SENTECH Erfolg durch Leistung

SpectraRay II and Application Tutorial

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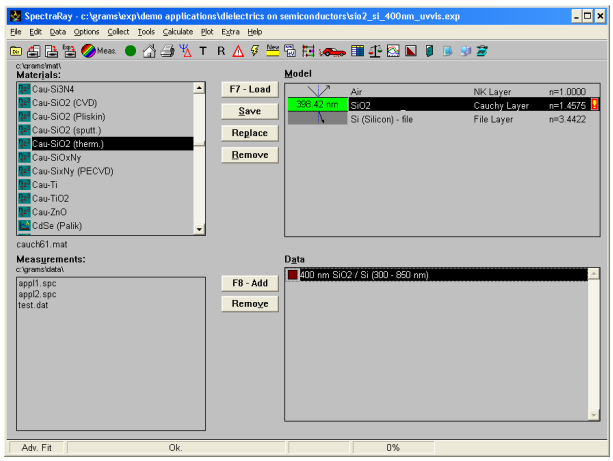
Version: 1.29

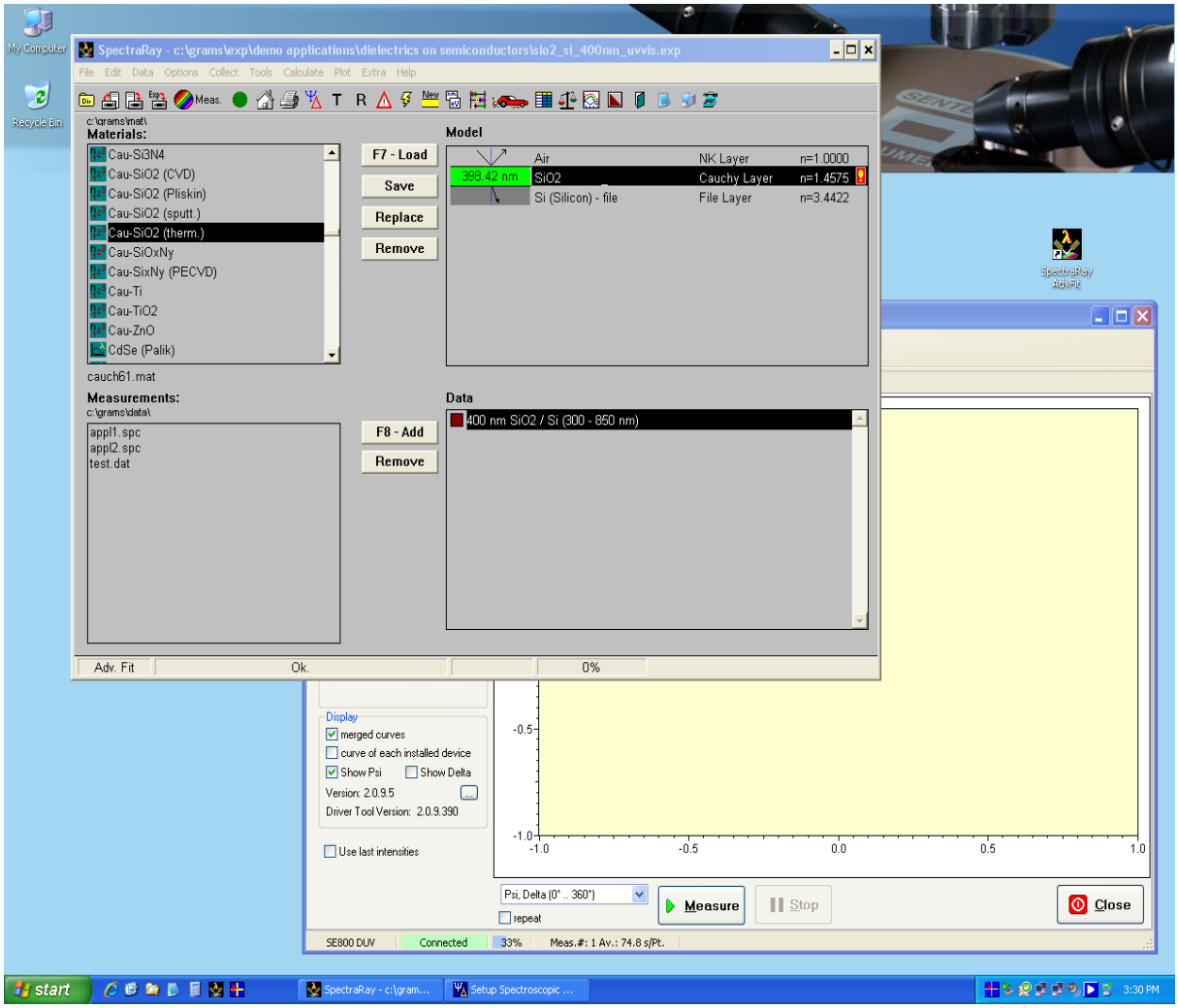


Content

1. Basic operation SpectraRay II software

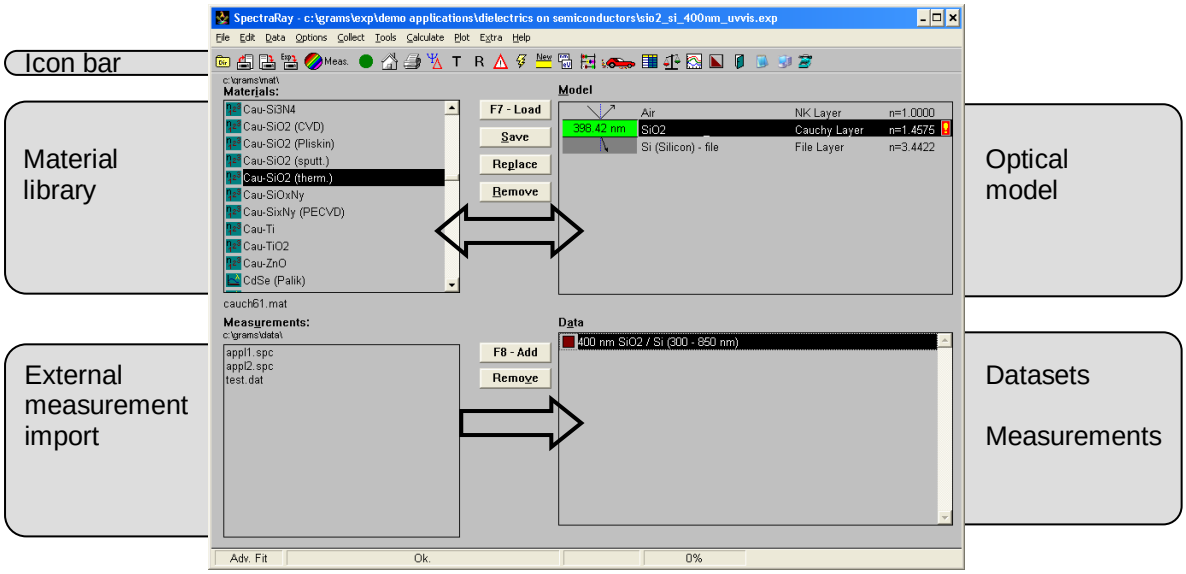
1.1. Starting the SpectraRay II software

The SpectraRay II software is started by double clicking the SpectraRay II icon on the desktop. Simultaneously the device drive software is started automatically. This software is necessary to operate the ellipsometer hardware. It shouldn't be closed. It will be reopened automatically, but some error messages will appear. Just press "OK" and proceed.



1.2. SpectraRay II Main Window at a glance

The SpectraRay II main window consists of the menu bar, icon bar and four sub-windows.



Icon bar:

The most important functions of SpectraRay II are represented in the icon bar for fast access like the measurement window 

, fitting window  or environmental parameters settings 

Sub-windows:

Materials:

It contains a comprehensive library of material dispersion. They can be moved by drag & drop to the Model sub-window to build the optical model. The material library can be extended with new material dispersions. The icon in front of the material name indicates the type of dispersion relation.

Model:

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.

Data:

Here all measured spectra are stored. Also data which are deduced from the existing model are stored in this window. Datasets can be exported e.g. to ASCII files. The box in front of the name of the dataset defines, whether the dataset is active (red) (used for the fitting procedure) or not (grey).

Measurements:

This window allows a fast import of external measurements (from other reflectometer or transmission tools)

1.3. Five basic steps of operation

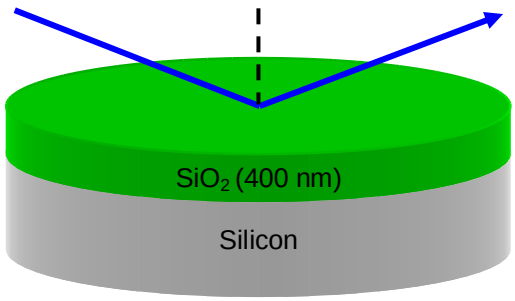
The sample measurement and analysis can be summarized in five basic steps of operation:

Five steps of SpectraRay 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 sample measurement and analysis will be discussed in the following chapters.

The following standard sample will be used as example:



1.3.1 Sample alignment

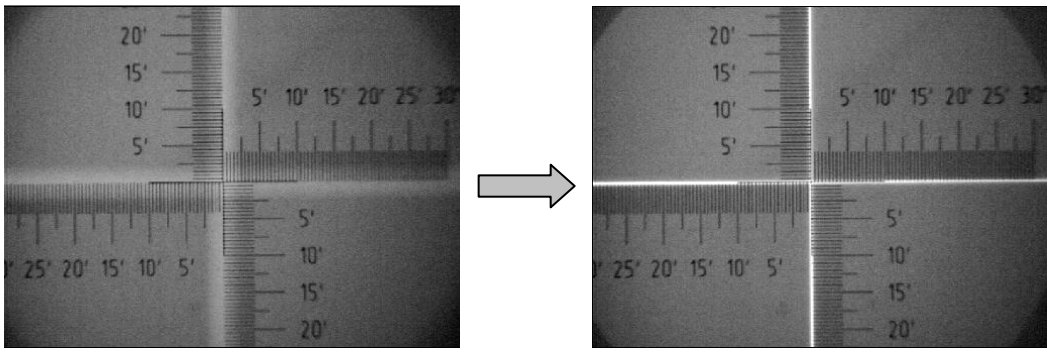
The Auto collimating telescope (ACT) in combination with the objective lens is used for the alignment.

The accurate alignment of the sample height and tilt are necessary to obtain the correct angle of incidence and PSI, DELTA spectra.

Alignment of ideal samples (perfectly flat and specular)

Step a) Height alignment

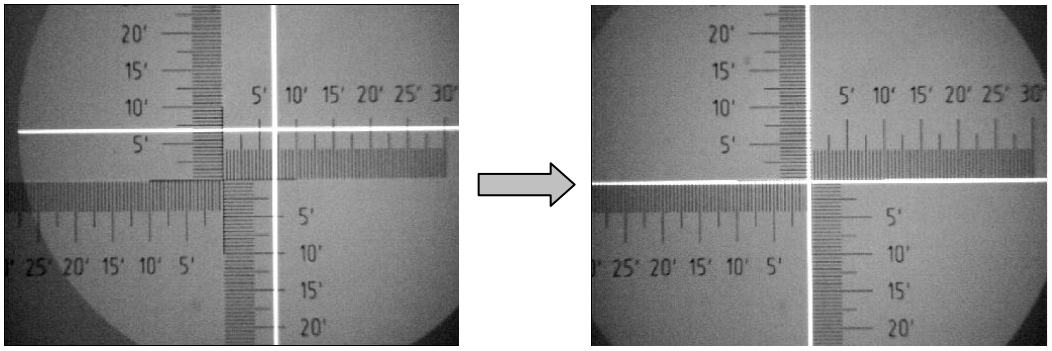
Move objective lens into "**sample height**" position
Use height alignment screw to focus the white cross



Wrong height (cross defocused) *Correct height (cross focussed)*

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).

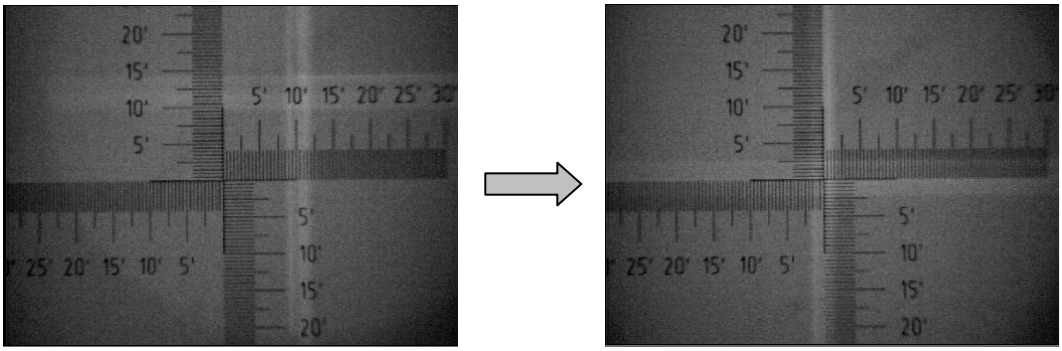
Alignment of non-ideal samples

- 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) 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) Move objective lens out to "**dark tilt**" position
Use the two tilt screws to align the tilt by aligning the white blurred cross to the crosshairs



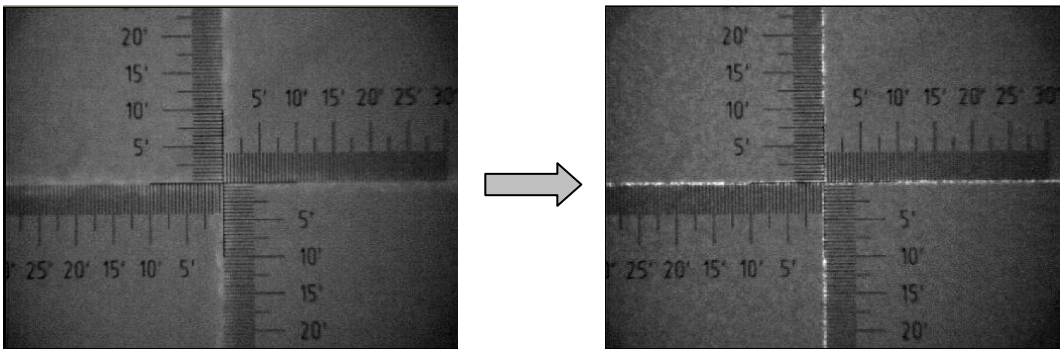
Wrong tilt (cross not on crosshairs) *Correct tilt (cross on crosshairs)*

- Alignment of non-ideal samples, not specular

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

Step a) 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) 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 focussed)*

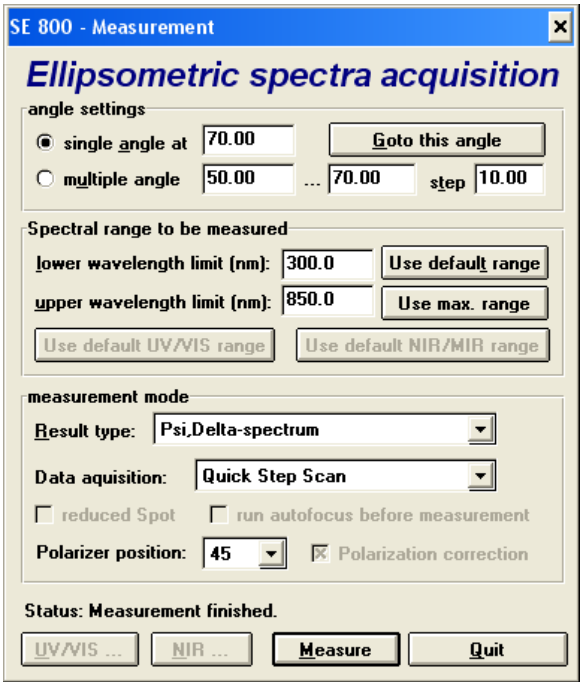
1.3.2 Ellipsometric measurement

Performing the measurement

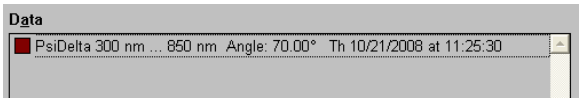
Press the "Measure" icon 

to open the "measurement window"
Select the standard settings as shown in the window below.
Press the "Measure" button

The measurement is performed now. The movements of "Analyzer", "Polarizer", "Shutter" and "Compensator" can be heard.
When the measurement is finished, leave the window with "Quit"



The measurement is saved into the "Data" section of SPECTRARAY.

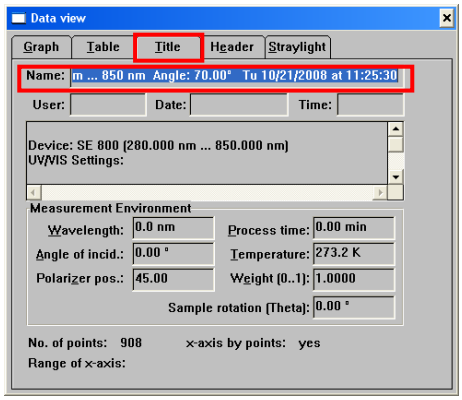


The measurement name contains the information about the spectrum type, spectral range, angle of incidence, date and time.

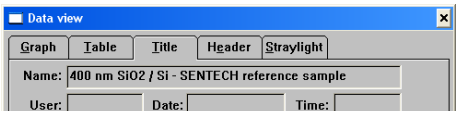
Renaming the measurement

Rename the measurement by using an informative name which describes the sample well:
Double click the measurement dataset and go to the "Title" tab.
Enter the name in the "Name:" section.

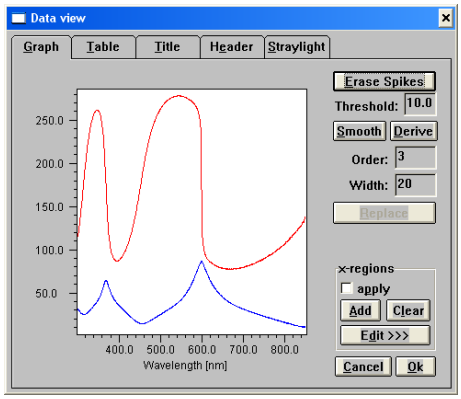
Standard name:



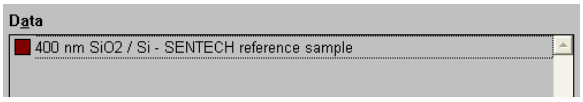
New name:



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



The new measurement name is shown in the "Data" section of SPECTRARAY.



1.3.3 Modeling

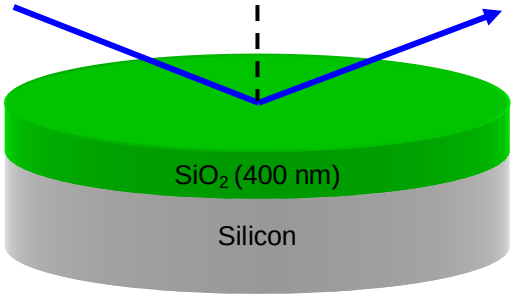
The optical model describes the optical and metrical properties of the sample. It consists of the substrate and the ambient (mostly air) and the layers inbetween. The dispersion of the optical constants n and k of ambient, layers and substrate is described by dispersion formulas. For different kinds of materials different kinds of dispersion formulas exist.

Creating a model

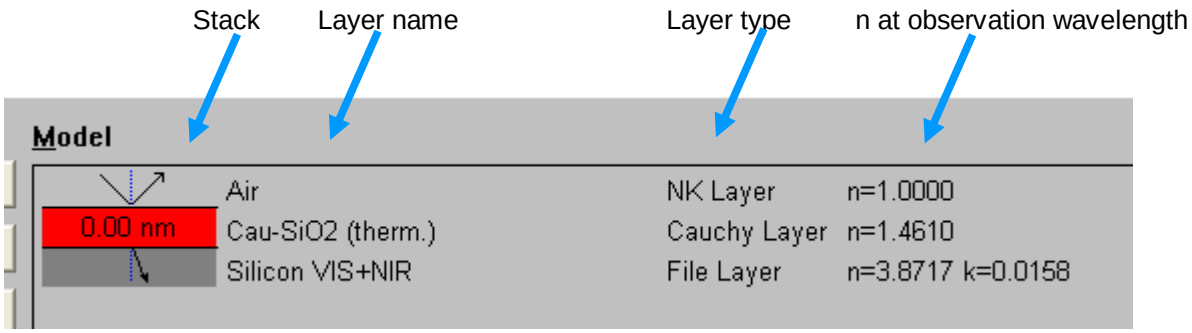
The optical model is now built by selecting the materials from the material library. In the following example the N,K fixed layer type is used to describe the ambient air, the Cauchy dispersion is used to describe the SiO_2 layer and the File layer type is used to describe the silicon substrate.

They are moved by drag and drop from the "Materials:" window to the "Model:" window.
If the resulting order of the layers isn't correct it can be changed easily by moving the materials by using the mouse.

A model for the standard sample is created:

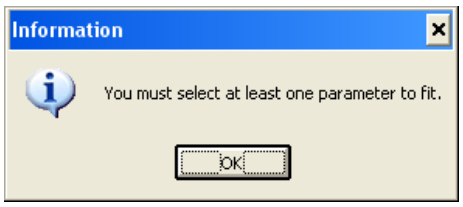


It will appear as follows in the Model section of SPECTRARAY:



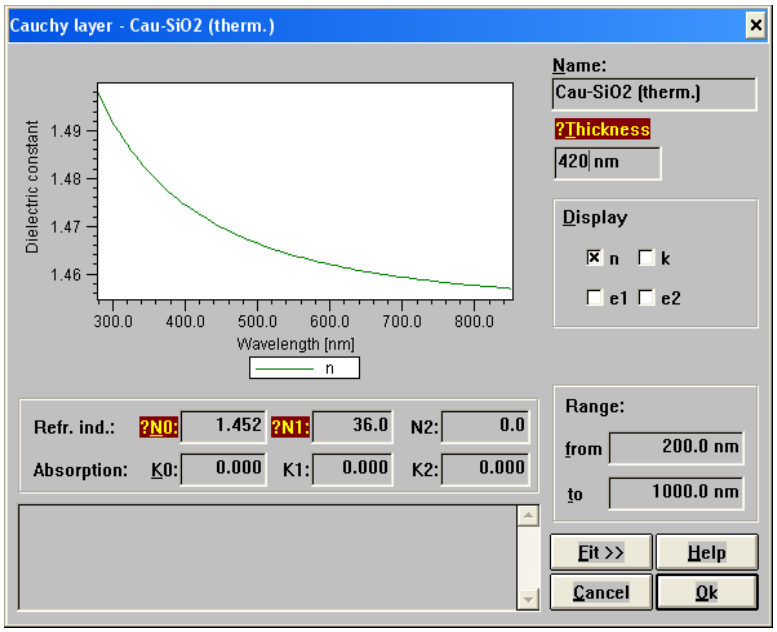
Now the fitting parameters must be selected.

