0		000	<u>n</u> ono		
Colo	r γ-Axis	z-Axis		z-Value	Use	View	Mod.	Minimum	Maximum	I
1	- S1	 Theta 	•	0,00	V	V	Г	-0,74342	-0,71444	×
2	- S2	✓ Theta	•	0,00		V	Г	0,67026	0,69929	
3	- S1	✓ Theta	•	15,00				-0,71135	-0,68468	
4	- S2	✓ Theta	Ŧ	15,00			Г	0,70280	0,73028	
5	- S1	🗕 Theta	Ŧ	30,00	V		Г	-0,69504	-0,66553	
6	- S2	🗕 Theta	-	30,00	V		Г	0,72044	0,74616	
7	- S1	🗕 Theta	•	45,00		V	Г	-0,70003	-0,66849	
8	- S2	🗕 Theta	•	45,00		×	Г	0,71435	0,74495	
9	- S1	✓ Theta	•	60,00		V		-0,72928	-0,69720	
10	- S2	✓ Theta	•	60,00			Г	0,68479	0,71777	
11	- S1	✓ Theta	Ŧ	75,00			Г	-0,77547	-0,73684	
12	- S2	🗕 Theta	Ŧ	75,00	V		Г	0,63193	0,67385	
13	- S1	🗕 Theta	-	90,00				-0,81694	-0,78306	
14	- S2	🗕 Theta	•	90,00		V		0,57595	0,61968	
15	- S1	🗕 Theta	•	105,00		>		-0,84366	-0,81339	
16	- S2	✓ Theta	•	105,00				0,53360	0,58068	
17	- S1	✓ Theta	•	120,00				-0,85067	-0,82167	-
18	- S2	 Theta 	•	120,00	V	~		0,52179	0,56436	₹ ⊻
19	R1	The second		405.00				.0.8/016	.0.81075	≚
		200.000		4- 0.40.000				_		
Currento	-Axis: from	300,289		to 840,298						
Т	ri <u>m</u> from	300,289		to 840,298	3		eac	h 1	Average	
										
			2	<u>D</u> K	<u> </u>	ancel				

Fig. 8-112 Header-tab of the measured data

The angle of incidence is shown in the tab "Title".

Data view					
Graph Tat	ole Ti	tle H <u>e</u> ader Sp	pecial Values Other Values		
Measureme					
Name:	Sample	rotation 0.00 36	0.00 [15.00] deg at angle = 70.00 c	leg / Th 03/25/2010 at 15:13:02	
User:			Date:	Time:	
Comment:		SE 850 (280.000 i Settings:	nm 2300.000 nm)	*	
	Wavele	ngth range [nm]: 3	300 840	~	
Measureme	ent enviro	onment			
Wavelengt	th:	0,0 nm	Process time:	0,0 s	
Angle of in	cidence:	70,00 *	Temperature:	0.6E-1 °C	
Polarizer p	osition:	45,000	Weight	1,0000	
			Sample rotation (theta):	360,00 *	
Change x-a	xis				
No. of poin	ts:	892	X-axis by points:	Yes	
			Make x-axis by points	Remove x-axis by points	
New range	of x-axis	300,289	840,298	Recalibrate x-axis	
				Flip x-axis direction	
<u></u>			<u>OK</u> <u>Cancel</u>		<u> </u>

Fig. 8-113 The "Title" tab shows the angle of incidence

SENTECH SpectraRay/4

The Tab "Graph" section shows all measurements:

010 Data view	
Graph Table Title Header Special Values Other Values	
0.5-	Smooth and derive Polynom order: 2 Width [points]: 30 Smooth data Derive data
0.0-	Erase spikes Threshold (y-value): 40 000000 Erase Spikes Beplace data permanent
0.5- 400 500 600 700 800	X-regions Apply x-regions Add sejected region Clear all x-regions
400 S00 700 S00	Edit x-regions >>>
QK Qancel	

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 CaCO₃ 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.