If no fitting parameters are selected, the fitting window can't be opened, an error is shown:



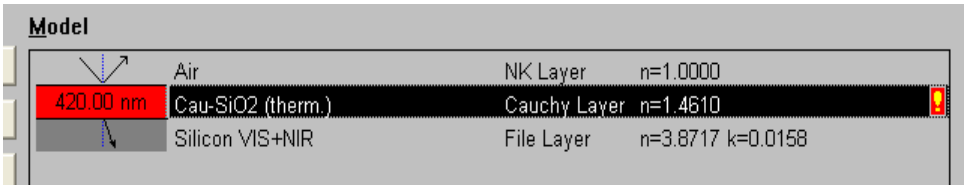
Selecting fit parameters

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.
The name of each parameter can be clicked once, then it gets highlighted (? yellow / red) which indicates that they are selected for fitting.
The film thickness is also selected for fitting.
If the approximate film thickness is known, it should be entered at "Thickness" (here: 420 nm)



The window can be closed now using "OK"

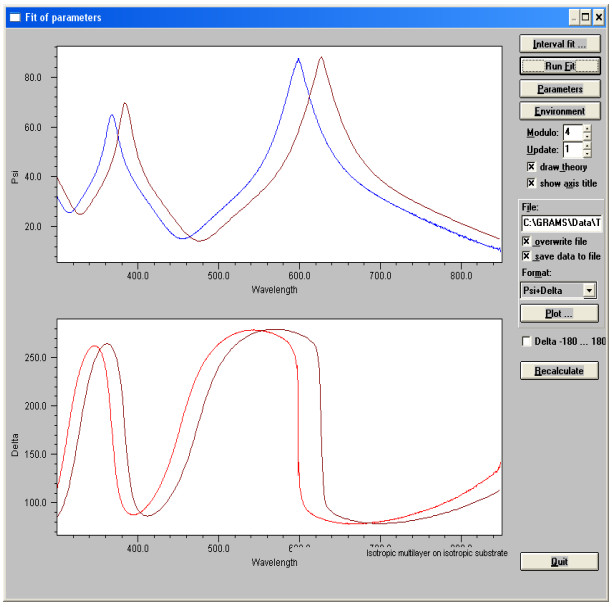
The model has changed its appearance:
The film thickness is 420 nm, the "!" at the end of the line indicates that fitting parameters are selected in this layer.



1.3.4 Fitting

The fitting window is opened by pressing the fitting button: 

The "fitting" window is opened:



Two graphs are shown in the “Fit of parameter” window. One for PSI, the other one for DELTA versus wavelength. Each screen contains two graphs. One represents the measurement the other one represents the modeled spectrum. Here the measured PSI, DELTA are displayed in blue and red colors, while the modeled PSI, DELTA spectra are displayed both in dark red color.

The "Modulo" value is used to increase the fitting speed.
Modulo = 1: every single point is used for fitting; slow but most exact.
Modulo = 4: every 4th point is used; faster but some points are skipped.

Use Modulo = 4 in general.

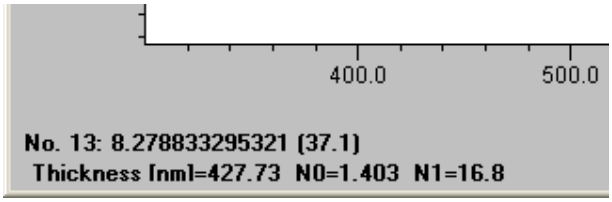
Rule of thumb: the more or the sharper structures in the PSI, DLETA spectra appear, the lower the modulo value should be to avoid loosing information.

The "Run Fit" icon is pressed to initialize the fitting procedure.

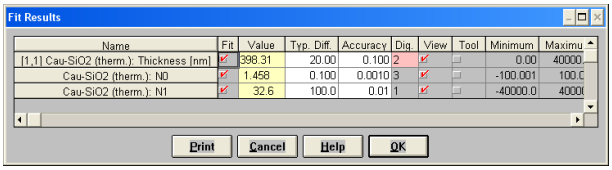
The software is now modifying the values of the selected fitting parameters thickness, N0, N1 in order to minimize the deviation between measurement and optical model. The goal is to achieve a perfect overlay of the measured and modeled spectra.

The deviation between the measured and modeled spectra is expressed in the MSE value. (MSE: Mean square error)

During the fit procedure the actual "iteration step" (No.), the MSE value and the fitting parameters are displayed in the lower left corner.



When the fitting procedure stops the results window is shown:



It can be closed with “OK” to return to the fitting screen:
Press "Recalculate" icon the see the MSE value again.

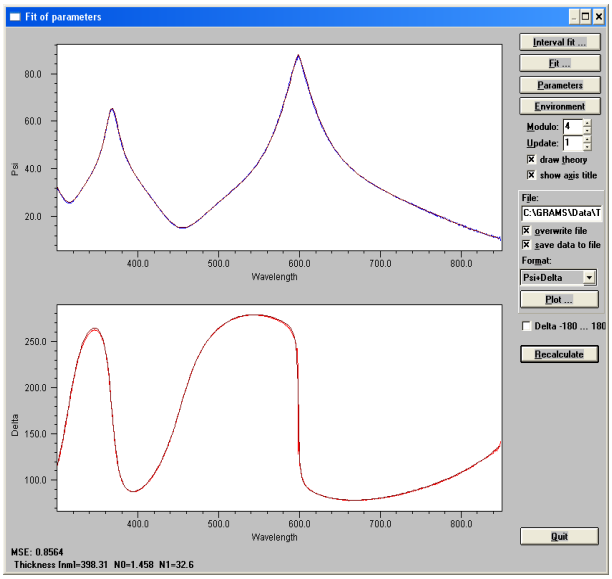


Figure: Each measurement and model appear as one spectrum

Now a decision is necessary:
Fit quality is good → ready → proceed with "Reporting"
Fit quality is below expectations → not ready → the optical model must be improved

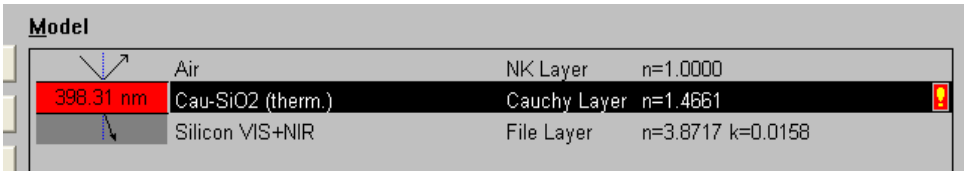
Here the actual fit is perfect. That means the mathematical equations of the optical model now exactly describes the measurement. We can proceed with "Reporting".

Leave the fitting window with "Quit" to return to the main window of SpectraRay II.

1.3.5 Reporting

No reporting

Without any reporting the main information of the fitted optical model can be read out from the Model window:
The optical model is updated with results from the fitting procedure.



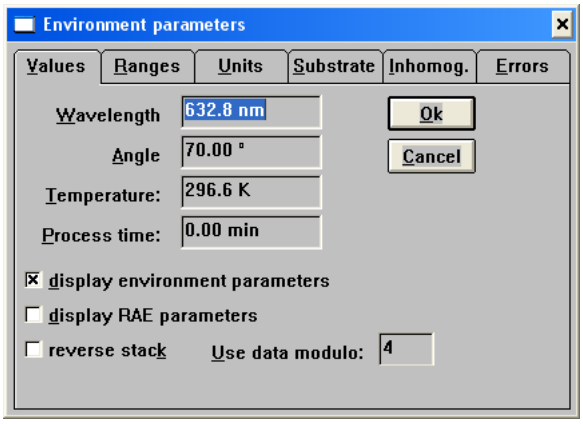
The correct film thickness and the refractive index n at the observation wavelength are displayed.
Because of the dispersion of the refractive index n it differs in every wavelength.

How to change the observation wavelength?

The observation wavelength is defined in the “Environmental parameters”:

Press the following icon: 

Select the Tab “Values”:
Enter e.g. 632.8 nm at “Wavelength”
Leave this window.

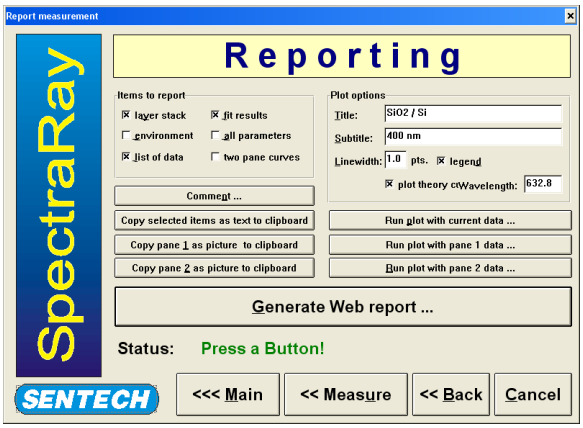


Measurement report

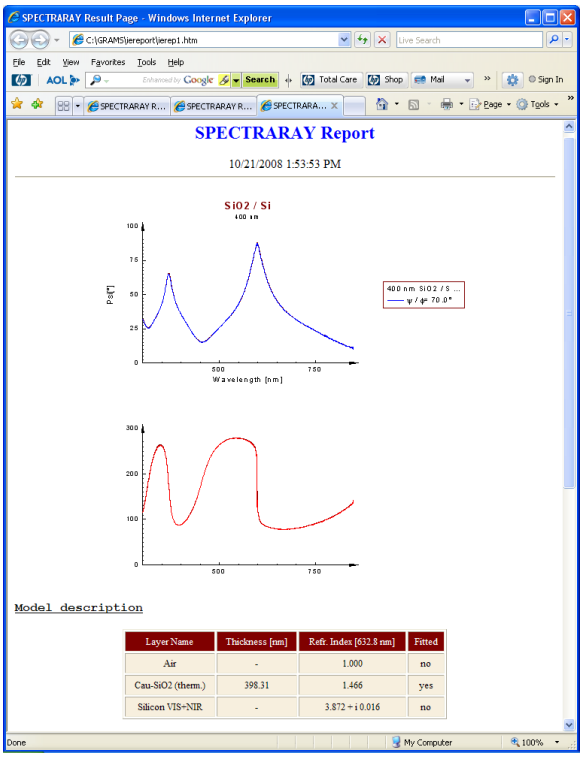
An automatic report can be created and displayed as html document in the Internet explorer.

Press the “printer” icon to open the “Report measurement”  window.

Enter the “Title” and “subtitle” in the “Reporting” window.
Switch on “legend” to show the legend in the plot
Switch on “plot theory” to show the modelled spectra.
Press “Generate Web Report”

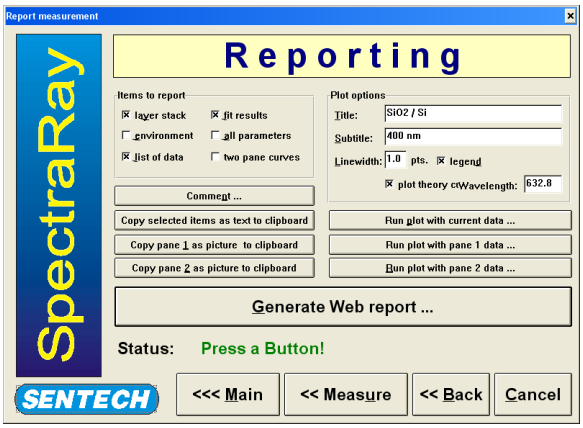


The web report is created now automatically and can be printed:

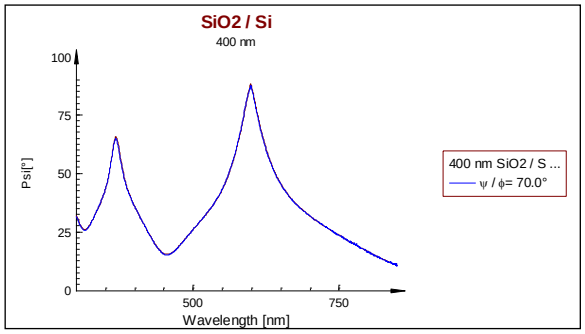


Creating a manual report

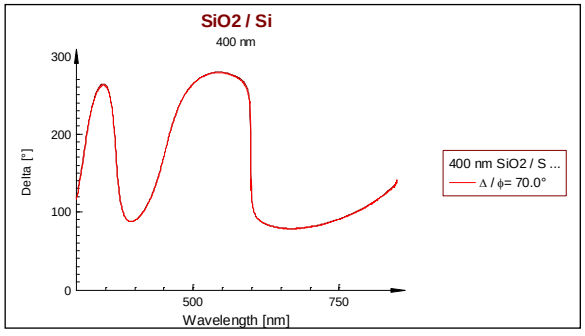
Using the “Measurement report window” the graphs and results can be exported to the clipboard.



Press **“Copy pane 1 as picture to clipboard”** copies the PSI spectra to clipboard:
CONTROL + V insert the graph into another application like WORD:



Press **“Copy pane 2 as picture to clipboard”** copies the DELTA spectra to clipboard:



Using the “Simulation” for reporting

The “Simulation” is used to calculate data on the basis of the actual optical model.
In this example the dispersion of n of the “Cau-SiO_2 (therm.)” layer versus wavelength will be calculated.

The “Simulation” is started by pressing the icon: 

The “Curve parameter” is the x-axis → Select “[0] wavelength [nm]”

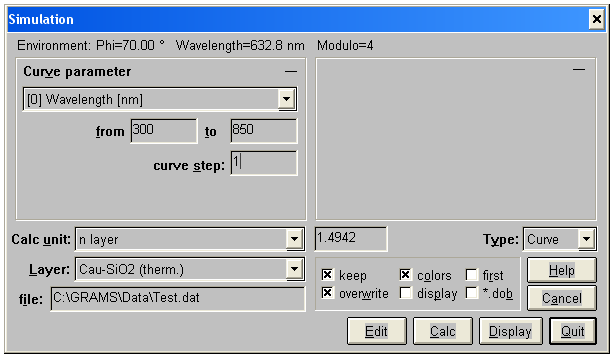
Set the wavelength range:
from: 300
to: 850
step: 1

The “Calc unit” is the y-axis → Select “n layer”

Select the “Layer”: Cauchy-SiO2 (therm.)

Switch on “keep”. This will create a new dataset in the “Data” window.

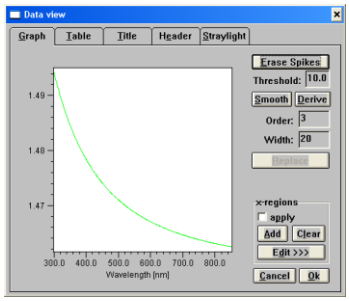
Press “Calc”. The data is now calculated and saved into the “Data” window.



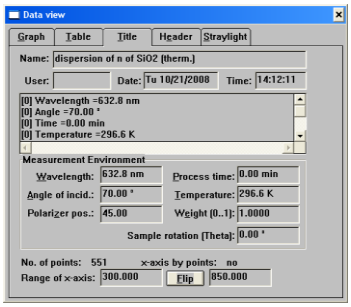
Leave the “Simulation” window with ”Quit” to return to SPECTRARAY.

The new dataset of the dispersion of n of “Cau-SiO2 (therm.)”:

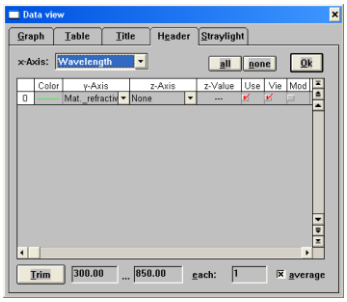
Graph:



Title:

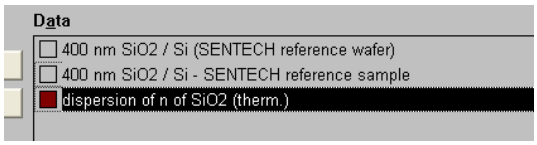


Header:

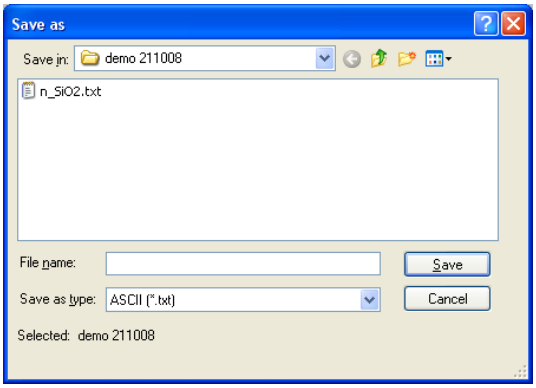


Exporting the dispersion data to an ASCII file:

The dataset is selected by a single mouse-click: it appears inverted.

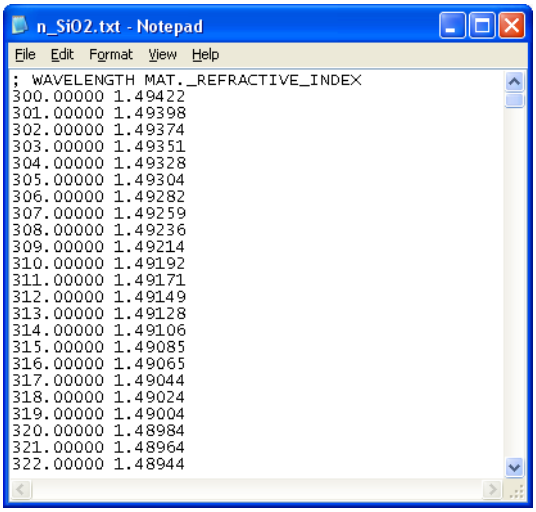


Select from the menu: "File" → "Save as … "



Select "ASCII (.txt)" as file type, the directory (free of choice) and filename (free of choice)

The file is now saved as an ASCII file which can be imported to other programs like EXCEL™ or Origin™.



2. Explanation of important SPECTRARAY features

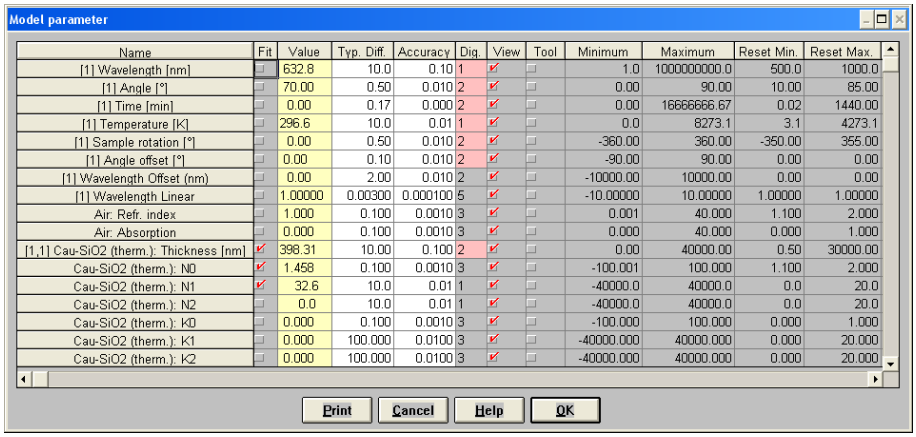
2.1. Parameter list

The parameters list allows the direct access to all fitting parameters of all layers in the stack and environmental parameters.

It allows selecting or deselecting fitting parameters, change their actual values and influence the fitting behavior.

There are two ways to open the parameter list.

1. from the icon bar: 
2. From the fitting window: “Parameter” button



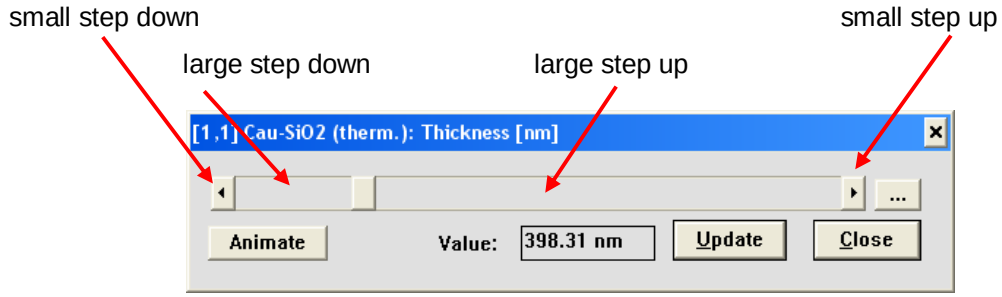
Columns	Explanation
Name	shows the fitting parameter name
Fit	indicates whether the value will be fitted or not
Value	actual value of the fitting parameter, starting value
Typical difference	This value is used in the beginning of the fitting procedure The actual value is either plus or minus the typical 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 then 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
Tool	Opens a slider bar window which allows an interactive and convenient variation of the actual fitting parameter for a manual modification of the selected value
Minimum	The smallest allowed value of the parameter
Maximum	The highest allowed value of the parameter
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. I 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

2.2. Slider bar

The slider is a convenient way to find proper starting values for fitting parameters.

It is selected in the “Tools” row of the parameter list.

This is the slider bar for the film thickness parameter of the SiO2 layer:

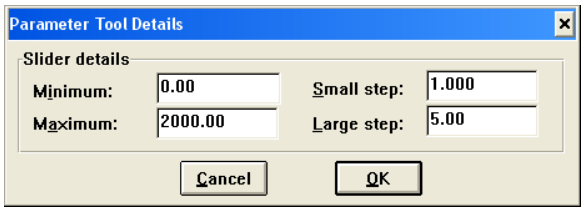


The slider can be moved by using the mouse. When it is released at a new parameter position the PSI, DELTA spectra will be updated using the new value of the parameter.

“Animate” does an automatic animation with “Large step” step size. It can be stopped when the correct value is reached.

The range and step size of the parameter are defined in: 

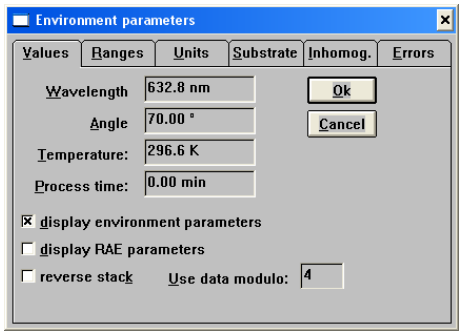
The window allows setting the minimum and maximum allowed range as well as the small and large steps.



2.3. Environmental settings

Explanation of the most important and most used environmental settings.

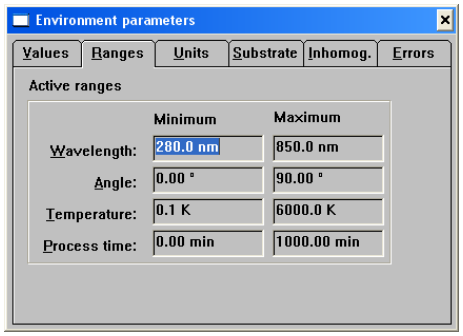
Tab: Values



"Wavelength" defines the observation wavelength of the display of the model

"Angle" defines the angle of incidence e.g. used for the "Simulation"

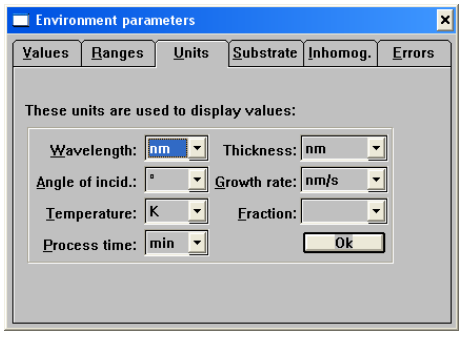
Tab: Ranges



"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 then to 450 to 850 nm. The spectral range below 450 nm is neglected and not displayed.

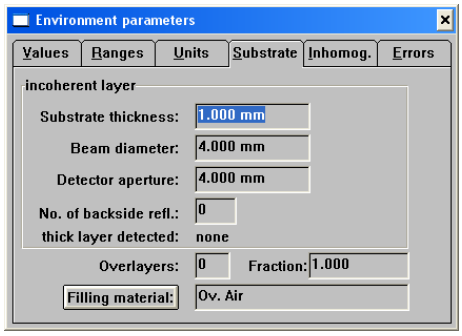
Attention: this restriction also applies for the export of data. In case the full spectral range of the measurement should be exported, the wavelength range must be extended to the measured range.

Tab: Units



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

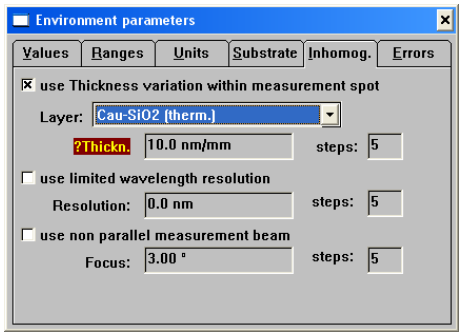
Tab: Substrate



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.

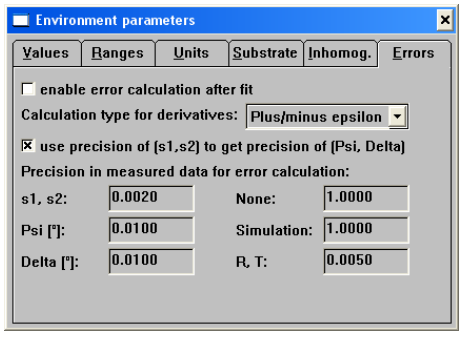
Tab: Inhomogeneities



This tab is used to model imperfections of the sample or equipment.

“use Thickness variation ...” describes a non uniformity of the layer (thickness variation) within the spot size of the ellipsometer.

Tab: Errors



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.

2.4. Simulation

The following example demonstrates the capabilities of the “Simulation”-Module of SpectraRay II.

The “Simulation”-module is based on the current optical model. It can e.g. calculate different values, like PSI, DELTA, R or T spectra for arbitrary angles of incidence in arbitrary spectral ranges.

Question:

How do the Ψ,Δ spectra behave in the spectral range from 300 to 850 nm for SiO_2 / Si for different film thickness of th = 0 … 20 nm with a 5 nm step size?

Stack:

Air - n and k are fix

SiO_2 - Cauchy

Si - File layer

Simulation:

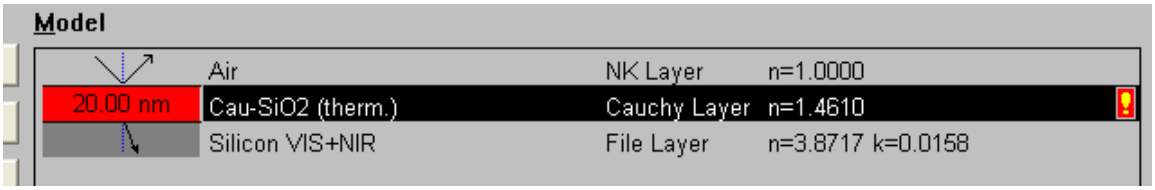
PSI, DELTA versus wavelength and film thickness of SiO_2

Spectral range: **300 … 850** nm

Angle of incidence: **70** deg

SiO_2 film thickness: 0 … 20 nm, step 5 nm

Creating the model

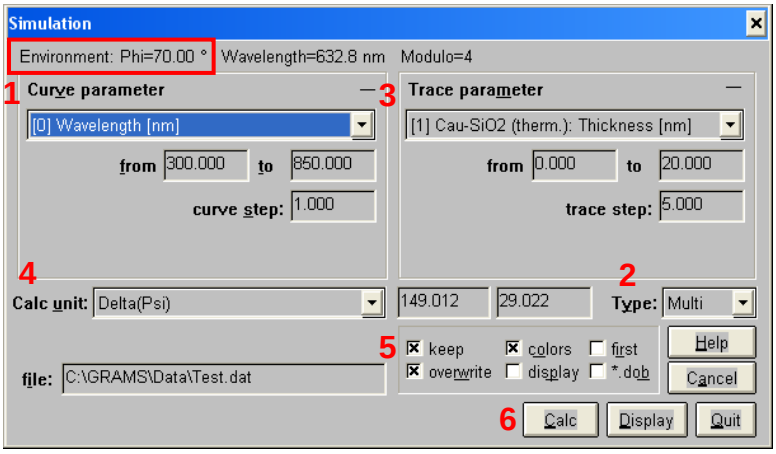


The actual thickness of SiO_2 in the model is not important, because it will be changed temporarily by the simulation.

Set the environment settings:

Set the angle of incidence to Φ=70°.

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 "Cau-SiO2 (therm.) Thickness [nm]"

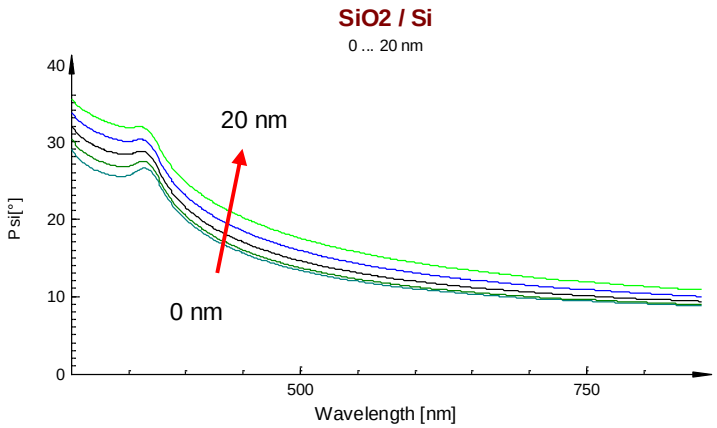
thickness range: 0 – 20 nm, 5 nm step size

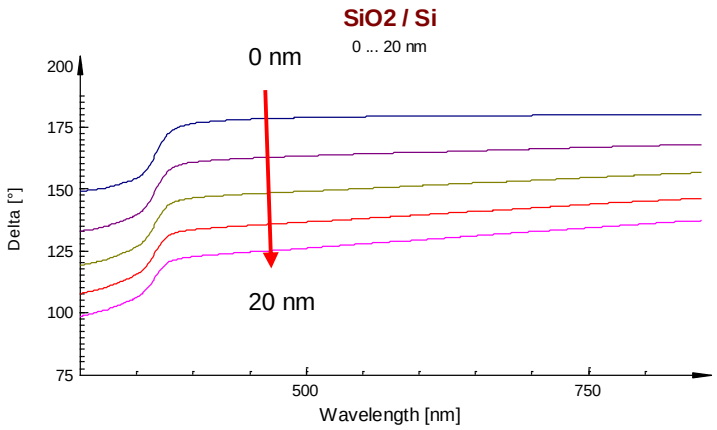
4) "Calc unit" is set to Delta(Psi) (defines y-axis)

5) "keep" is switched on to store the calculated data to the Data sub-window.

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

Results of the simulation





The effects in Delta are very strong. With each nm in film thickness a change of about 4 deg in Delta is obtained. This is the reason for the high sensitivity of ellipsometry against film thickness.

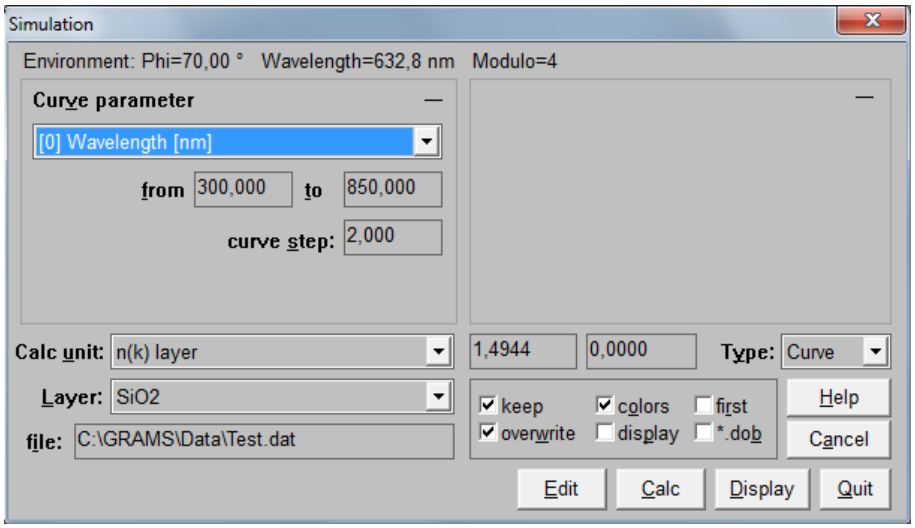
Question:

How to calculate the dispersion of n and k of a material using the "Simulation"

(This procedure ia alerady expained in "Using Simulationfor Reporting")

The dispersion of n and k of the SiO2 layer of our current model should be calculated:

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



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) "keep" is switched on to store the calculated data to the Data sub-window.

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

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

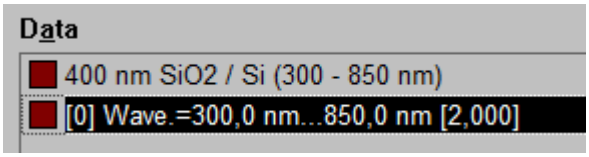


Figure: dispersion as new dataset

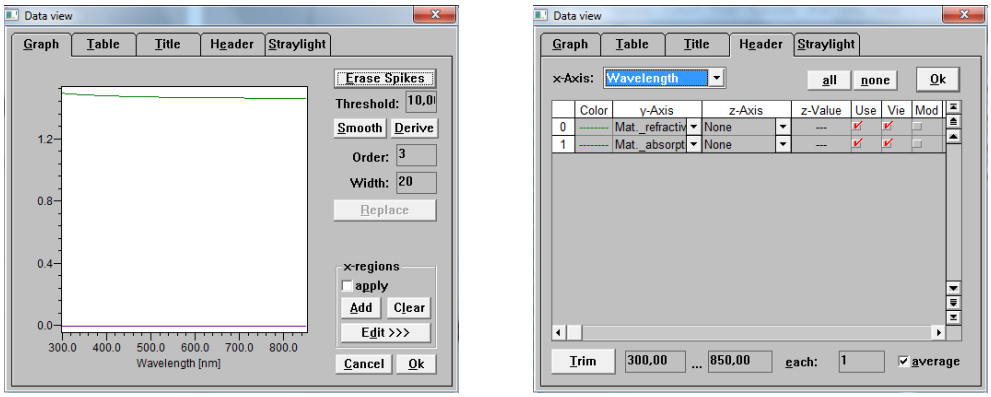


Figure: dispersion of n and k of SiO2and header tab

The dataset can be exported now as ASCII file as described in section “Import and Export of datadifiles”

3. Conversion of different wavelength or energy scale units

Conversion of wavelength ↔ photon energy (nm ↔ eV)

$$\frac{1239.85}{nm} \mathrel{\hat{=}} eV \quad , \qquad \frac{1239.85}{eV} \mathrel{\hat{=}} nm$$

Examples:

300.0 nm = 4.13 eV

400.0 nm = 3.10 eV

632.8 nm = 1.96 eV

1239.85nm = 1.00 eV

Conversion of wavelength ↔ wavenumber (nm ↔ cm^{-1})

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

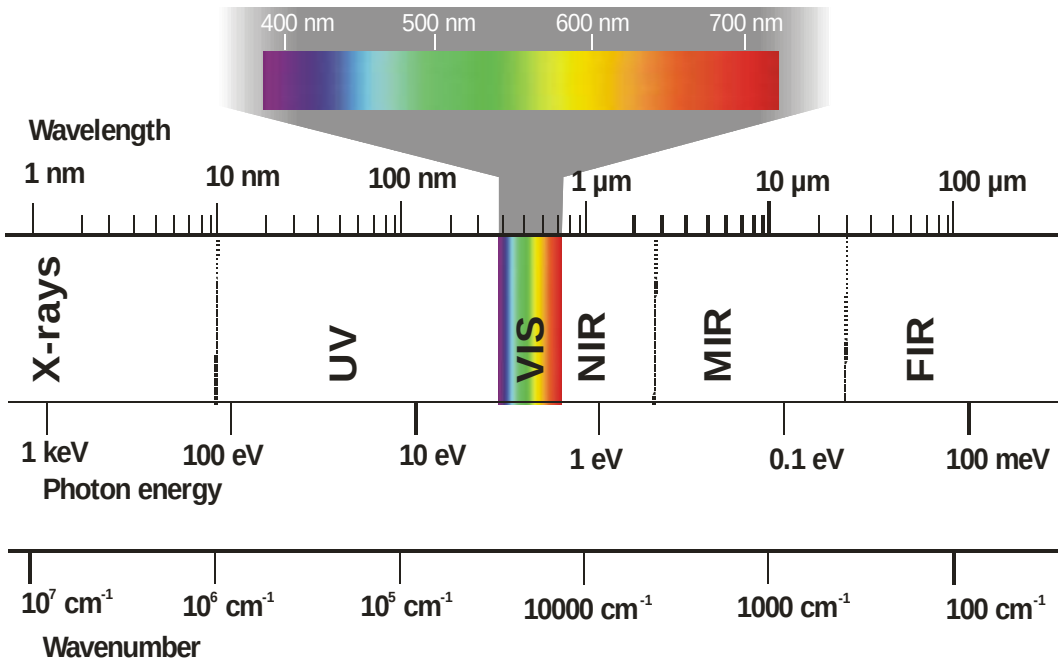
Examples:

200 nm = 50000 cm^{-1}

500 nm = 20000 cm^{-1}

1000 nm = 10000 cm^{-1}

2000 nm = 5000 cm^{-1}



4. Import and export of data

4.1. Import of external measured data

The results of external measurement devices like reflectance, transmission or ellipsometric measurements can be imported into SPECTRARAY II.

The external data must exist as ASCII datasets. The file extension *.txt is recommended.

The data must be split into different columns.

The first column contains the x-axis. Usually it is the wavelength axis.

The following units for x-axis are possible:

- Wavelength / nm
- Photon energy / eV
- Wavenumber / cm^{-1}

Further columns contain the y-axis data. The following units for y-axis are possible:

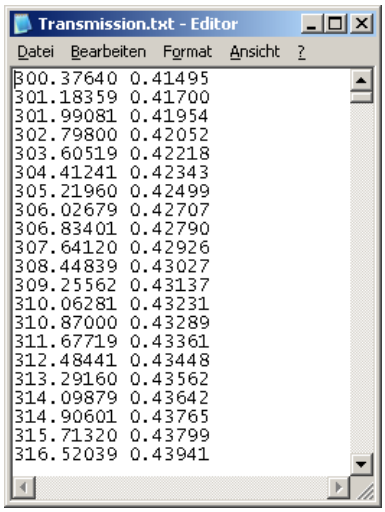
- Reflectance: 0 … 1 (0% to 100% is not supported)
- Transmission 0 … 1 (0% to 100% is not supported)
- Ψ, Δ spectra /°
- tan Ψ, cos Δ
- Fourier coefficients s1, s2

The individual rows are separated by either spacebars or tabs.

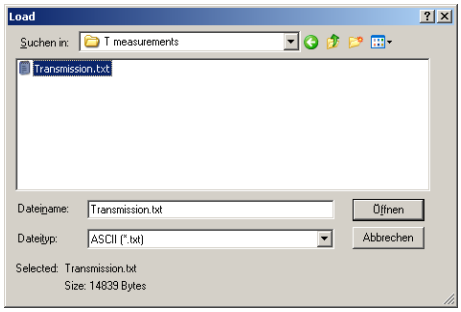
A header line is not necessary.

Example: import of a transmission measurement

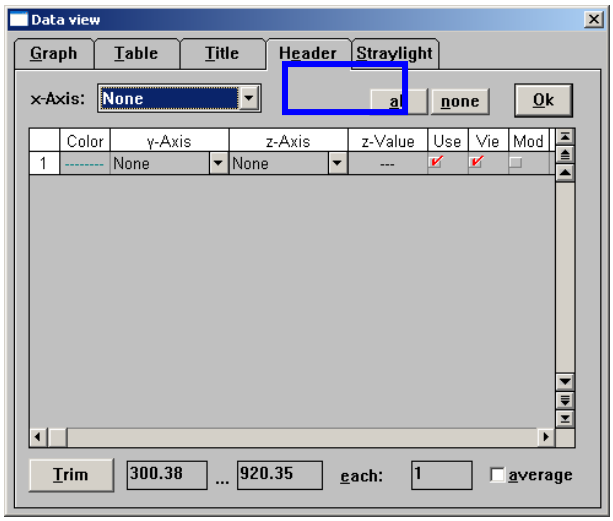
The following example shows the file format for a transmission measurement from 300 to 920 nm. The first column contains the wavelength / nm. The second column contains the transmission data:



The file is imported into the data section of SPECTRARAY II by Menu → File → Load …

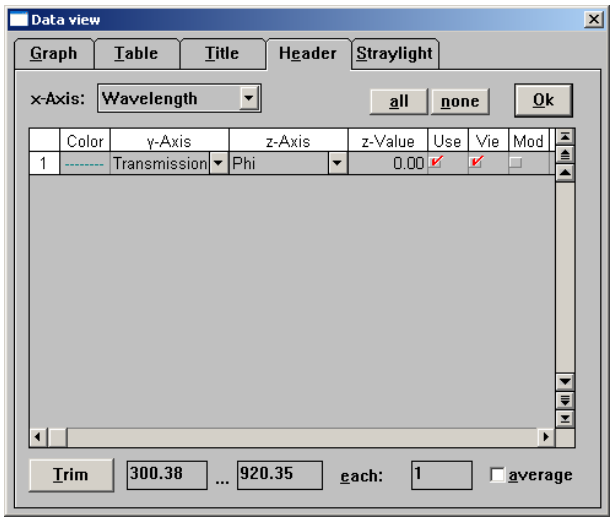


The units of the imported files must be set. The transmission measurement is double clicked and the "header" tab is selected.



For this Transmission file the following settings are necessary:

x-Axis: "Wavelength"
y-Axis: "Transmission"
z-Axis: "Phi" (unit of the angle of incidence of T measurement)
z-Value: "0.00" (the value of the angle of incidence)



Now this dataset can be used for the modeling procedure.

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 (sinply click once with left mouse button) so it apperas invderted

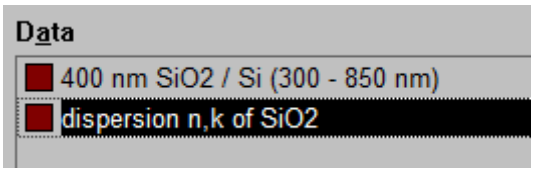


Figure: selected dataset

Important: Only “used” data will be exported

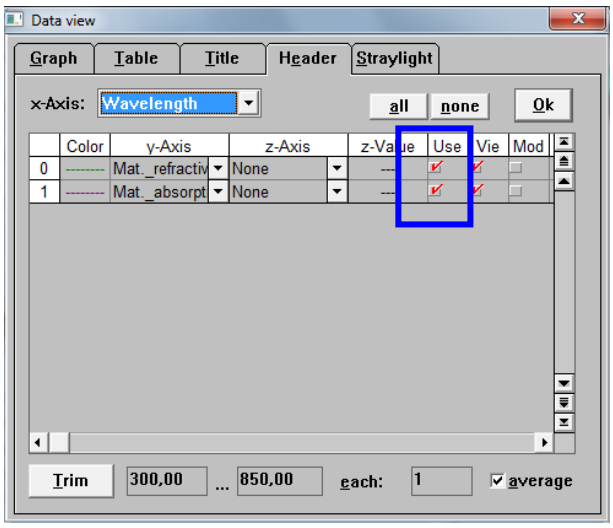


Figure: the data with selected “Use” will be exported

The spectral range set in the Environemtal settings must be equal or broader than the spectral range of the dataset. Otherwise the export will be cut to the environemtnal settings.

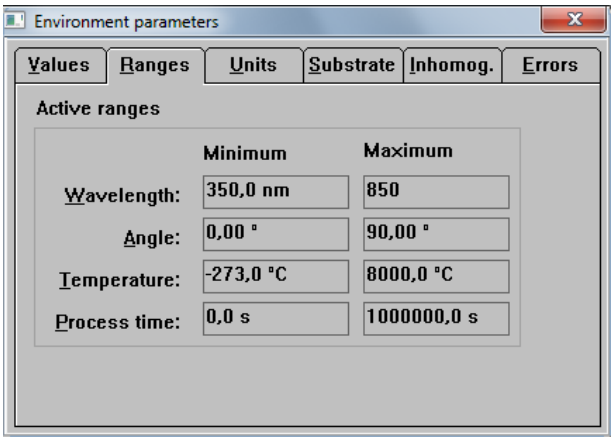


Figure: Spectral range in “Environemntal settings”

Now the File → “Save As ...” menu entry is selected

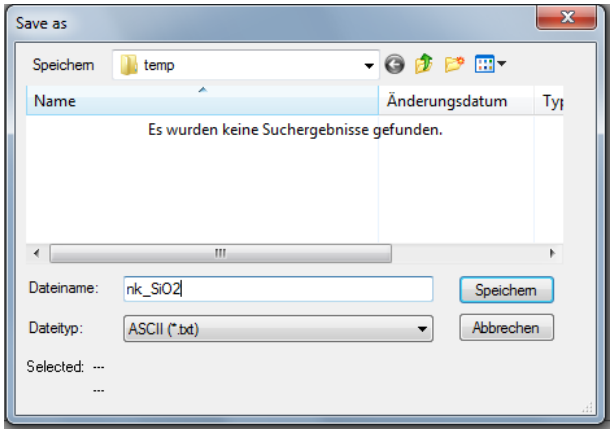


Figure: Filename and extension ASCII(*.txt) are selected

The file extension “ASCII(*.txt) and a filename are selected and saved.