945 Data view	
Graph Table Title Header Special Values Other Values	
x-Axis: Wavelength Use <u>a</u> ll Use <u>n</u> one	
Color y-Axis z-Axis z-Value Use View Mod. Minimum Maximum	
1 S1 ▼ Theta ▼ 0.00 ▼ ▼ 0.74342 -0.71444	-
2 S2	× 4
3 S1 ▼ Theta ▼ 15.00 ▼ ▼ □ -0.71135 -0.68468	
4 S2 ▼ Theta ▼ 15,00 ▼ ▼ □ 0,70280 0,73028	
5 S1 ▼ Theta ▼ 30,00 ▼ ▼ □ -0,69504 -0,66553	
6 S2 ▼ Theta ▼ 30,00 🗹 🗹 🗂 0,72044 0,74616	
7 S1 - Theta - 45,00 - S - 0,66849	
8 S2 • Theta • 45,00 🗹 🔽 🔲 0,71435 0,74495	
9 S1 • Theta • 60,00 🗹 🔽 -0,72928 -0,69720	
10 S2 • Theta • 60,00 🗹 🔽 🔲 0,68479 0,71777	
11 S1 🔻 Theta 💌 75,00 🗭 🗭 🗂 -0,77547 -0,73684	
12 S2 - Theta - 75,00 - O.63193 0.67385	
13 S1 🗸 Theta 🗸 90,00 🔽 🔽 -0,81694 -0,78306	
14 S2 • Theta • 90,00 🔽 🔽 0,57595 0,61968	
15 S1 • Theta • 105,00 🗹 🗹 🗔 -0,84366 -0,81339	
16 S2 • Theta • 105,00 🗹 🔽 🗌 0,53360 0,58066	
17 S1 • Theta • 120,00 🗹 🗹 -0,85067 -0,82167	-
18 S2 ▼ Theta ▼ 120,00 ▼ ▼ □ 0,52179 0,56436	¥ X
19	•
Current x-Axis: from 300,289 to 840,298	
Trim from 632,800 to 632,800 each 1 🛛 🖉 Average	
QK Cancel	

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.

No.	Wavel.[nm]	S1	S2	S1	S2	S1	S2
		THETA:0,0000	THETA:0,0000	THETA:15,0000	THETA:15,0000	THETA:30,0000	THETA:30,000
548	628,580	-0,72538	0,68652	-0,69550	0,72041	-0,67569	0,73657
549	629,196	-0,72605	0,68839	-0,69220	0,71840	-0,67620	0,73617
550	629,812	-0,72363	0,68906	-0,69343	0,72175	-0,67229	0,73891
551	630,428	-0,72457	0,68887	-0,69365	0,72103	-0,67573	0,73709
552	631,044	-0,72551	0,69094	-0,69258	0,72181	-0,67321	0,73730
553	631,660	-0,72551	0,69222	-0,69395	0,72360	-0,67252	0,73913
554	632 276	-0 72327	0.69161	-0.69035	0 72331	-0.67305	0 73967
555	632,892	-0,72313	0,68834	-0,69177	0,72278	-0,67290	0,73901
556	633,508	-0,72129	0,69111	-0,68916	0,72198	-0,67499	U,74143
557	634,123	-0,72418	0,68841	-0,69316	0,72322	-0,67274	0,73716
558	634,739	-0,72441	0,69126	-0,69196	0,72168	-0,67521	0,73840
559	635,355	-0,72376	0,68957	-0,69173	0,72228	-0,67429	0,73889
560	635,971	-0,72379	0,68951	-0,69205	0,72089	-0,67310	0,73737
561	636,587	-0,72207	0,68872	-0,69037	0,72244	-0,67290	0,73866
562	637,203	-0,72482	0,68989	-0,69163	0,71964	-0,67370	0,73770
563	637,819	-0,72207	0,68955	-0,69111	0,72337	-0,67311	0,74058
564	638,435	-0,72343	0,69146	-0,69127	0,72355	-0,67123	0,74024
565	639,051	-0,72435	0,68868	-0,69323	0,72074	-0,67459	0,73697
566	639,667	-0,72402	0,68976	-0,69230	0,72156	-0,67226	0,73674
567	640,283	-0,72268	0,69172	-0,68751	0,72071	-0,67171	0,73944
568	640,898	-0,72358	0,68995	-0,69229	0,72287	-0,67471	0,74012
569	641,514	-0,72416	0,69051	-0,69007	0,72076	-0,67245	0,73561
570 571	642,130 642,746	-0,72273 -0,72369	0,68920 0,68888	-0,69061 -0,69333	0,72014 0,72074	-0,67341 -0,67372	0,73983 0,73753
	m		1	1			•
				ancel			