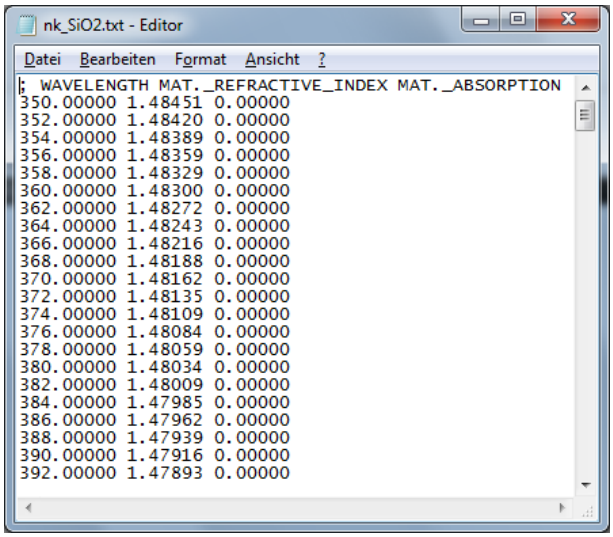


Figure: Exported dataset in ASCII format

5. Dispersion formula examples

The dispersion relation (short: dispersion) describes the dependency of the refractive index n and extinction coefficient k with the wavelength: n(λ) and k(λ).

Different types of materials show different types of dispersions. Four different kinds of materials illustrate the variety of different dispersion relations:

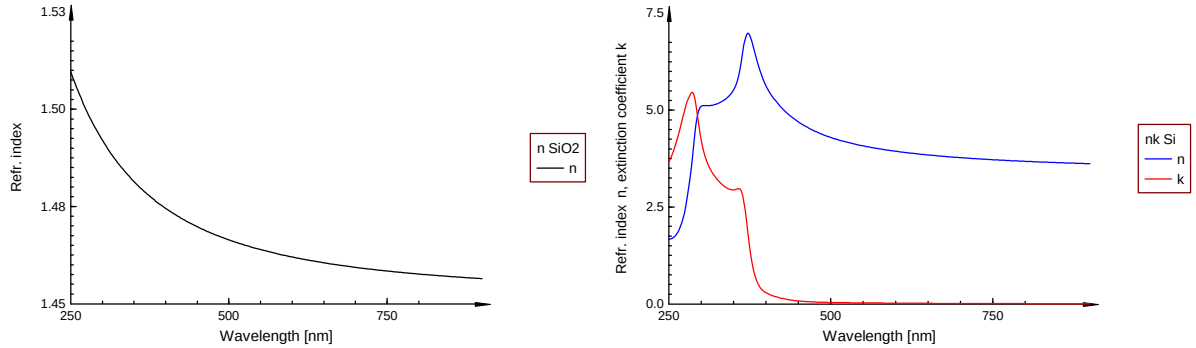


Figure: Typical dispersions of a dielectric (SiO_2, left) and a crystalline semiconductor (Si, right)

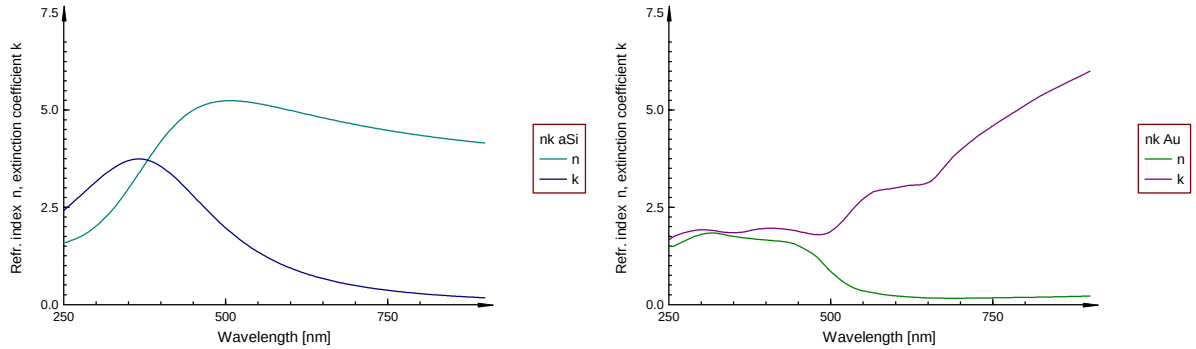


Figure: typical dispersions of an amorphous semiconductor (aSi, left) and a metal (Au, right)

For different kinds of material types different kinds of mathematical descriptions are necessary. The following chapter gives an overview of the dispersion relation available in SpectraRay II.

5.1. Overview of dispersion formulas and layer types

By pressing the “New” icon a new material can be inserted into the model:

L	Dispersion	Used for ...	Example
H	Fixed n and k	Constant dispersion	Only air
H	Cauchy	transparent dielectric materials Photoresist Glass	SiO_2, Al_2O_3, Si_3N_4, TiO_2 PMMA BK7, quartz
H	Tauc-Lorentz	Absorbing dielectric materials amorphous materials	Si_3N_4, TiO_2 a-Si, a-C
H	Drude-Lorentz	Metals TCO (transparent conductive oxide)	Au, Ag, Cu, Cr, Ni ITO, ZnO:Al
H	File-Layer	Table of wavelength, n, k, no fit parameters substrates	Good for all Si, Ge, GaAs, quartz
M	Leng-Lorentz	Crystalline indirect semiconductors polycrystalline indirect semiconduct. conjugated polymers (OLED, OFET)	c-Si, c-Ge, c-SiGe poly-Si MEH-PPV, P3HT
M	Brendel	Absorption (vibration) bands in the MIR	SiO2, SiN, CH-bonds
M	Sellmeier	Like Cauchy but for broader spectral range (VIS + NIR)	SiO_2
M	Tanguy III/V	Bandgap of direct semiconductors, also II/VI	GaAs, GaN, AlGaN ZnSe
L	Hamberg Sernelius	TCO (transparent conductive oxide)	ITO, ZnO:Al, SnO_2:F
L	Afromovitz	III/V semiconductors (specific)	GaAs, InP, InGaAsP
L	Formula	New non implemented dispersions	Good for all
L	Schott glass	Specific for glasses from Schott	AF45

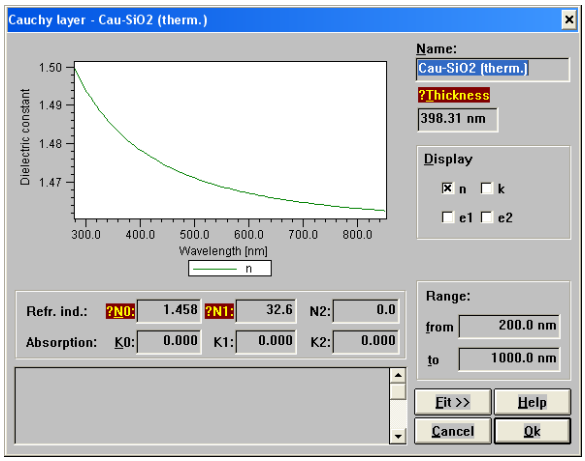
L	Layer type	Used for ...	Example
H	EMA (effective medium approximation)	Mixture of two materials Roughness Interface Gradient	 mixture: Air / layer mixture: layer1 / layer2
M	Biaxial anisotropic	Direction dependent dispersion	Crystalline quartz
M	Periodical group	Bragg reflectors	20x (SiO_2 / TiO_2)
L	Table (2D)	Parameter dependent data of e.g. - Temperature - composition	 Si (0 deg C … 1000 deg) Si_xGe_{1-x}
L	Homogeneous growing layer	In-situ applications, thickness changes with time	Good for all
L	Nuclei growth	In-situ applications, island growth	Metallic film growth
L	Epitaxial Si profile	MIR, Si epitaxial layer growth	Si doping concentration and gradient

L: Level of usage, High (used very often), Medium (sometimes) Low (seldom)

5.2. Cauchy dispersion

The Cauchy dispersion is mainly used for transparent materials like dielectrics e.g. SiO_2, Al_2O_3, Si_3N_4 and TiO_2.

The Cauchy – window appears as follows:



There are three Cauchy coefficients N0, N1 and N2 which describe the dispersion of the refractive index n.

Additionally there are three Cauchy coefficients K0, K1 and K2 which describe the dispersion of the extinction coefficient k. In general all K0, K1 and K2 are set to zero when transparent materials are described.

The Cauchy formula is as follows:

$$n(\lambda) = n_o + C_0 \frac{n_1}{\lambda^2} + C_1 \frac{n_2}{\lambda^4} \qquad \lambda \text{ in nm}$$

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

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

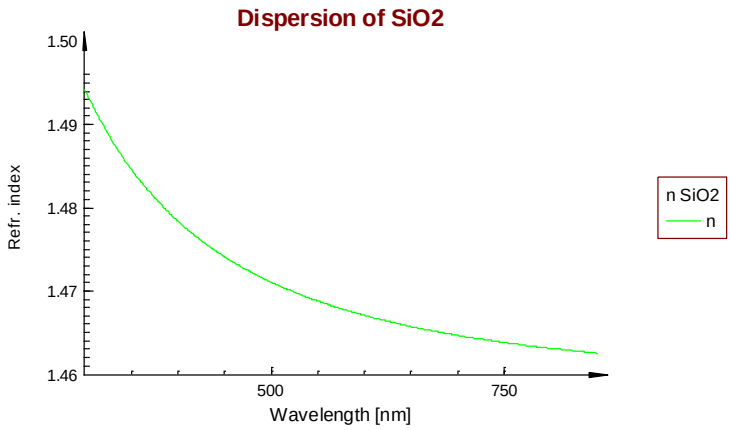
The n_0 (k_0) value is simply a constant value. It is not dependant from the wavelength.

The n_1 (k_1) and n_2 (k_2) are dependent from the wavelength. They are defining the dispersion of the refractive index n (extinction coefficient k).

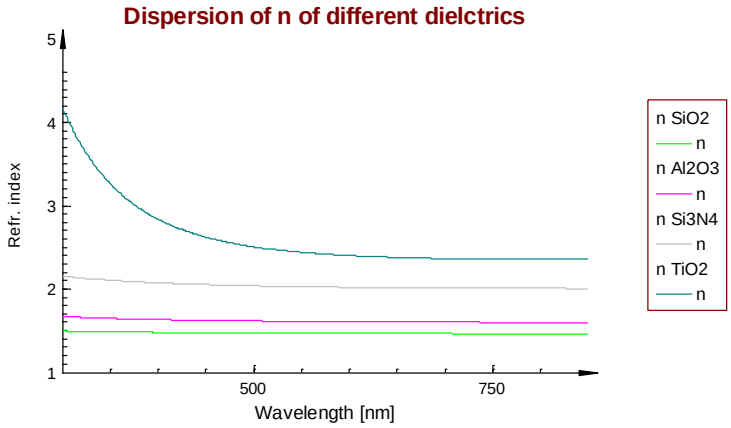
Attention: n_0 is frequently confused with the refractive index at 632.8 nm!

Normal dispersion:

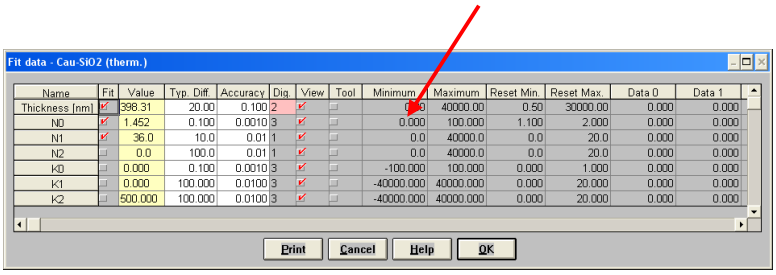
The refractive index is increasing towards shorter wavelength. The following graph shows the normal dispersion of SiO_2. The refractive index is increasing from n=1.46 at λ=850 nm to n=1.49 at λ=300 nm.



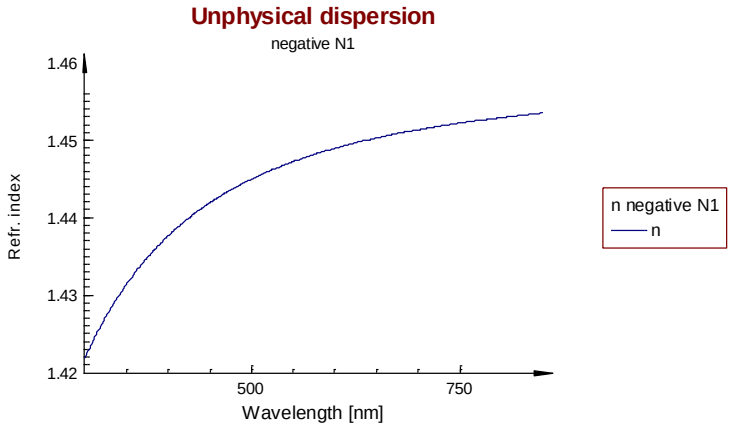
In general the dispersion is getting stronger when the refractive index is increasing. This behavior can be seen in the following graph where the dispersion is shown for different dielectric materials.



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).

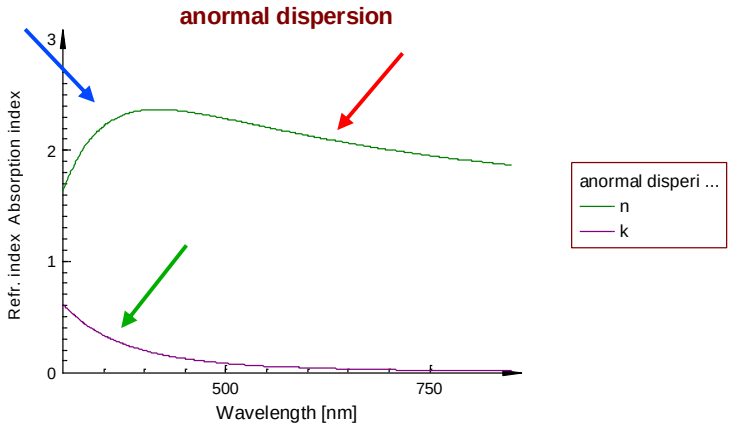


Otherwise the following behavior might happen: the dispersion becomes negative. This is called abnormal dispersion. It is an allowed and physical correct solution only when an extinction k is present. It is a physical incorrect solution when k=0.



Abnormal dispersion:

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



The red arrow 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 it exist a 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 as mentioned above.

5.3. Tauc-Lorentz oscillator

The Tauc-Lorentz oscillator dispersion formula (TL) is mainly used to describe transparent dielectric materials with absorption in the short-wavelength range.

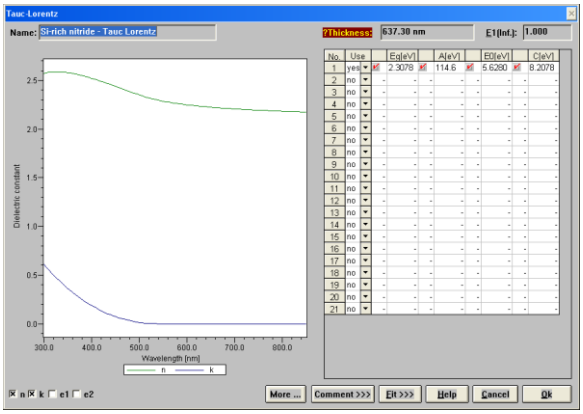
It can also be used to describe the dispersion of:

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

The following graph shows the dispersion of n and k of Si rich Nitride described by a TL oscillator. It also represents the principal dispersion dielectric material which absorbs in the short wavelength range.

X-axis:

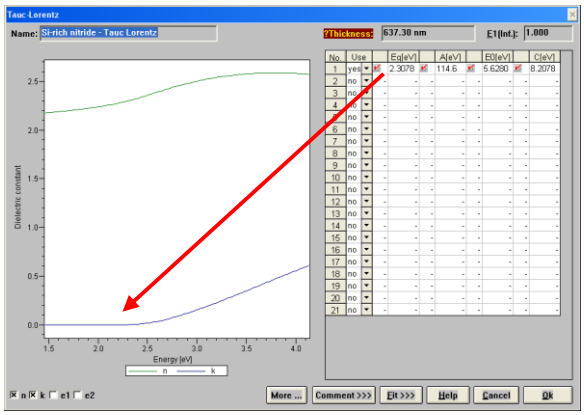
Wavelength / nm



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

X-axis:

Photon energy / eV

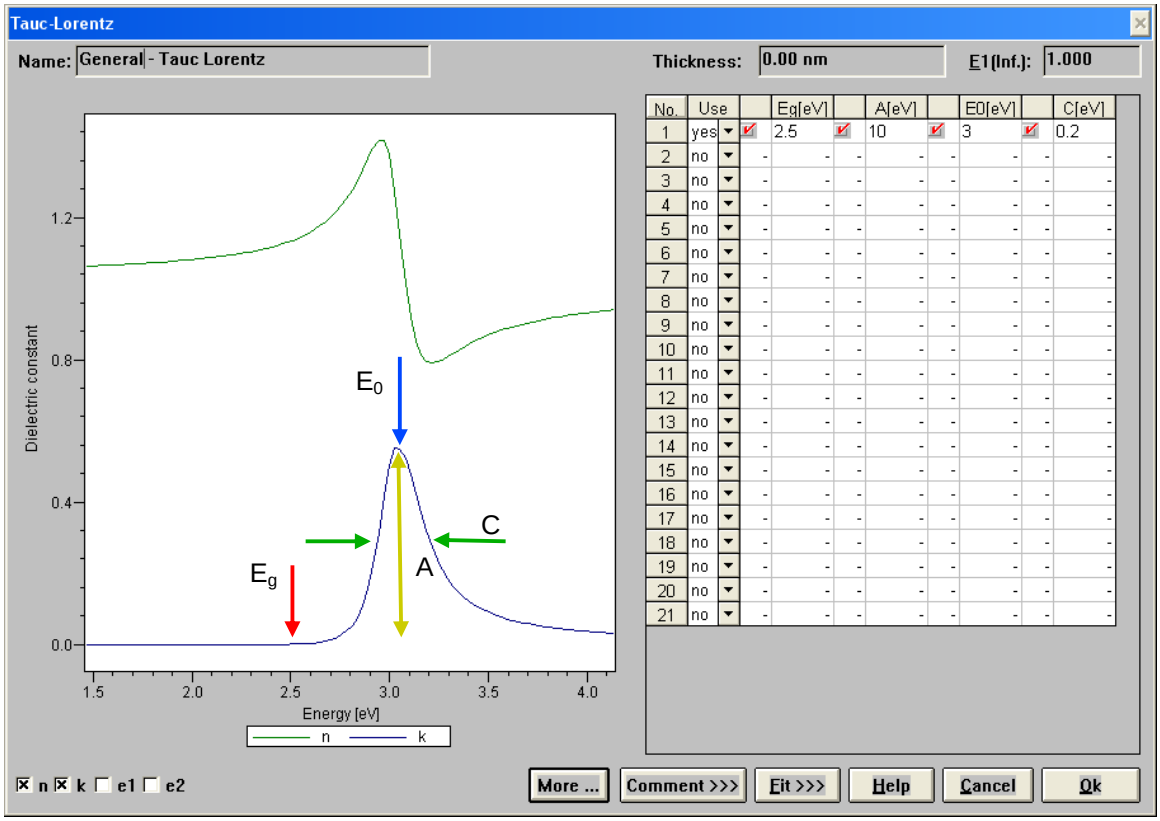


There are four parameters which describe the dispersion of n and k.

The phenomenal description of these parameters is given in the following table:

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

General example of the TL-oscillator to visualize the effect of the parameters:



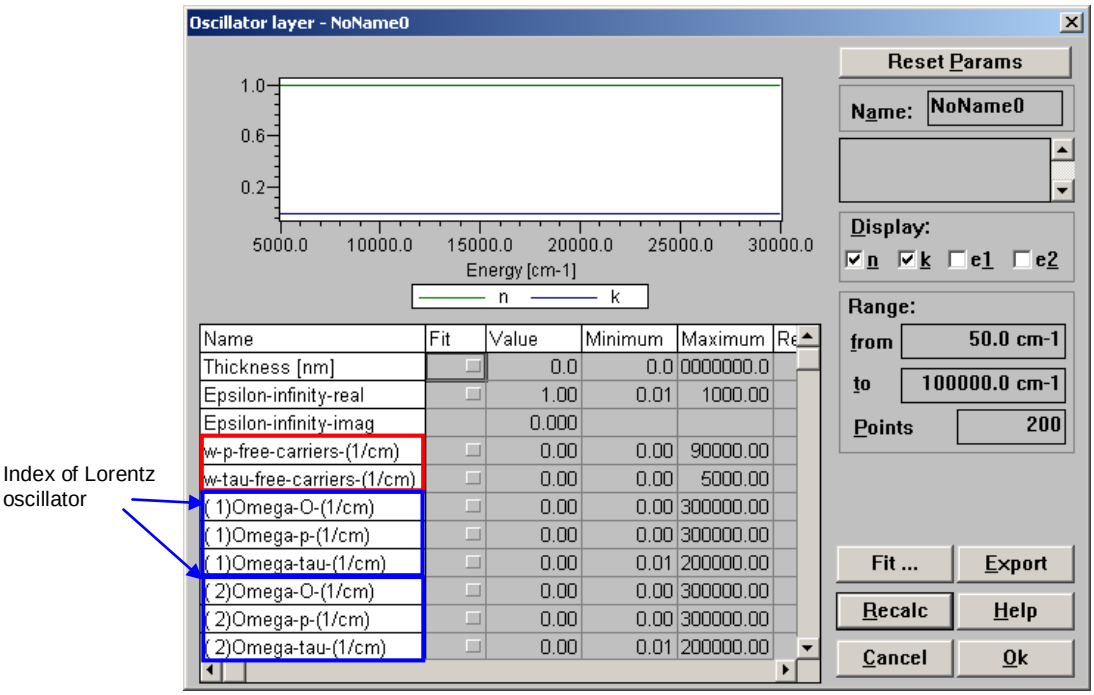
5.4. Drude-Lorentz oscillator

The Drude-Lorentz oscillator is a combination of two dispersion types: the Drude absorption of free charge carriers (see 4.4.2) and a Lorentz-oscillator model (4.4.1) .