Fig. 8-116 Wavelength closest to the selected value

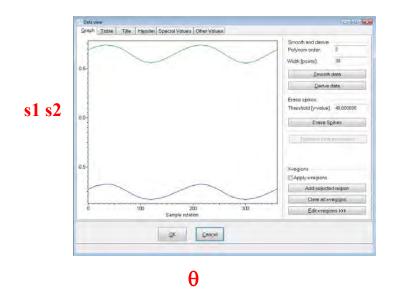
When "Trim" is pressed a new dataset is created containing s1, s2 at 632.9 nm as a function of the rotation angle θ indicated by "Swap" in the name of the dataset.

I	Data	≥€
	Sample rotation 0.00 360.00 [15.00] deg at angle = 70.00 deg / Th 03/25/2010 at 15:13:02	
	Trim: Swap: Sample rotation 0.00 360.00 [15.00] deg at angle = 70.00 deg / Th 03/25/2010 at 15:13:02	
	I construction of the second se	

The units were changed now. The x-axis is changed to "theta" and the "z-axis" becomes the wavelength in nm.

Data view Graph Table Tple Hgader Special Values Other Values	- • •
Glabu Taple Line Line Special values Other values	
x-Axis: Theta - Use gli Use none	
Color y-Axis z-Axis z-Value Use View/Mod Minimum Maximum 1 S1 ▼ Wavelength ▼ 632,3 ▼ □ -0,62934 -0,67305 2 S2 ▼ Wavelength ▼ 632,3 ▼ □ 0,55690 0,73967	
1	K (a)
Currentx-Axis: from 0,000 to 360,000	
Trim from 0.000 to 360.000 each 1 VAverage	
QK Qancel	

Fig. 8-117 New axis for the trimmed data



These measurements are now performed between $\varphi=50^{\circ}$ and 70° (steps: 5°) angle of incidence.

Data	₩.
Sample rotation 0.00 360.00 [15.00] deg at angle = 70.00 deg / Th 03/25/2010 at 15:13:02	
Trim: Swap: Sample rotation 0.00 360.00 [15.00] deg at angle = 70.00 deg / Th 03/25/2010 at 15:13:02	
Sample rotation 0.00 360.00 [15.00] deg at angle = 65.00 deg / Th 03/25/2010 at 15:20:45	
Trim: Swap: Sample rotation 0.00 360.00 [15.00] deg at angle = 65.00 deg / Th 03/25/2010 at 15:20:45	
Sample rotation 0.00 360.00 [15.00] deg at angle = 60.00 deg / Th 03/25/2010 at 15:29:04	
Trim: Swap: Sample rotation 0.00 360.00 [15.00] deg at angle = 60.00 deg / Th 03/25/2010 at 15:29:04	
Sample rotation 0.00 360.00 [15.00] deg at angle = 50.00 deg / Mo 03/29/2010 at 10:14:23	
Trim: Swap: Sample rotation 0.00 360.00 [15.00] deg at angle = 50.00 deg / Mo 03/29/2010 at 10:14:23	
Sample rotation 0.00 360.00 [15.00] deg at angle = 55.00 deg / Mo 03/29/2010 at 10:20:55	
Trim: Swap: Sample rotation 0.00 360.00 [15.00] deg at angle = 55.00 deg / Mo 03/29/2010 at 10:20:55	

The spectra are shown in the following plot.