The units of the parameters in the Drude-Lorentz oscillator dispersion is wavenumbers. Therefore it is best to change the wavelength scale to wavenumber 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.



The red box indicates the two parameters for the Drude-oscillator model.
The blue boxes indicate the three parameters for the Lorentz-oscillator model. Up to 10 Lorentz-oscillators can be used simultaneously.

5.4.1 The Lorentz-oscillator

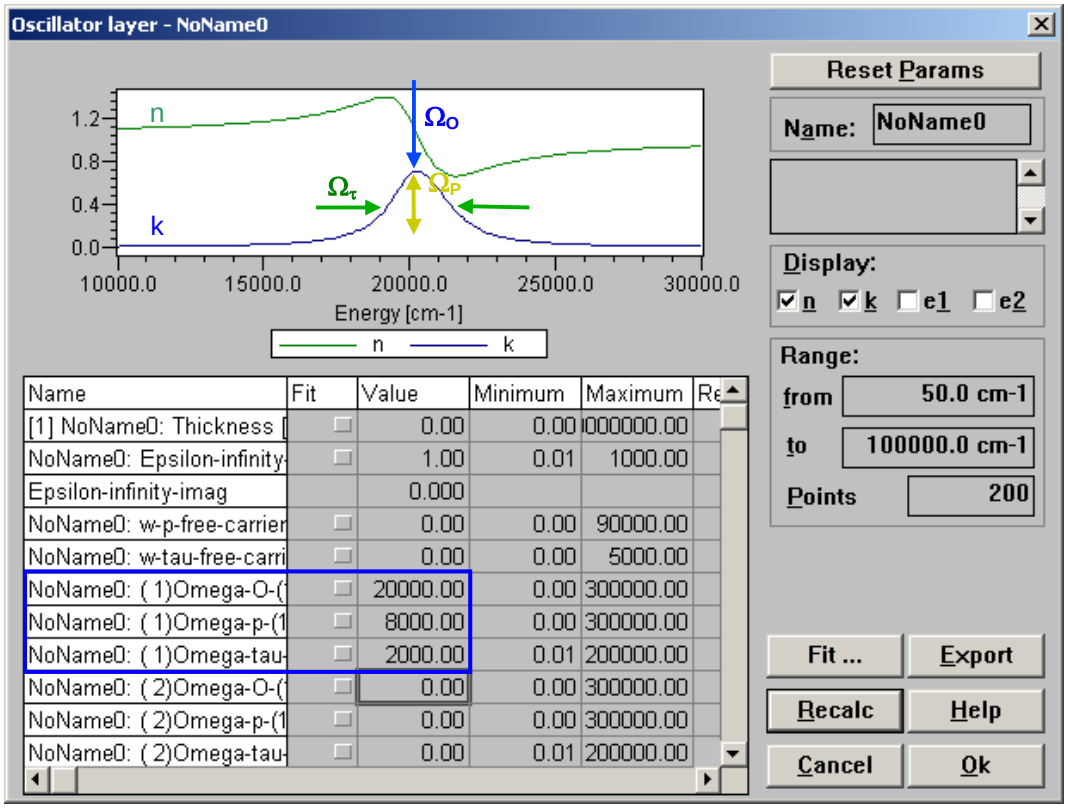
The Lorentz-oscillator consists of three parameters for the spectral position, strength and damping.

Its contribution to the dielectric function ε is:

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

Its parameters are summarized in the following table.

Lorentz-Oscillator	
Parameter	Description
Ω_O	Center frequency of the oscillator in cm^{-1}
Ω_P	Strength of the oscillator (amplitude)
Ω_τ	Damping of the oscillator



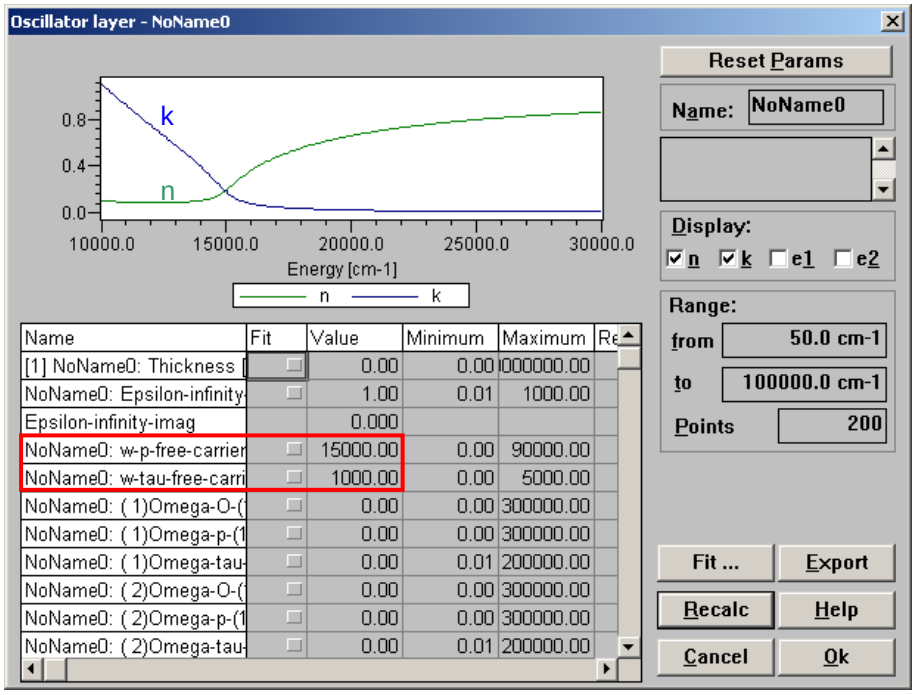
5.4.2 The Drude-free carrier absorption

The free carrier concentration in a material leeds to an oscillator with a center frequency of ω_0=0.

Its contribution to the dielectric function ε is:

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

Drude-oscillator	
Parameter	Description
ω_P	is dependant from the concentration N and the effective mass m* of the free carriers: $\omega_P = \sqrt{\frac{N e^2}{\varepsilon_0 m^*}}$ N: free carrier concentration m*: effective mass
ω_τ	is dependant from the mobility μ and the effective mass m* of the free carriers: $\omega_\tau = \frac{e}{m^* \mu}$ μ: mobility of the free carriers m*: effective mass



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) .

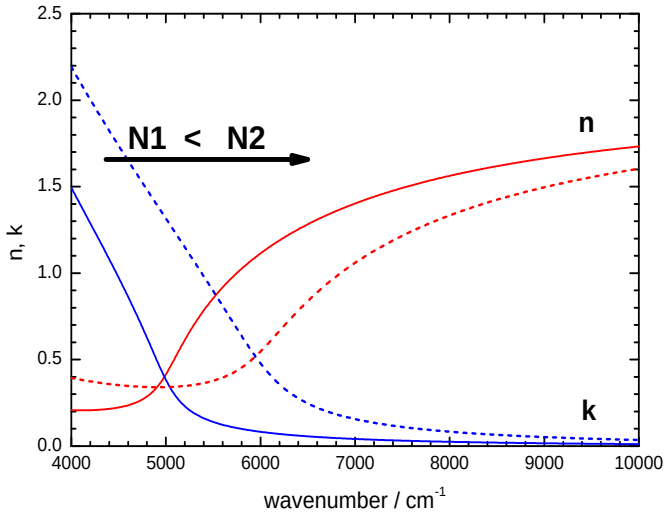


Figure: influence of carrier concentration N to the dispersion on n and k

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

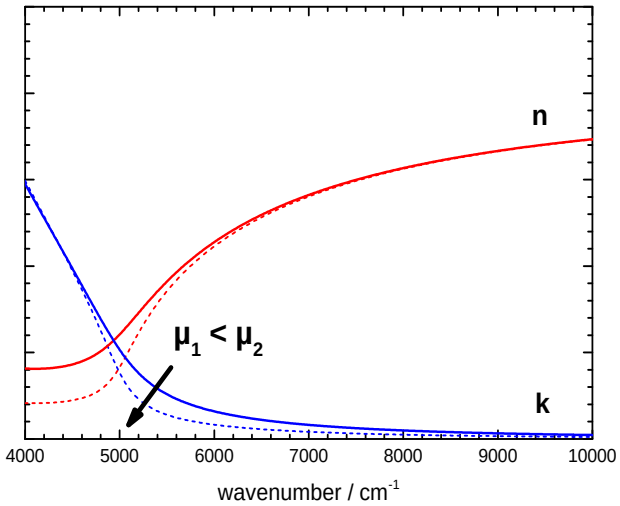


Figure: influence of carrier mobility µ to the dispersion on n and k

→ With increasing mobility µ of the free carriers the oscillator structure gets sharper.

5.5. Brendel oscillator model

The Brendel oscillator model is designed to describe vibration absorption bands of molecules in the MIR spectral range. It is based on a harmonic 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 harmonic oscillator.
Beyond that it is very useful to describe also metallic films. Especially metals like gold are showing strong benefits when described using the Brendel oscillator model.

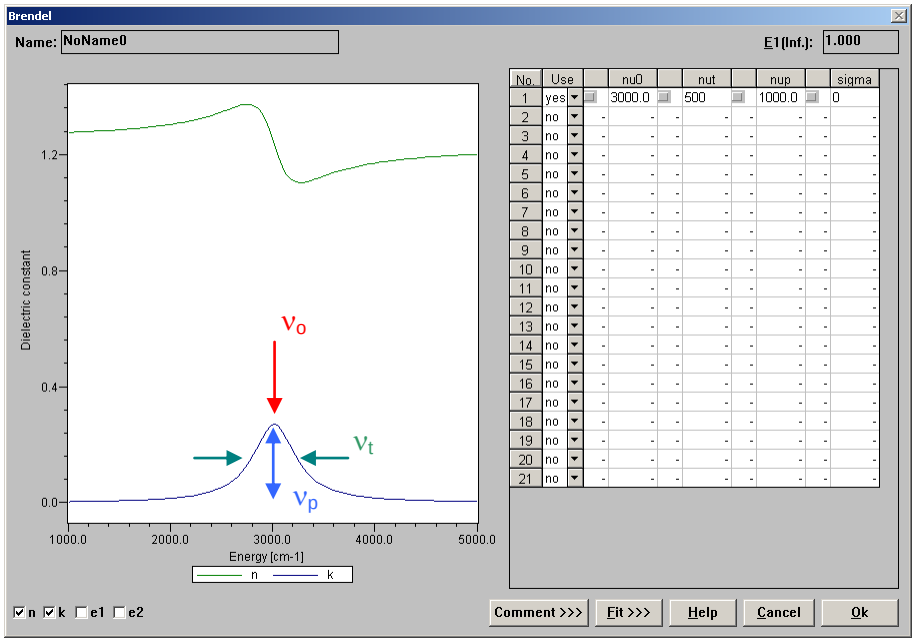
$$\varepsilon(\nu) = \varepsilon_\infty + \sum_{k=1}^{m} \chi_k(\nu)$$

Gaussian distribution — Harmonic oscillator

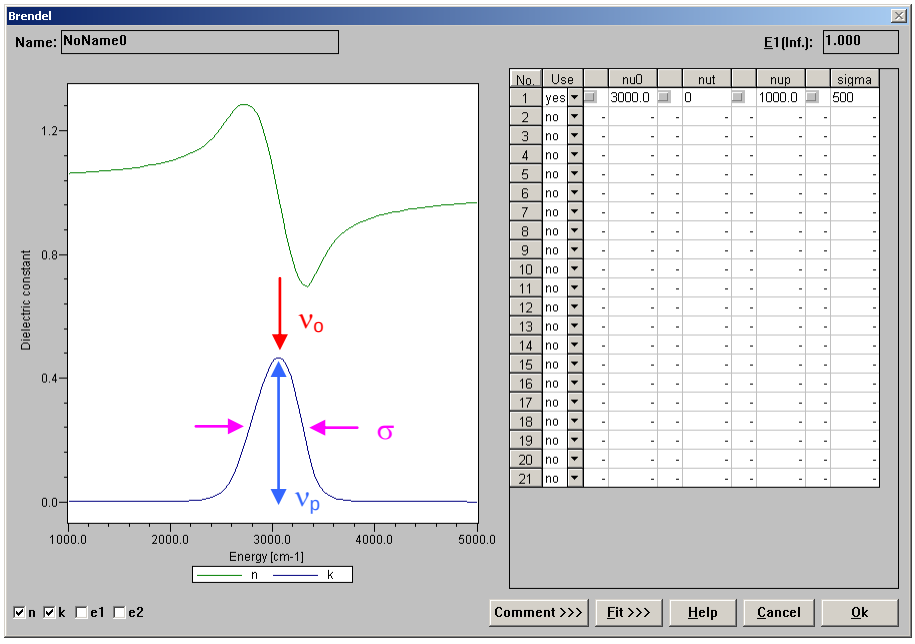
$$\chi_k(\nu) = \frac{1}{\sigma_k\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left\{-\frac{(x-\nu_{0k})^2}{2\sigma_k^2}\right\} * \frac{\nu_{Pk}^2}{x^2 - \nu^2 + i\nu_{Tk}\nu}\, dx$$

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

The Brendel oscillator becomes a standard harmonic oscillator exactly like the Lorentz-oscillator model, when the standard deviation becomes 0.



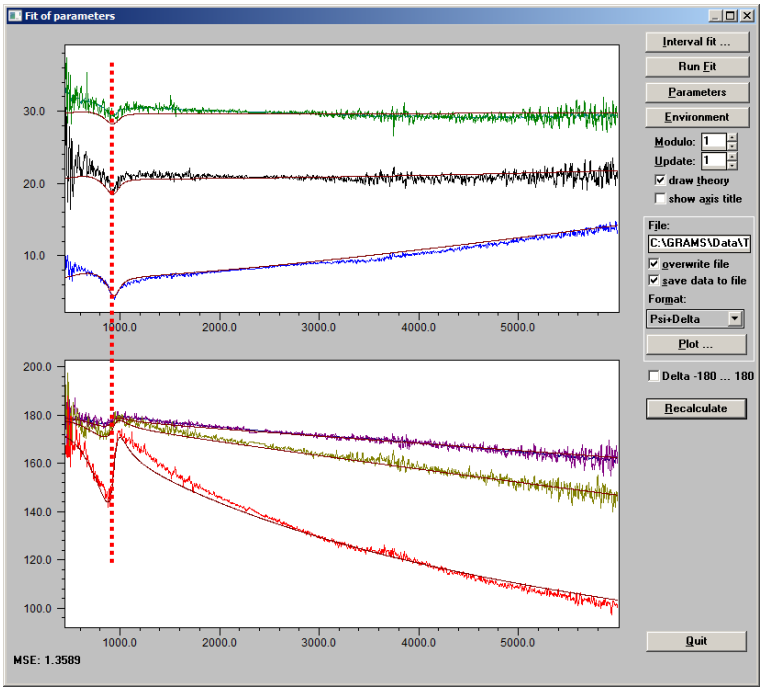
The Brendel oscillator becomes the shape of a Gaussian oscillator when the damping of the harmonic oscillator becomes zero and the standard deviation is not zero.



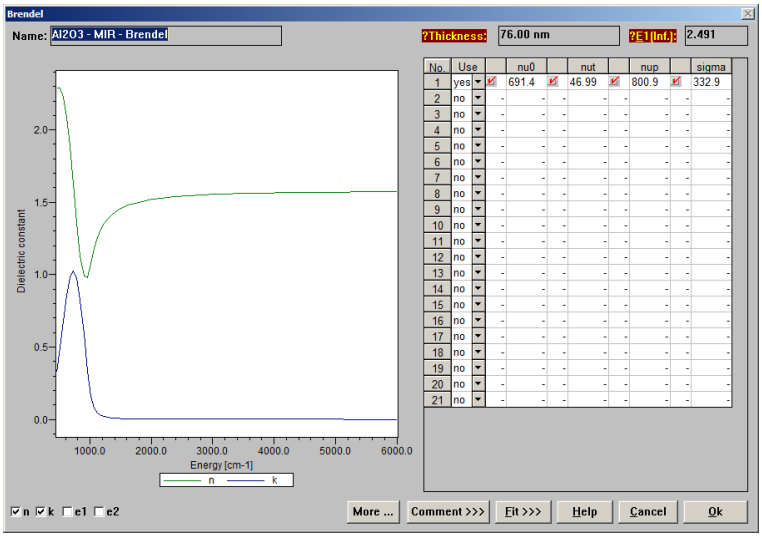
5.5.1 Brendel oscillator examples

Dielectrics the MIR spectral range

The following examples 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.



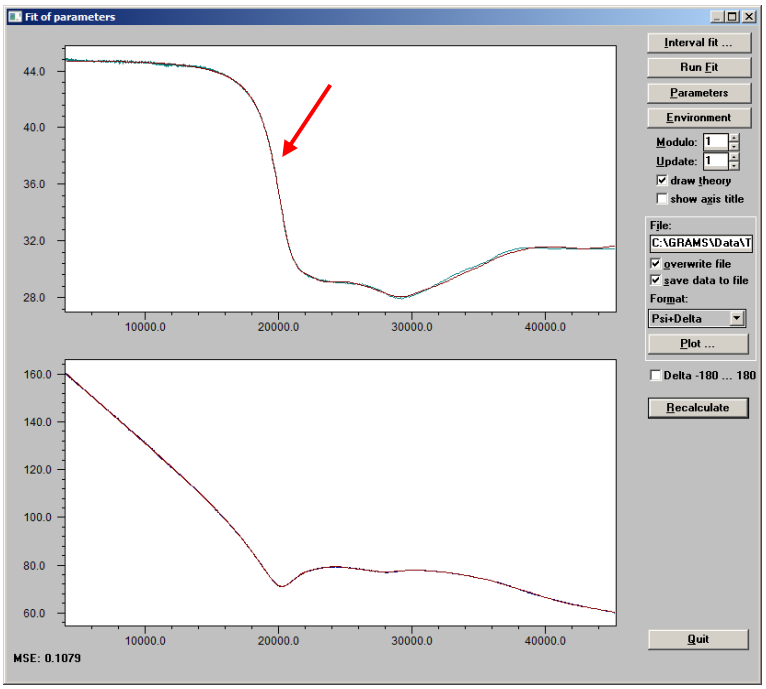
The screenshot of the Brendel dispersion window for Al_2O_3 shows the dispersion of n and k using a single Brendel oscillator.



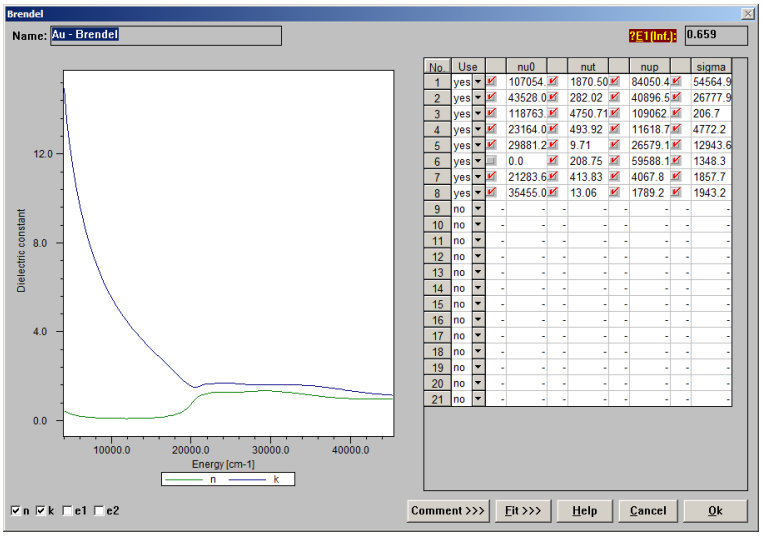
Metals in the UV-VIS-NIR spectral range

For the modelling 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 modelled 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.



The following screenshot shows the dispersion of Au. A total number of 8 oscilaotrs 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.



Glass in the VIS-MIR spectral range

Glass 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 PSI of an ellipsometric measurement and a transmission measurement are combined in one experiment.

SLG example
The upper graph of the screenshot shows the PSI 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.