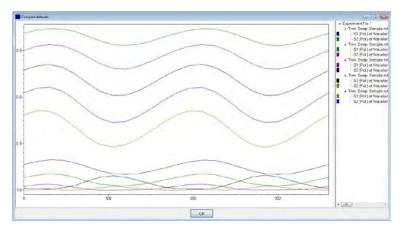


Fig. 8-118 (s1, s2) in dependence of θ for different angles of incidence

Modeling of CaCO₃:

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):

tle Air	\checkmark	Thick	ness	State		.aye K la	er Type yer		Info n=1,	[633,1 0000	0 r
, .	CaCO3	Fig. 8-119-8	3-120	Moc				ropic la	n=1,!	5949	
- Dispersion - Bi	avial anisotropic lay									- 0	
Lavername: C					Name	Fit	Value	Scroll valu	e M	mmum	1.
naver name. C	10000				Alpha [*]	9	91.02	* III		-369,00	
		Anisotropy option is available			Beta [*]	m	0,00	9. 11	+	-360,00	
Discontinues	na 7 (Example)	a sufficient of a support of the support	unin mater	1	Gamma [*]	0	0,00	3 💷		-360,00	
	ang 2 (E-vector i	s z-direction perpendicular to sar			N0		1,650	* HI	,	-100,001	F
CeCO3.o			Edi	tZ	N1		0,0	· Gi	1	0,0	
Alpha 12	91.02	From moterials .	Fromb		N2	1	0,0		-	-40000,0	
		From morenais .	From k	aheis -	K1 K1	H	0,000	A 11		100,000	
		of Alpha and Theta	10		KI K2	H	0,000			0006,000	
					ND	7	1,485	4 11		/100,001	8
Dispersion all	ang Y (E-vector i	n sample surface and parallel to	plane of in	cidence)	NI	i÷.	0,0	411	2	0.0	10
CatCO3 e			Edi	N 1	N2	i-i	0.0	1 1-1		-40006.0	
			La	() J	RD	H	0.000	1		-100,000	
Eeta [']	0.00	From materials _	Fromle	syers_	KI		0,000	*	_	0000,0000	
					K2	m	0,000	1 1.5		0000,000	
Dispersion ald	beg X (E-vector in	sample suitace and normal to p	lane of inc	idence):	NU	P	1,650			100.001	
CaCO3 a			Ed	dX_	N1	m	0,0	×10.		0.0	
	0.00		And a second		N2		0,0	 inf 		40000,0	
Gamma [']	.0.00	From materials	From	layer_	KD	10	0,000	A. 11	+	-100,000	1
					K1	101	0,000	·	1 .4	000,000	
	ample rotation T				K2	1	0.000		1 -4	0000,0000	E
Comment	600 m. Vin Vik ⊡ ets Copy eps d	Wavelength[nm]	00 Solution h	-							
	- Company		OK								

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 CaCO₃ 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°.

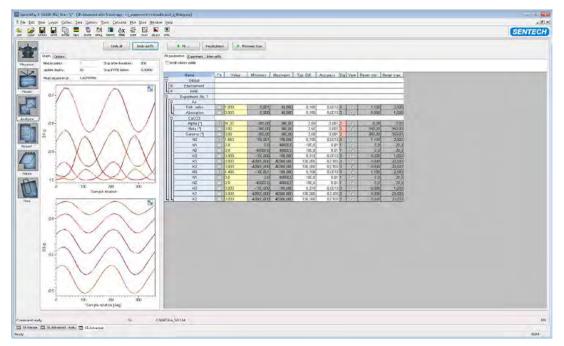


Fig. 8-123 Fit results

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.

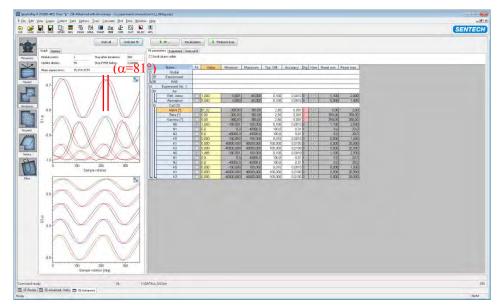
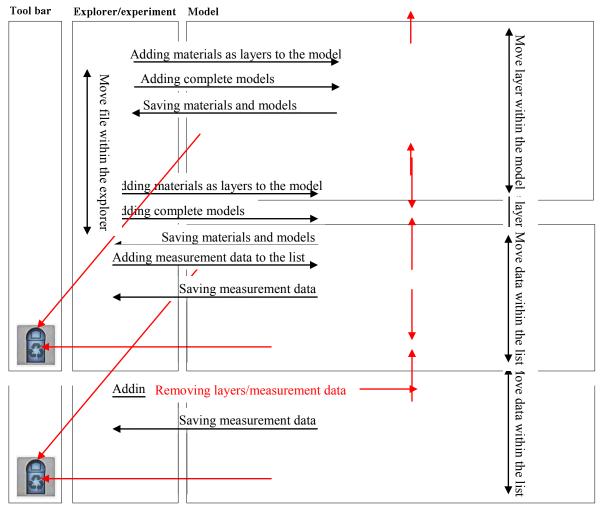