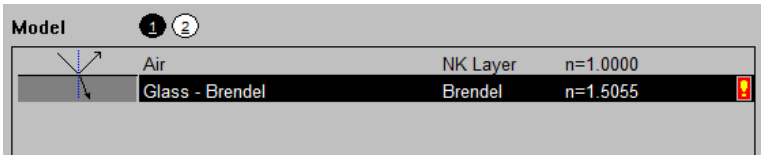


Figure: ellipsometric model without backside reflections

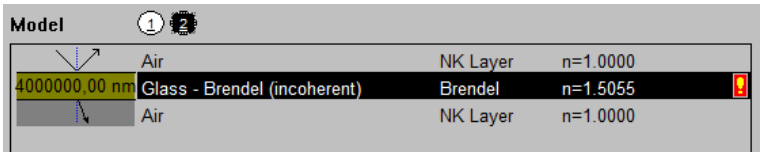


Figure: transmission model without backside reflections

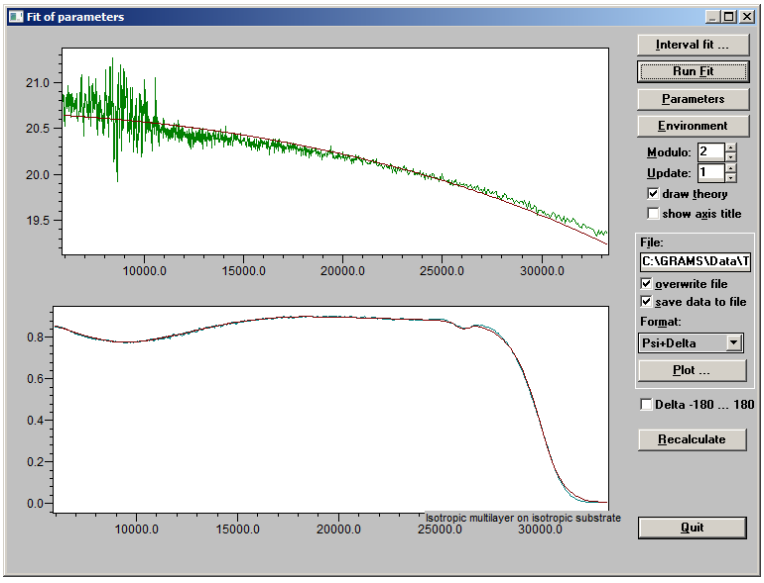
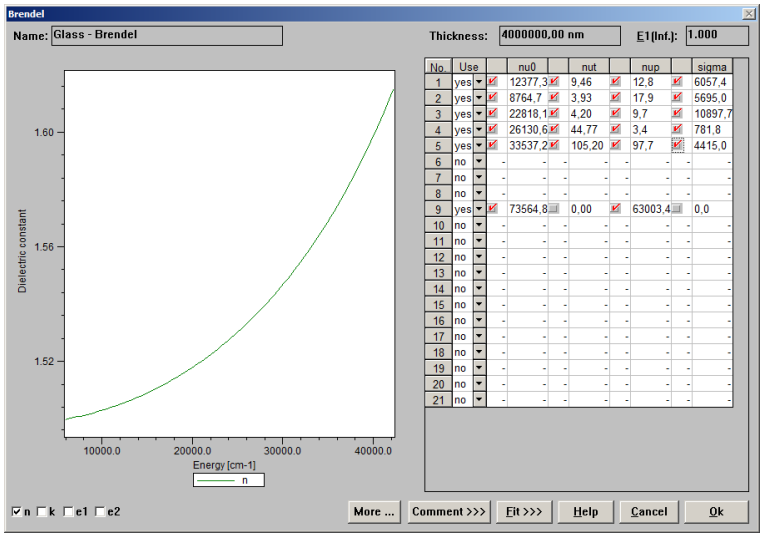
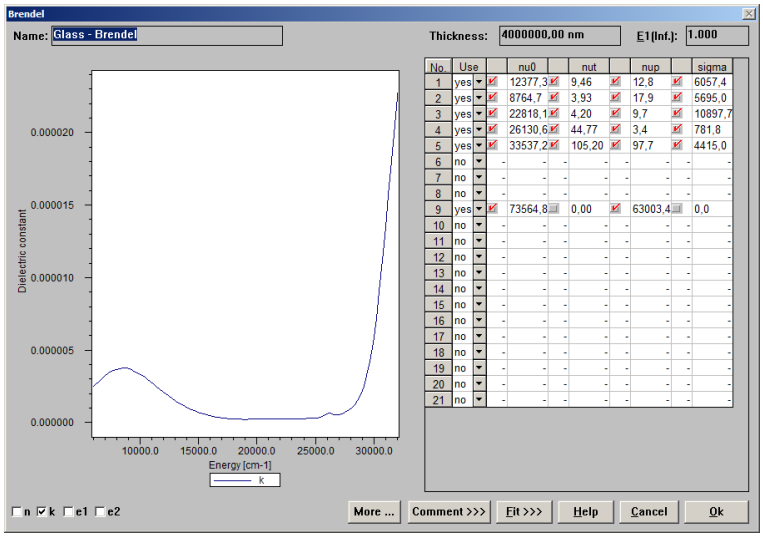


Figure model and measurement of PSI (top) and transmission (bottom)

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 is will always be too large and will suppress the weak absorption structures in the VIS and NIR.



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}!



More topics …

Layer types:

EMA (example: 50/50 and graded films (ZnO / glass)
Leng-Lorentz (example: ???)
Tanguy: (example: AlN bandgap from Bilkent)

6. Hackers guide for scripts

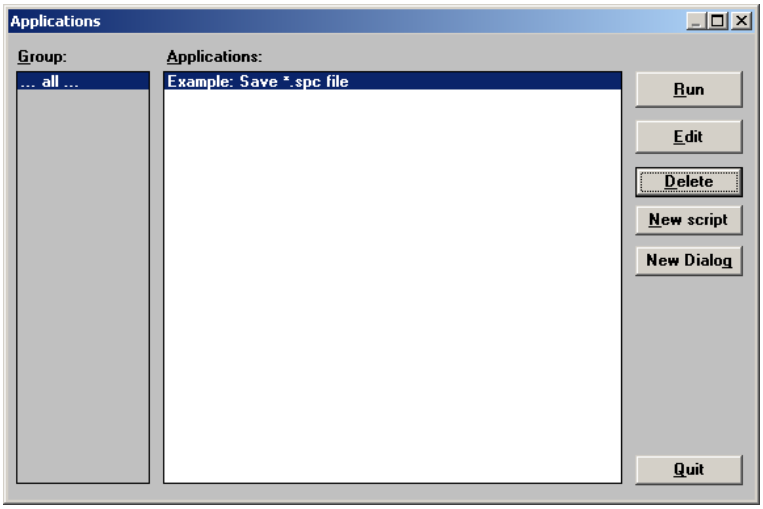
Scripts can be used to automate procedures in SPECTRARAY. They can be applied for many kinds of applications like e.g. automatic measurements, fitting, import or export of data. This chapter gives an overview how to build scripts using some useful short examples.

6.1. Starting the script editor to build a new script

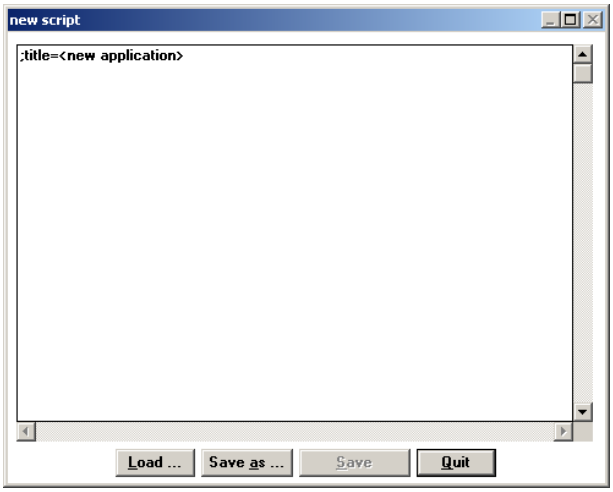
The script editor can be opened in two different ways:

- Menu → Extra → Applications
- Single mouse click on the script icon: 

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



“New script” opens the script editor where the scripts can be developed, executed, loaded or saved.



In the beginning a title is defining which is displayed in the “application runner” window. It is not absolutely necessary to save the script, because it will be automatically saved using a default name created automatically by SPECTRARAY II. In order to prepare the first example the title is set to:

;title=Example 1: 10 consecutive fits

The editor is closed and the new script appears as a new entry in the “application runner”

6.2. Script examples

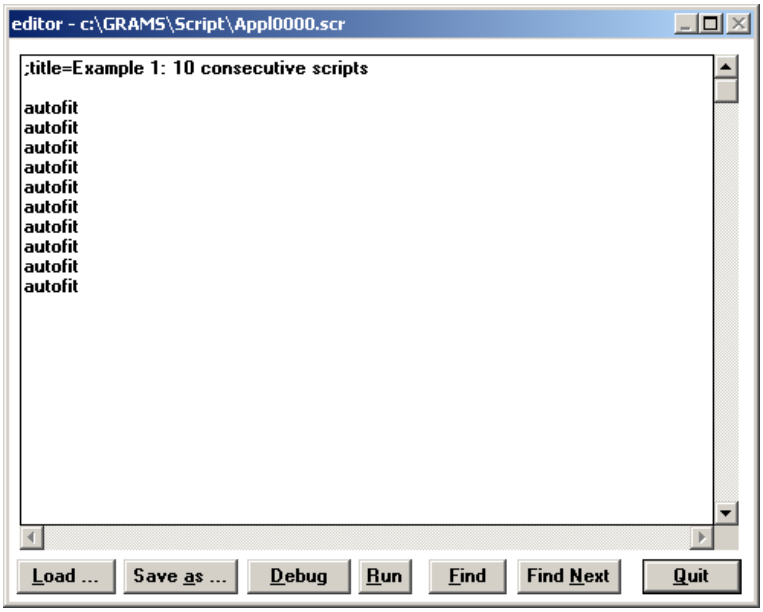
6.2.1 Script for numerous consecutive automatic fittings

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.

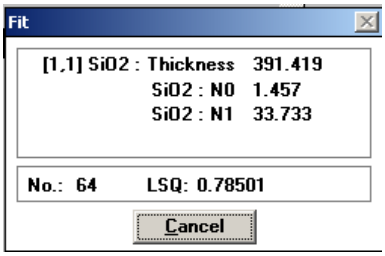
This example will be programmed using two different scripts. The first shows the trivial case the second uses a loop to execute the fitting procedure.

The script command which is used to execute the fitting procedure is called "*autofit"*. There are no parameters for this command.

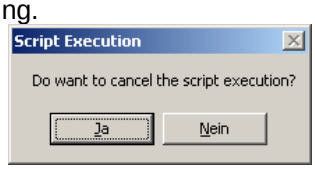
Trivial script:
The trivial script will be to simply copy the *"autofit"* command ten times into the script editor.
The new script "10 consecutive fits" is opened by "Edit"



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 now shows a small window with information about the progress of the actual fit run.

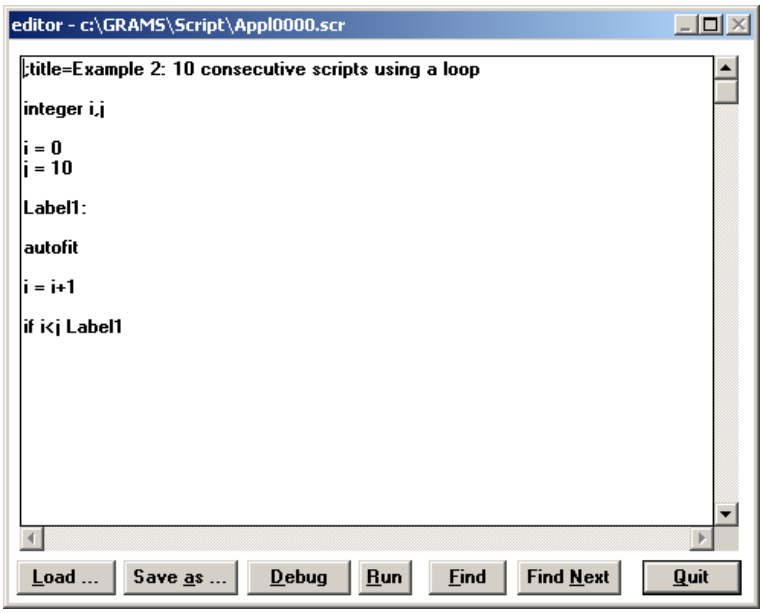


The script can be cancelled before it automatically ends by holding the "CTRL" key. Then a window appears asking to confirm the cancelling.



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:



This is the same script but with comments:

```
;title=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:

autofit

;the variable i is incremented
i = i+1

; now it is checked whether I is still lower than j, then the script jumps to Label1
; here no colon ":" is used at the end of Labe1
if i<j Label1
```

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.

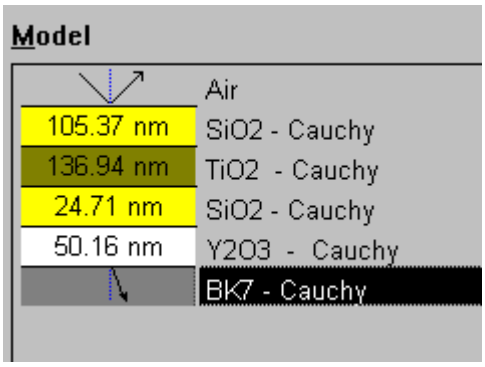
Please obey the following scripting rules:

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. Assigning a value to a variable needs to use space in front and after the equals sign “i = 0”
6. Comparison of variables need to use no space in front and after the comparison sign “i<j”
7. Comments can be introduced with a semicolon “;” in the beginning of a row

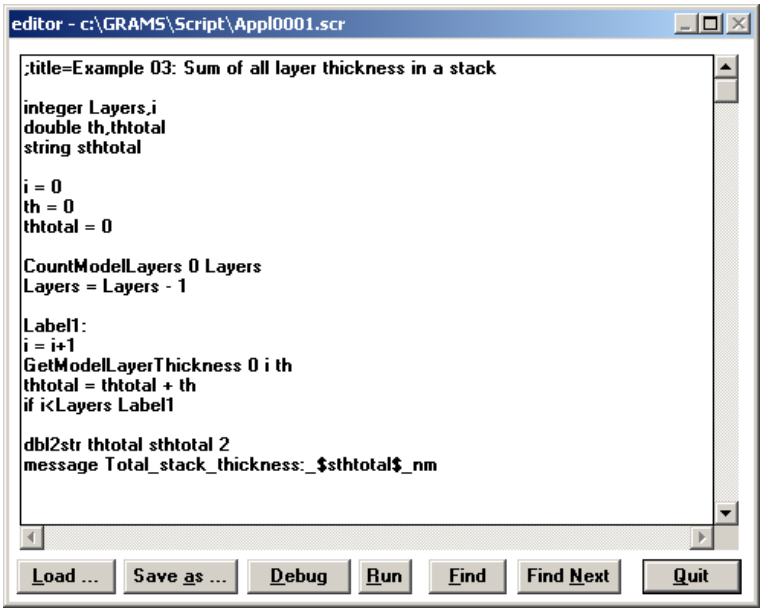
6.2.2 Calculation the sum of all films in a stack

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.

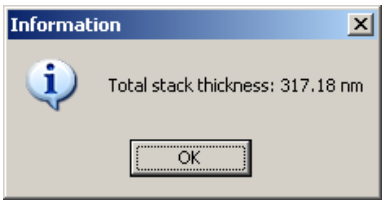


The scripts will read out the amount of layers in a stack, add them up and prints out the sum in a window. Additional commands are used to convert floating point variables into string variables.



It is important to know that the command “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”. Therefore

This result window is shown when the script is executed:



This is the script with comments:

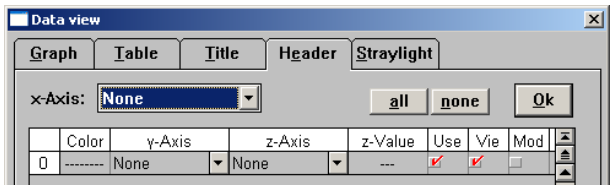
```
;title=Example 03: Sum of all layer thickness in a stack

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”
CountModelLayers 0 Layers
;
Layers = Layers - 1

Label1:
i = i+1
GetModelLayerThickness 0 i th
thtotal = thtotal + th
if i<Layers Label1

; the double variable is converted into a string. The digits are cut to 2 digits
dbl2str thtotal sthtotal 2

;message opens the result window
; “_” underscores are used to print a spacebar
; the variable is put in $$ to give the content of the variable
message Total_stack_thickness:_$sthtotal$_nm
```

6.2.3 Import of external data with unit assignment

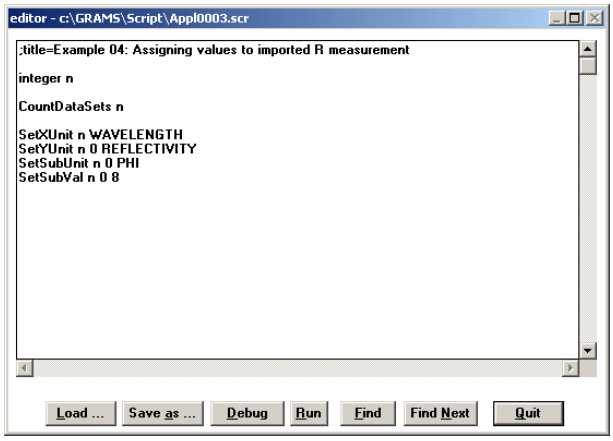
It was already explained how to import external measured data which is existent as ASCII data of e.g. two columns of wavelength and reflection data. The following script shows how to assign the units using a script.

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 $\Phi = 8°$.

The important information of the measurement are not set yet: “None”
x-Axis: None – (this will become: wavelength / nm)
y-Axis: None – (this will become: reflectivity)
z-Axis: None – (this will become: angle of incidence)
z-Value: --- – (this will become: value of the angle of incidence: 8°)



The fit script needs to count the amount of datasets to know which will be the last one in the row. Then the four parameters will be assigned to this dataset.



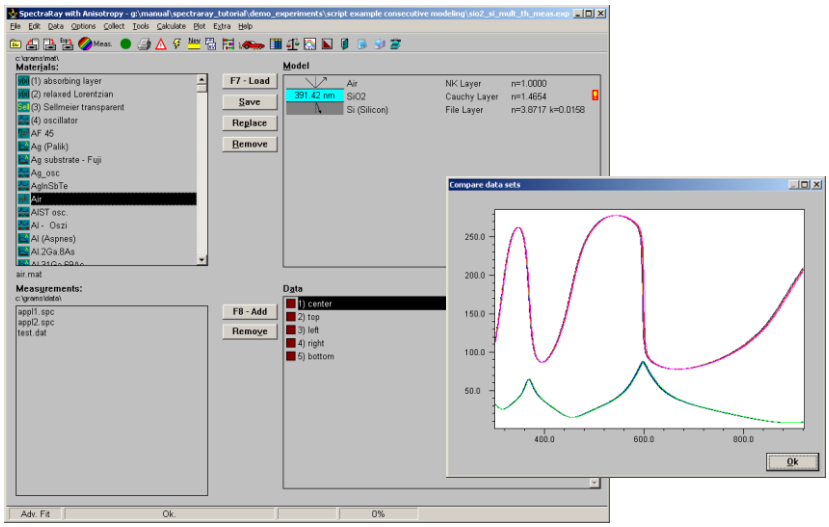
Script with comments:

```
;title=Example 04: Assigning values to imported R measurement

integer n

; the amount of datasets is saved to the variable n
CountDataSets n

; the x-axis is set to wavelength / nm
SetXUnit n WAVELENGTH

; the y-axis is set to wavelength / nm
; 0 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
SetYUnit n 0 REFLECTIVITY

; the z-axis is set to the angle of incidence "PHI"
SetSubUnit n 0 PHI

; the value of the angle of incidence is set to 8°
SetSubVal n 0 8
```

After executing the script all units and values are assigned as shown in the following screenshot.

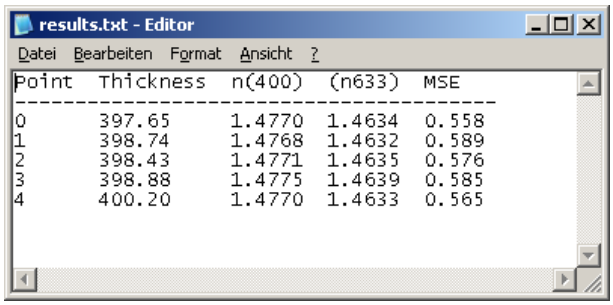
6.2.4 Consecutive fitting of n datasets using the same optical model

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.



The script shares the writing of messages into a file with SPECTRARAY II. That means SPECTRARAY uses a logfile which is used to write messages into it. The script also can write into the same logfile. To overcome this problem, the filename of the logfile is renamed to the one the script wants to every time when a message is written into it. After that the logfilename is restored to the one SEPCTRARAY II is using.

The result file is called results.txt and it is saved into the same directory where SEPCTRARAY II is located. It shows a unit name header and the columns with the results:



This is the script file with comments:

```
;title=Example 05: Consecutive fitting of multiple measurements

integer i,n
double th,n400,n633,k,MSE
string sth,sn400,sn633,sMSE

; *************************
; Deleting the old logfile
; *************************

logfile {.}\results.txt
eraselogfile
logfile {.}pmodell.log

; *************************
; Writing logfile header
; *************************

logfile {.}results.txt
logmessage Point__Thickness__n(400)__(n633)__MSE
logmessage ----------------------------------------
logfile {.}pmodell.log

; Initial settings of the variables
i = 0
CountDataSets n
n = n+1

; ****************************
; Deselecting all datasets
; ****************************
; Begin of the loop1
Label1:

SetDataUse i 1 0
SetDataUse i 2 0
i = i+1

if i<n Label1
; End of the loop1

i = 0

; ****************************
; Fit of all measurements
; ****************************

; Begin of the loop
Label2:

; Selecting the actual dataset
SetDataUse i 1 1
SetDataUse i 2 1

; Starting the fit
autofit
```

```
; Reading the film thickness of the first experiment (0) of the first layer (1)
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
getmodellayerrefrindex 0 1 400 n400 k
getmodellayerrefrindex 0 1 633 n633 k

;Reading the MSE value
MSE = GetLSQ

; 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
logfile {.}results.txt
logmessage $i$_____$sth$_____$sn400$__$sn633$__$sMSE$
logfile {.}pmodell.log

; Deselecting the actual dataset
SetDataUse i 1 0
SetDataUse i 2 0
; incremenent of the actual dataset
i = i+1

; Jump to label 2
if i<n Label2
; End of the loop

; ***********************************
; End of Fit of all measurements
; ***********************************



; display of the results by starting the external notepad program
shell notepad.exe {.}\results.txt
```

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=consecutive measurements

double CurrentAngle
integer i,number,tinitial,tellapsed,tdiff
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
tinitial = timedifference

;****************************
;label, loope begins here
;****************************
jumphere:

tdiff = timedifference
tellapsed = tdiff - tinitial

dbl2str i snumber 0
dbl2str tellapsed stellapsed 0

; writes status information of measurement number
; and ellapsed time into the status bar of SPECTRARAY II
STATUSTEXT Current measurement number:_$snumber$__ellapsed_time:_$stellapsed$_s

; start the ellipsomtric measurement
runscript {.}sysscr\\meastool.scr SingleMeasurement

; delay if necessary (waits now for 1000 ms)
delay 1000

i = i +1
if i<number jumphere
;******************
; loop ends here
;******************
```

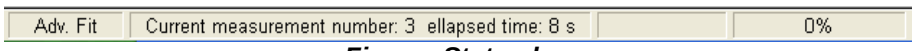


Figure: Status bar

6.2.6 Calculation of the sheet resistance of conductive films

Films like TCO's or $SrTiO_{3-x}$ show conductivity due to free carrier absorption. This is mostly observed in the NIR spectral range. The Drude equation of the Drude-Lorentz model is used to describe this absorption. Its parameters can be used to calculate the sheet resistance of the film using the following formula.

$$R_s = 6 \cdot 10^8 \cdot \frac{\omega_\tau}{\omega_p^2 \cdot d}$$

ω_p and ω_τ are the Drude parameters. They are read out from the parameter list of the current experiment and Rs is calculated then. It is necessary to have the experiment ready where the model fits the measured data well based on the Drude model.

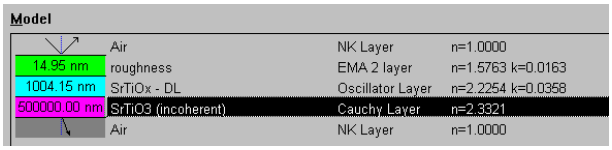


Figure: Optical model

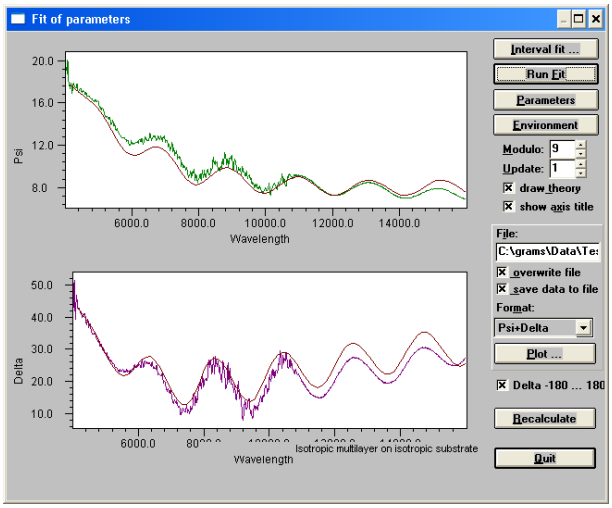


Figure: Model and fit in fitting window

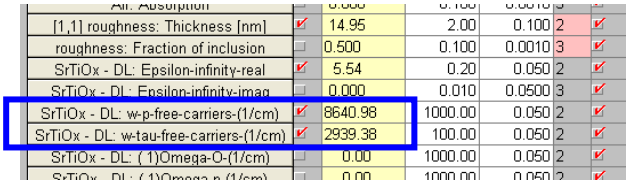


Figure: parameter names of wp and wt of the Drude part in the parameter list

```
;title=Calculation of sheet resistance Rs

double Rs,wp,wt,d

; The SrTiOx film is the second film in the stack - thickness is read
d = getparameter [1,2]

; wp and wt are read from the SrTiO3 film
; the parameter names don't need to be complete
; it is sufficient if they can be clearly distinguished from other parameter names

wp = getparameter  SrTiOx_-_DL:_w-p-
wt = getparameter SrTiOx_-_DL:_w-tau-

; Calculation of the sheet resistance
Rs = 600000000 * wt / wp / wp / d

; Message box showing result
message Rs=_$Rs$_Ohm_square
```

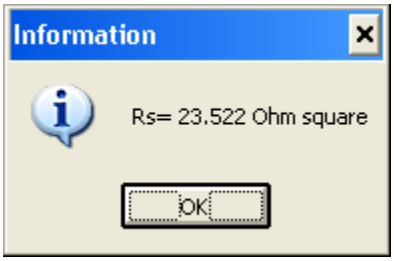
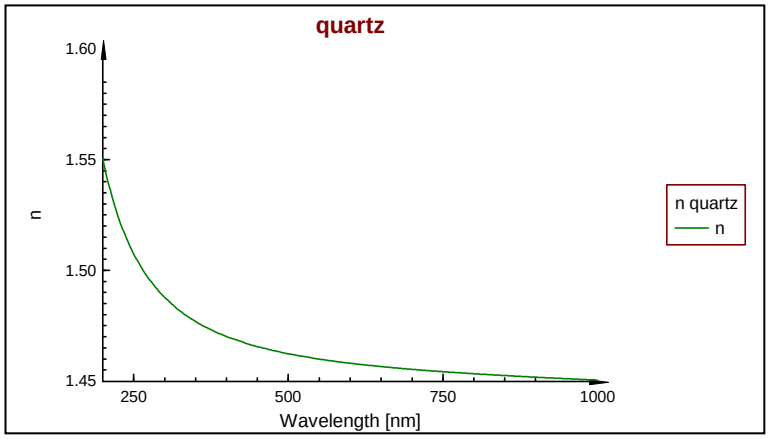


Figure: message box with Rs result

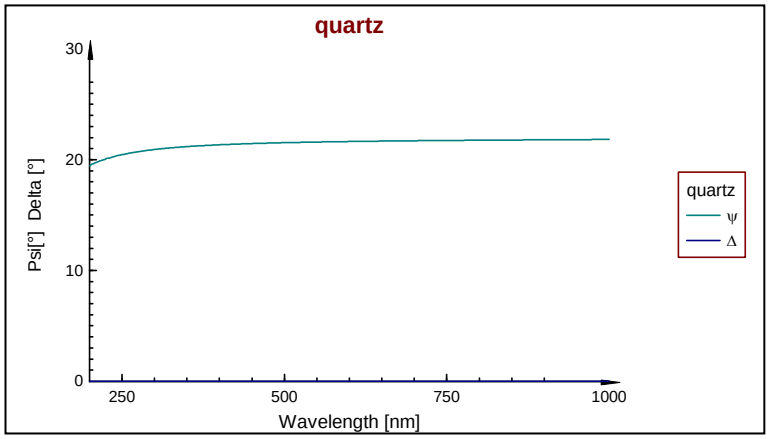
6.3. Measurement of substrates

6.3.1 Transparent substrates

The dispersion of transparent materials is strictly increasing to lower wavelength (higher photon energies). There is no additional structure in the transparent spectral range.

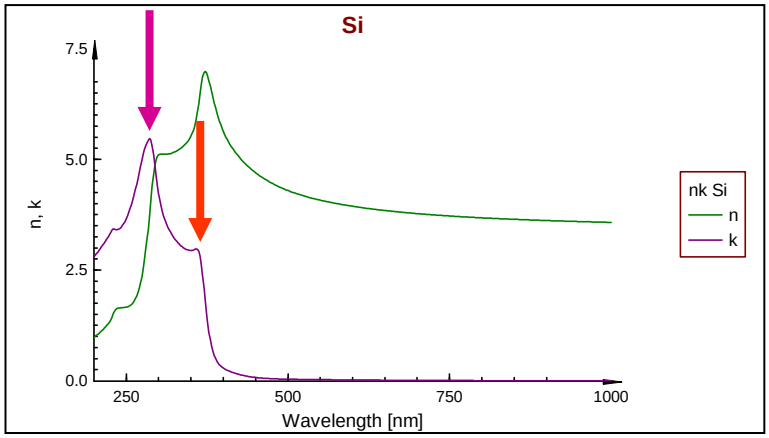


This results also in monotone spectra (here at Φ=70°). Ψ shows no particular structures. Δ is constant at 0°. It can also be constant at 180° when the angle incidence is lower than the brewster angle.

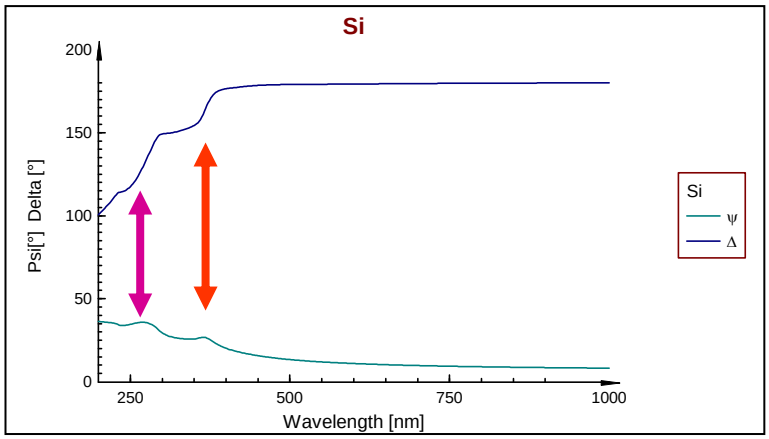


6.3.2 Absorbing substrates

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.

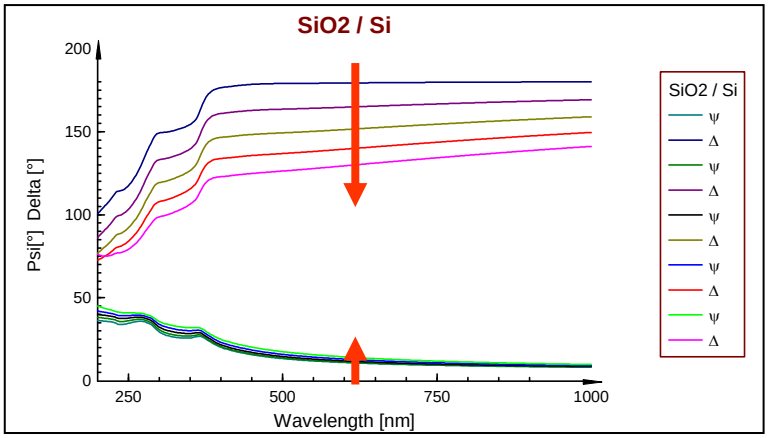


These characteristic structures appear also appear as structures in the ellipsometric spectra Ψ and Δ.



6.3.3 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 an a strong and almost constant shift with increasing SiO_2 film thickness. On the other hand Ψ shows only a little change, which is rather higher in the UV than in the NIR spectral range.

The huge effect in Δ is the reason for the enormous sensitivity of ellipsometry to very thin films compared to reflectivity measurements.

The weak effect in Ψ is the reason why for thin transplant films in the thickness range below 25 nm the optical constants are fixed and the remaining fitting parameter is just the film thickness.

7. Application examples

7.1. CET procedure

CET :(**C**ombined **E**llipsometry and **T**ransmission)

Example: P2000 (polymer / C60 fullerenes blend)

7.1.1 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 ca 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 70deg). This measurement was performed on a roughened substrate so no backside reflections occur.

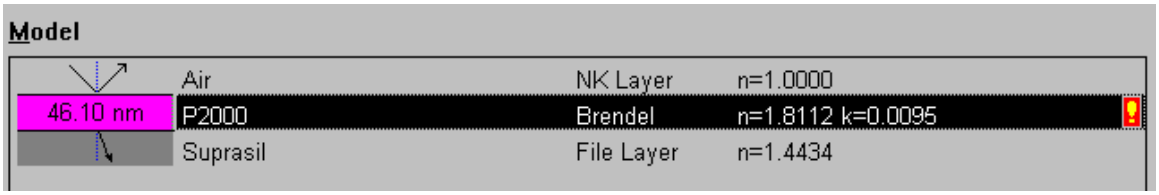
The transmission measurement is done with a polished substrate of course. It is saved as an *.spc file.

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 PSI, DEL 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.

7.1.2 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.



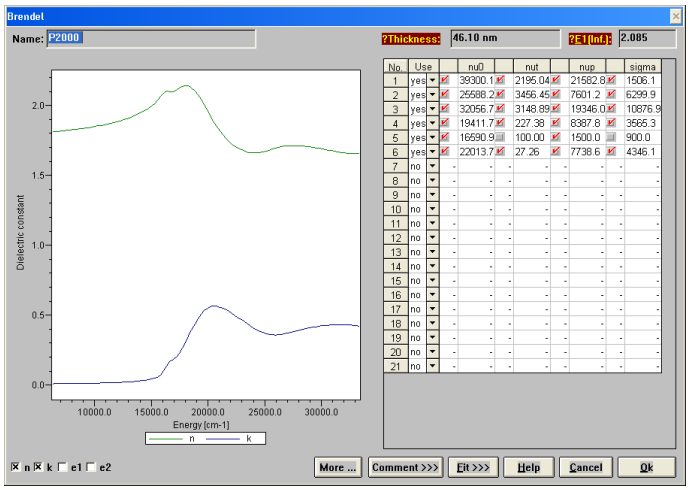


Figure: Dispersion of P2000 describe using Brendel oscillator model

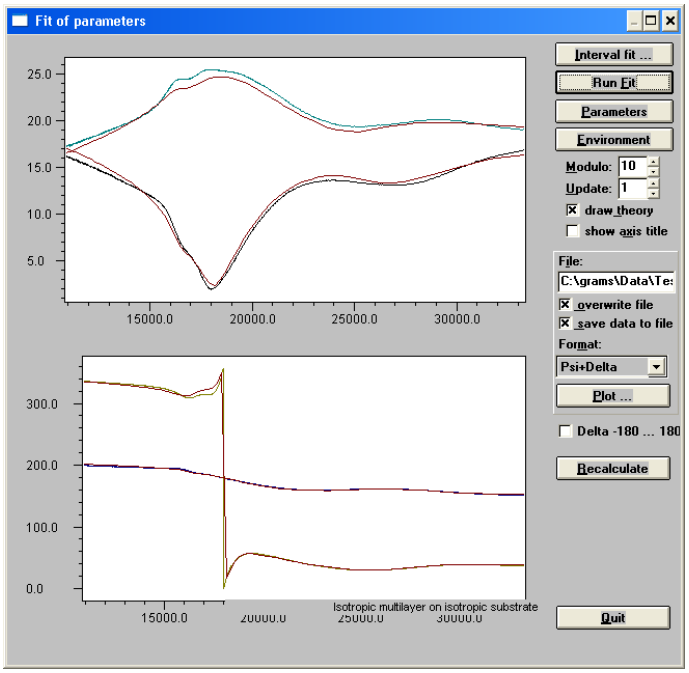
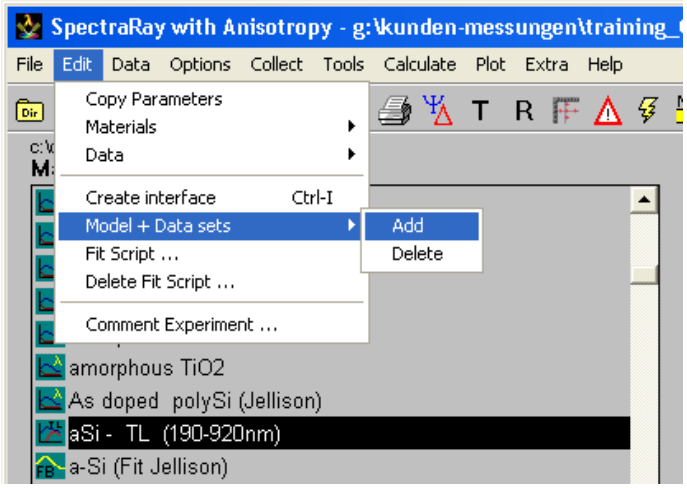


Figure: Measurement and model at Phi = 50and 70deg

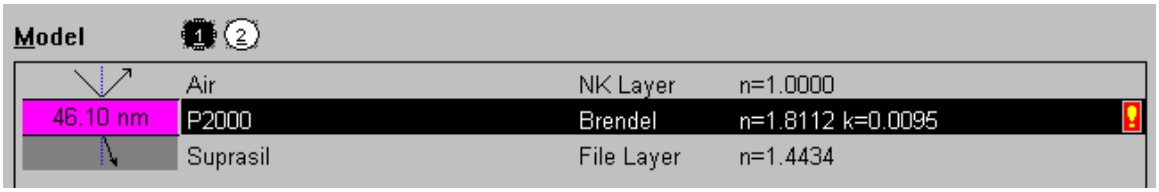
7.1.3 Second experiment for transmission

Creating the second experiment

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



On top of the model window two icons appear (1) and (2) . By selecting an icon it can be switched between both experiments.



The inverted icon represents the selected experiment.

Building the model for the second experiment
The model is practically identical with some extensions. The model from the first experiment is coped to second one by:

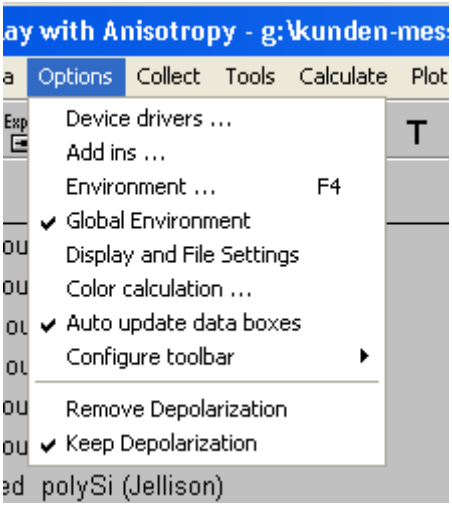
- Selecting the first experiment
- Menu → Tools → Make equal models

Then the second experiment is selected
Air is copied below the “Suprasil” (e.g.: “CTRL” + moving Air with mouse cursor) and the correct substrate thickness is entered for suprasil.

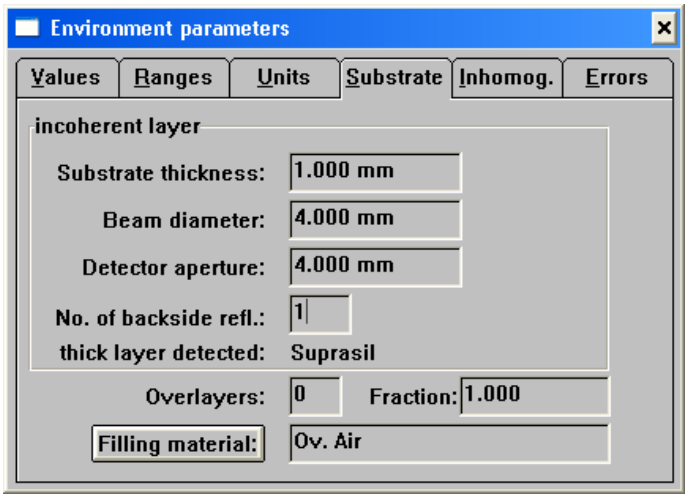
7.1.4 Setting the environmental parameters for the second experiment

Then the incoherent calculation must be activated for the second experiment. Momentarily the environmental conditions are valid for all experiments. They are “global”.

This is switched off by Menu → Options → Deselecting “Global Environment”
The checkmark must disappear



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



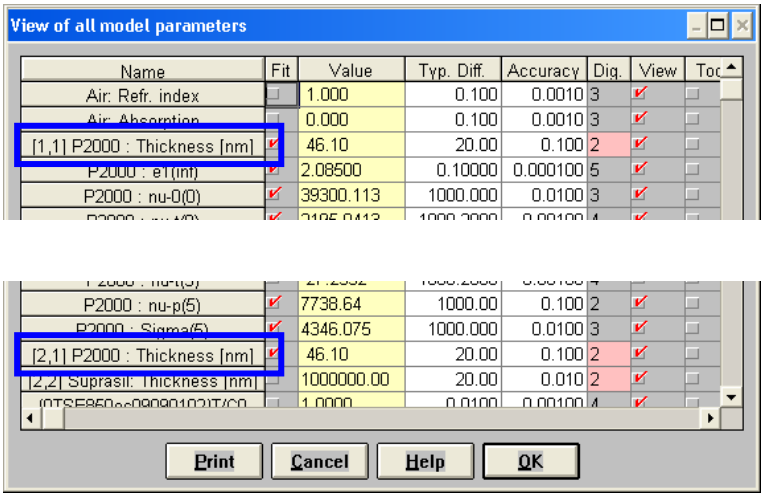
The transmission measurement is loaded into the dataset of the second experiment by Menu → File →Load (*.spc extension is selected)

The two experiments appear as shown in the screenshot:

All materials having the same name also have the same parameters with on exception: the film thickness is independent in both experiments. But the thickness also must the same. Otherwise this combination doesn't overcome the ambiguity problems.

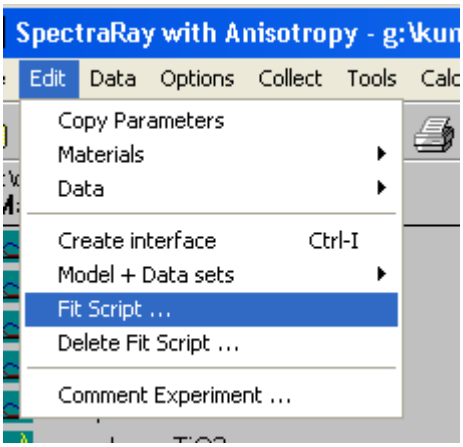
7.1.5 Creating the “fit script”

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:



It is not necessary to use the full name for the fit script. SO many character are necessary until it can be is identically recognized by the fit script. Therefore “[1,1]” and “[2,1]” are sufficient to be used in the fit script.

The fit script is now created by: Menu → Edit → Fit script …



Currently no fit script exists. Therefore the following message appears:

After confirming the message box a basic fir script is created. Momentarily this fir script has no effect.

The fit script must be completed using the necessary commands inserting at the correct positions:

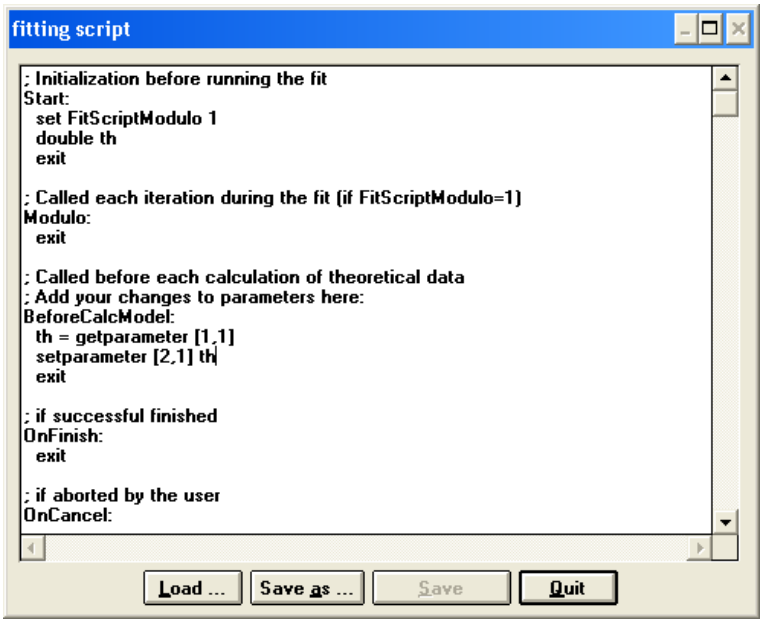
A variable for the thickness must be declared in the “Start:” section using the command:

double th

The thickness is read out from the first experiment and copied to the second in the “BeforeCalcModel:” section:

Th = getparameter [1,1]
Setparameter [2,1] th

The fit script appears as follows:



The fit script can be closed using “Quit”. It is not necessary to save it separately. It will be automatically saved with then actual experiment file.

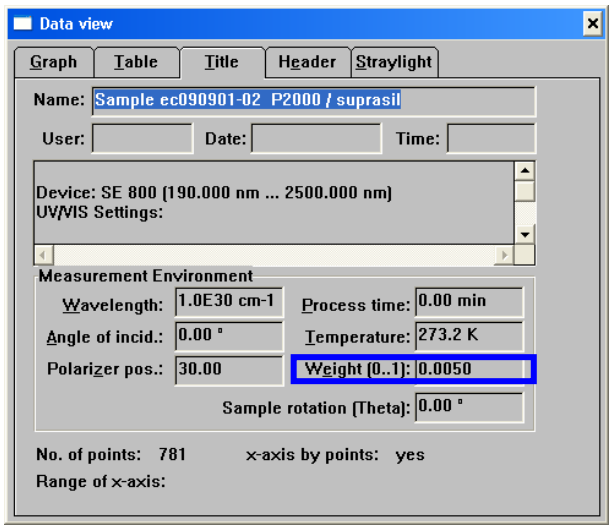
7.1.6 Fitting the CET model

The range of values of the PSI, DELTA measurement is 0 … 90 and 0 … 360 deg while transmission is only between 0 … 1.

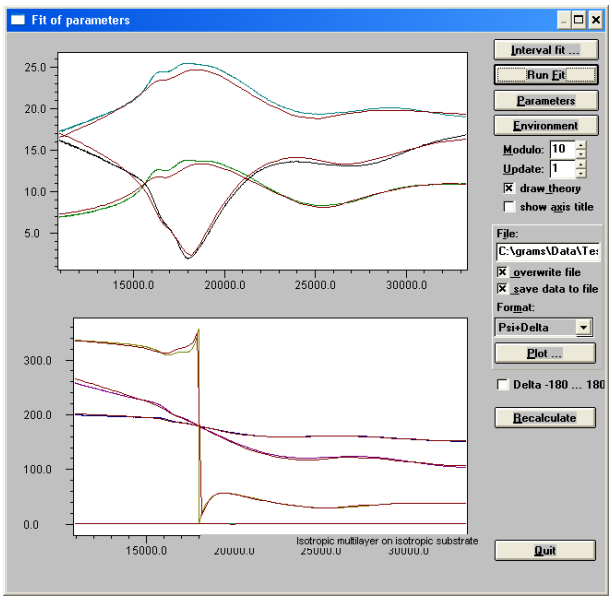
The will lead to a strong overestimation of the PSI, DEL measurement and the transmission measurement won't have an effect.