Fig. 8-124 Results for a wrong rotation angle

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:



Removing layers/measurement data _____

Appendix B: Icon reference

Layer types:

Afromovitz III-V layer H Biaxial anisotropic layer ²³ Cauchy layer Effective medium and index gradient layer y(x) 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 N Silicon epitaxial layer Tanguy III-V layer ¹Uniaxial anisotropic layer

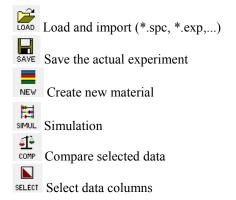
Icon bar functions:

Image: Directories for materials and dataImage: Directories for materials and export (*exp, *.csv,...)Image: Directories

Data selections:

all columns selected no column selected

AGA	AlxGa(1-x)As layer
	Brendel oscillator layer
<u>.</u>	Drude-Lorentz oscillator layer
	File layer
FB	Forouhi-Bloomer layer
Ô	Homogeneous growing layer
16AP 10P	In(1-x)GaxAsyP(1-y)on InP layer
IGA	InxGa(1-x)As layer
Ser	Ito Sernelius layer
nk	NK layer
	Parametric file (2D) layer
1	Polynomial layer
Sel	Sellmeier transparent layer
	Spectral combination layer
⊠	Tauc-Lorentz layer





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	····, ···/0'
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 From materials ... 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

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 From layers ... 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 " μ m". 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 curves (PLOT) and smoothed curves Theory=000000FF Grayed=00C0C0C0 disabled x-regions Fit=0000080 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=0000080 Curve8=0000FF00 Curve9=00FF00FF Curve10=00808080 Curve11=00808000 Curve12=00800000 Curve13=00008000 Curve14=00800080 Curve15=0000000 . . . 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 curve area background grcntl CurveBk=gray axis background grcntl AxisBk=lightgray color of scale grcntl Scale=black 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=0000080 k - curves in layer editors Ed E1=00FF0000 ε_1 - curves in layer editors Ed E2=000000FF ε_2 - 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 lay-
	er in the model and the layer below
Ctrl+R	Create an roughness layer between the selected lay-
	er 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 (cop-
	ied 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
CCIIIDIagging	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
e	directory where you dropped the file in the explor-
	er

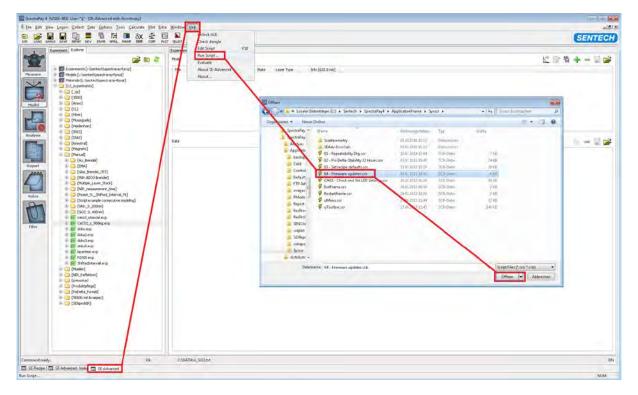
Appendix I: Firmware Updater

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).



art Stop	IPAddr:	192,168,90,24	6	Update Firm	iware	ļs	<u>p</u> s <u>s</u>	alliserv	Ctrl-C
elliser									
lliServ/	Linux V	ersion 3.	89-1 for 1	ADNP/1520,	build Mar 16	5 2012 12	:13:16,	optimized	1

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)

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SENTECH

- 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:

Entries:					
ID: Pa	th:			Absolute position:	
Text:					
Description:					
Userlevel:		-	State:	<u>E</u> dit	
	New	Delete	Cancel	ОК	

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 prede-fined 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"

SENTECH

E Custom N Entries:			n menu ent	ries			
	L Path:	2				Absolute position: -1	
					re implemen State: 0 Cancel	ted by script)	

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.

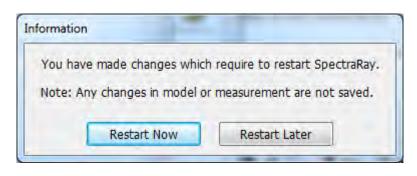
	Editor - Vers	-	-		-	-	-	-		-	-	_		-	-	-
	autoexec *			()	14	R 16	₩ B	un	⊒ Debug	Pros	funç	& <u>N</u>	E	-	€.	1
1	FRAMEWOF	K.Cust	OMGUIC	all 20	1: //	Edit/	Custom	men	u editor						-	
2	RunScr	ipt "c	:\\Sen	tech\S	pectr	aray3\1	Applica	atio	nFrame\S	ysScr\	ume	nu.	scr"			
3	exit															
3 4	exit															
	exit															
	exit															
	exit															
	exit															
	exit															
	exit															

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 appears¹⁵:

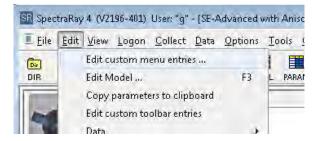
¹⁵ For setups newer than 102, this is no longer necessary and no message appears.



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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:

Custom Menu Entries	X
Entries:	
[201] Edit \ Edit custom menu [202] File \ Exit	entries
(D: 202 Path: File	Absolute position: 0
Text: Exit	
Description: Exit	
Userlevel:	State: 0 Edit
New	Delete Cancel OK

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:

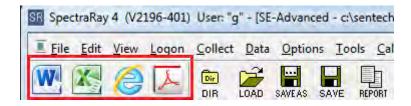
The script editor also allows to drop files on its window. When you drag a file from the Windows Explorer onto the editor the following happens for each file in the drop:

- 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 ..."
 - o 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)

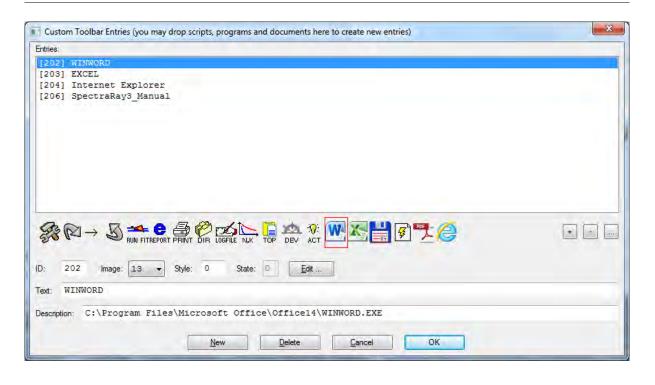
The best method is to add the editor to the menu in a first step. Please fill out the window as shown below (or just drag the file "uToolbar.scr" from within the windows explorer and drop it onto the menu editor). Close the editor, allow a restart and use the "Edit" menu to open the toolbar editor.

ntries:	
[200] Edit \ Edit custom menu entries [201] File \ Exit	
[205] Edit \ Edit custom toolbar entries	
205 Path: Edit	Absolute position: -1
	Absolute position: -1
d: Edit custom toolbar entries	Absolute position: -1
205 Path: Edit xt: Edit custom toolbar entries scription: Edit custom toolbar entries erlevel: Stat	

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).

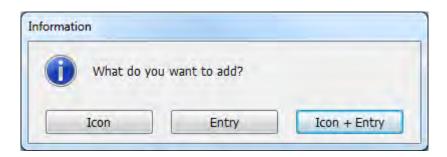
Support for Drag and Drop:

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").