Two ways are possible to overcome this problem:
1) The PSI, DEL measurement can be converted to the fourier-coefficients (s1, s2). Their range is from -1 … +1 and therefore very similar to the transmission range.

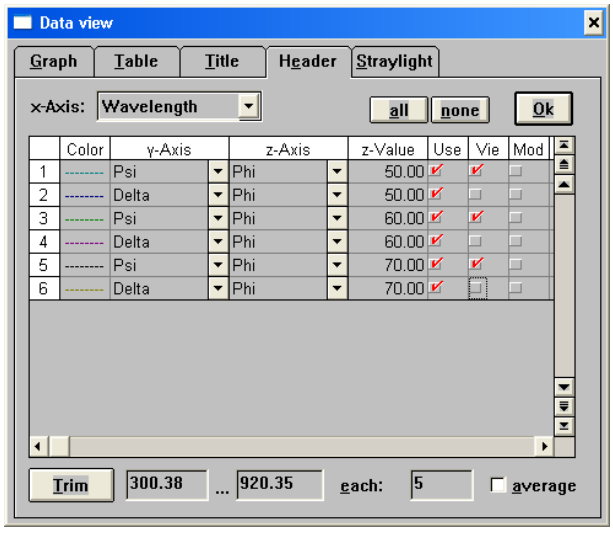
2) If this conversion is not wanted, then the weight of the PSI, DEL measurement for the MSE value of the fitting procedure must be reduced strongly.
This is done in the "Title" tab of the PSI, DEL measurement. In this example it is reduced from 1 to 0.005.



When the fitting screen is opened then PSI, DEL is displayed as usual. The transmission measurement is displayed in the DEL window. It is hard to see it because it is just a straight line at zero and fitting quality can't be estimated.

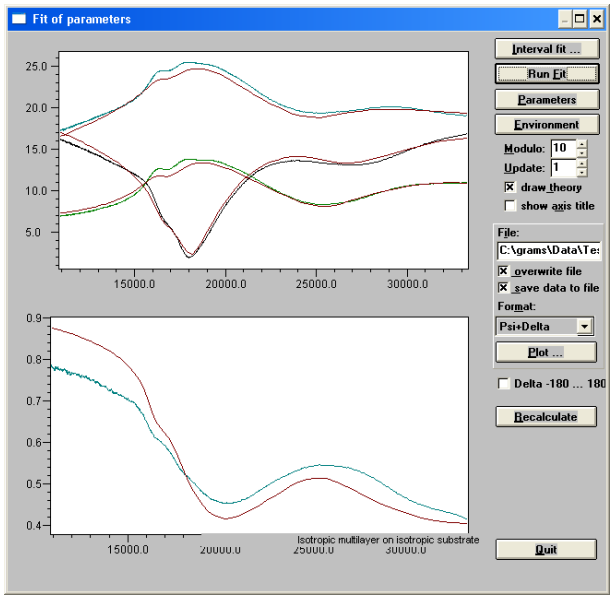


In order to make Transmission visible the DEL measurement can be hided from this display. This is done in the “Header” tab of the PSI, DEL measurement



The checkmarks for DEL are deselected I the “View” column. Now the DEL 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.



7.2. Shifted Interval Fit + Parameterization with Tauc-Lorentz oscillator model

A photoresist film should be measured. 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 obtain the dispersion of n and k of 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 example shows the analysis of the dispersion of n and k in the full spectral range using the “Shifted Interval fit” procedure.

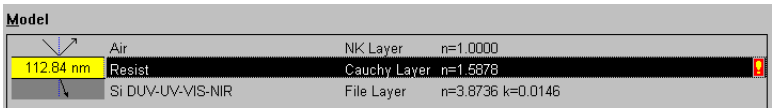
This is followed by fitting the Tauc-Lorentz oscillator dispersion to the dispersion obtained from the interval fit.

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 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 to 920 nm.

The fit parameters of the resist film are the film thickness and Cauchy coefficient N0, N1, N2.

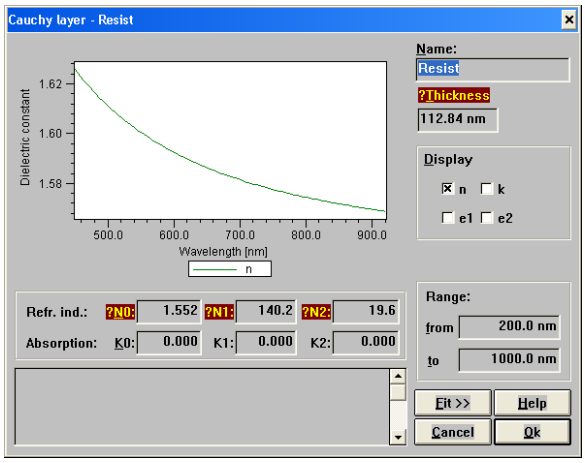


Figure: Cauchy model of the resist film

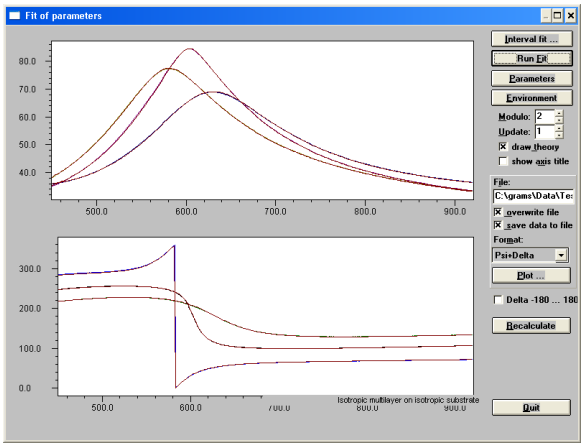


Figure: The measurement and model after fitting

The model shows an ideal fit to the measurement.

A film thickness of **112.8 nm** is obtained.

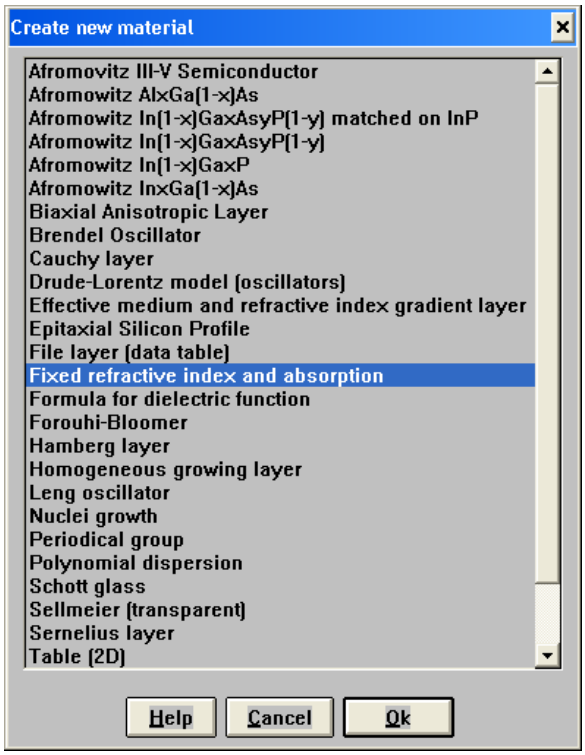
Step 2) Setup of the model for the “Shifted interval fit”

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 “Fixed refractive index and absorption” type and Press “ok”.

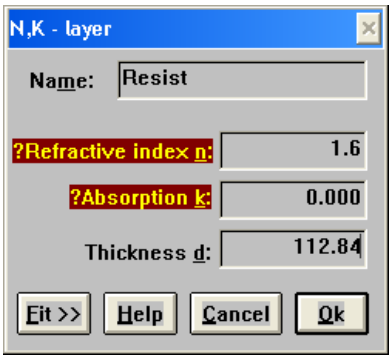


Double click the “Fixed refractive index and absorption” layer. The “N,K layer” window is opened.

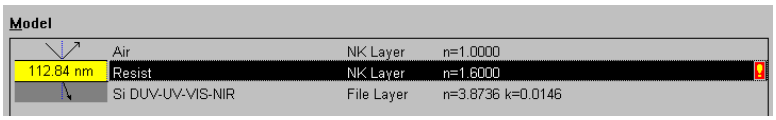
Enter the film thickness obtained from the former modeling (Here: th = 112.84 nm)

Select n and k as fit parameter.

Set a starting value for n of n=1.6



Press “Ok”. The layer is inserted now into the model. Move it to the correct position. The model appears now as follows:



Step 3) “Shifted interval fit”

The used spectral range is set to 240 to 920 nm.

The fitting window is opened now.

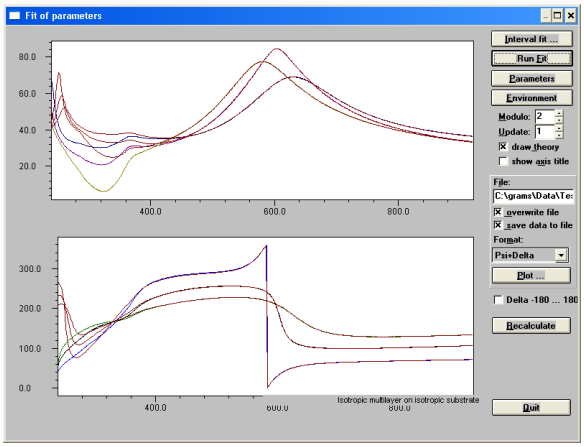


Figure: Measurement and model with new model with fith “N,K layer”. The model fits well in the VIS. The UV shows deviations because the absorption of the resist isn’t described in the model

Press the “Interval Fit …” button. The Shifted Interval Fit window is opened. Select 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 an structures in the spectrum)

width: 5 nm (width of the fitted interval, it It should be sufficiently narrow in order not to average the structures in the spectrum)

Max. Iterations: 100 (the fitting of each interval will be stopped at least after 100 steps of iteration

Stop fit if MSE if less than: 0.00 (the Fit quality is not used to limit the amount of fit iterations)

Press clear results: (in case old results are shown in the results section)

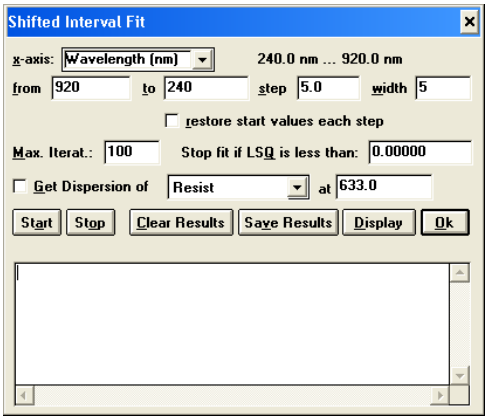
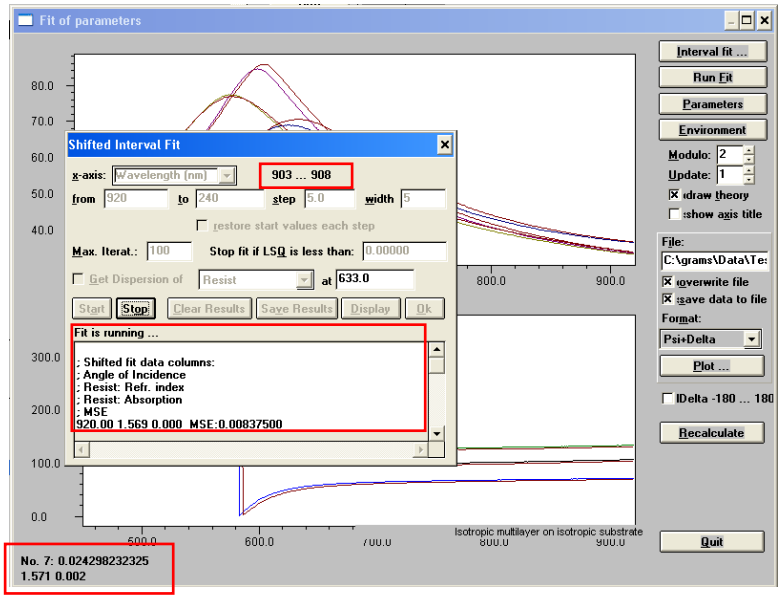


Figure: “Shifted interval fit” window

The “Start” button is pressed to initiate the fitting procedure. The fit is now done step by step. The progress is shown in the “Shifted interval fit” window, where the actual interval is displayed. 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 can be displayed by pressing the “Display” button. The dispersion of n and k as well as the MSE value are displayed.

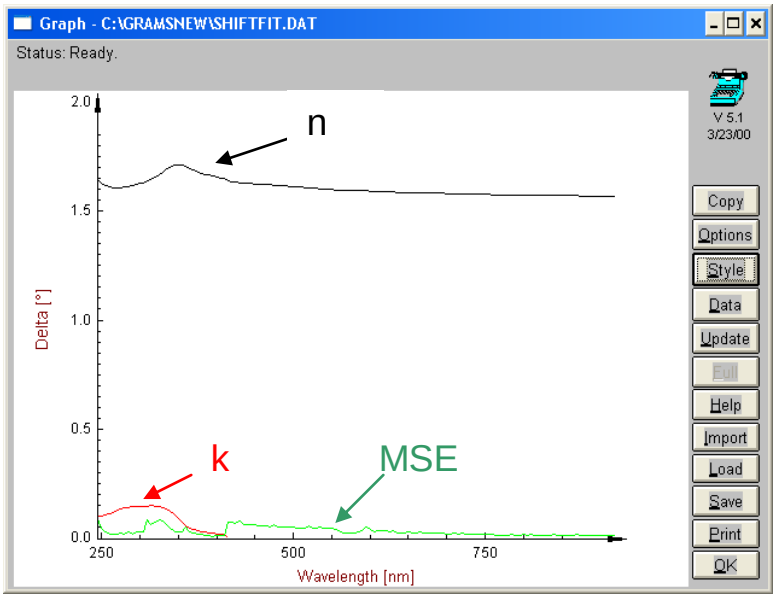
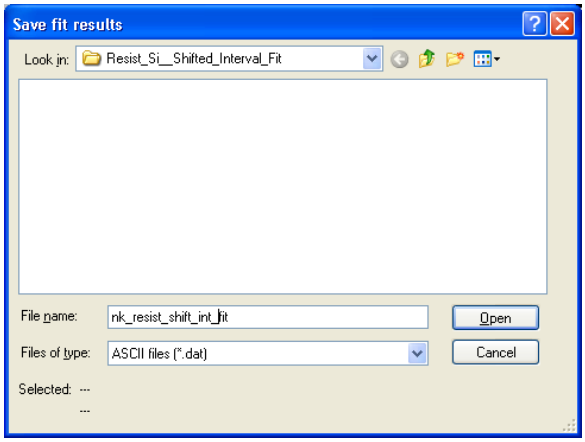


Figure: “Shifted Interval Fit” results

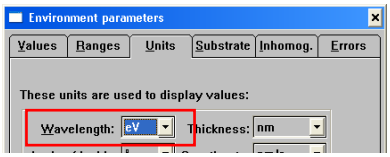
The results of the fitting procedure are saved now as a “dat” file: press the “Save results” icon and select a meaningful filename for the results file.



The “shifted interval fit” and the “fitting” window can be closed now. The experiment can be saved.

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).



Import of the dispersion data

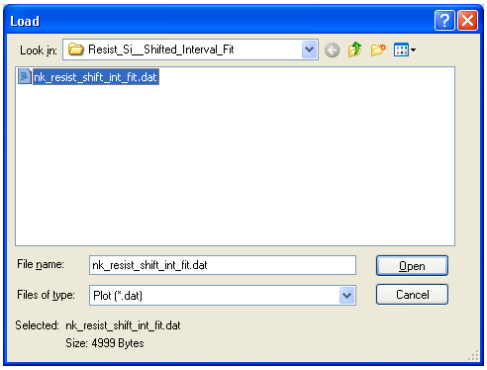
The dispersion data must be imported now to the “Data” section of SPECTRARAY

Select from menu: File → Load File …

Select File extension: (*.dat)

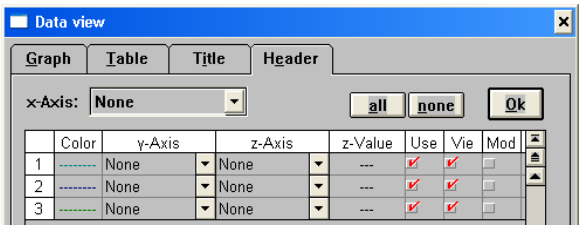
Select the results file.

It is imported to the Data section.

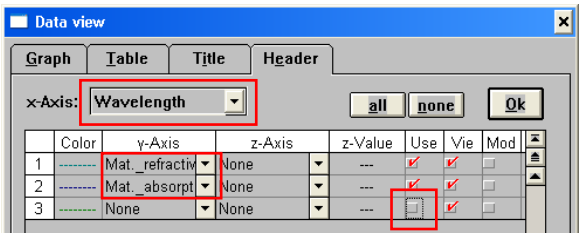


When the file is imported the unit of each parameter is unknown. It must be set manually.

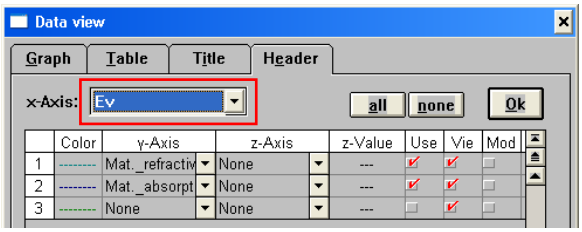
Open the results file and enter the “Header” tab.



Assign the units of the parameters. The 3rd row is the MSE value. It can be neglected. Simply switch off “Use” for the 3rd row as shown in the screenshot:



It is recommended to convert the x-Axis from “wavelength” scale to “eV” (photon energy) to simplify the next step of modeling. This is simply done by selecting “eV” instead of wavelength. The conversion is done automatically now.

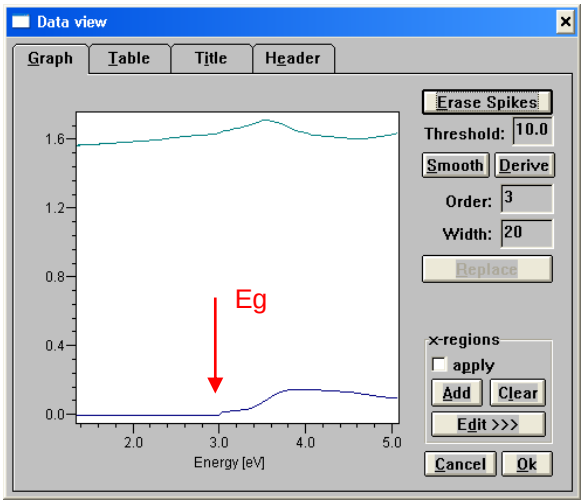


Step 5) Modeling

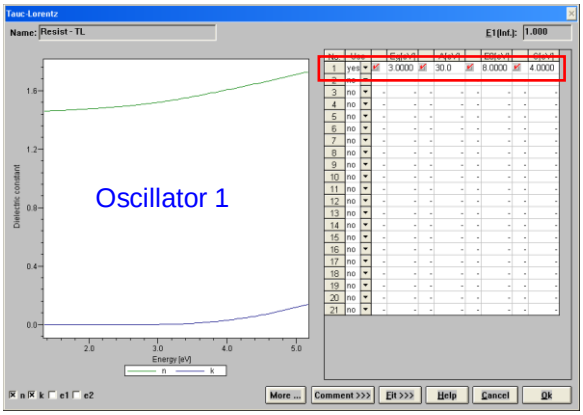
A model with ambient “Air” and a new “Tauc-Lorentz” layer is created. The Tauc-Lorentz Layer is renamed to “Resist – TL”

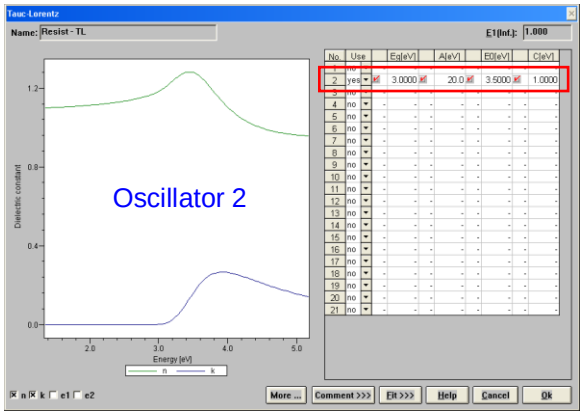
The next step is to find starting values for the Tauc-Lorentz oscillator.

The result of the “shifted interval fit” is investigated. The absorption (bandgap E_g) 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.

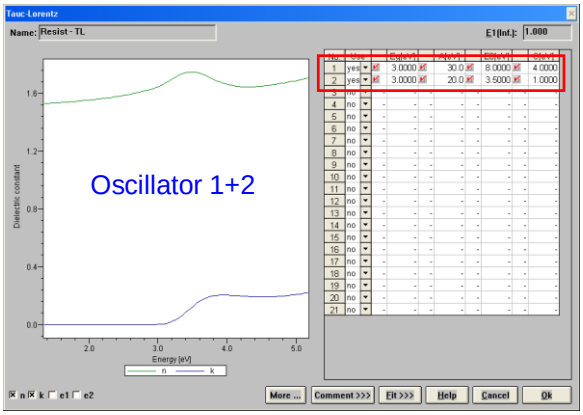


The following two oscillators are build up using the Tauc/Lorentz oscillator model:





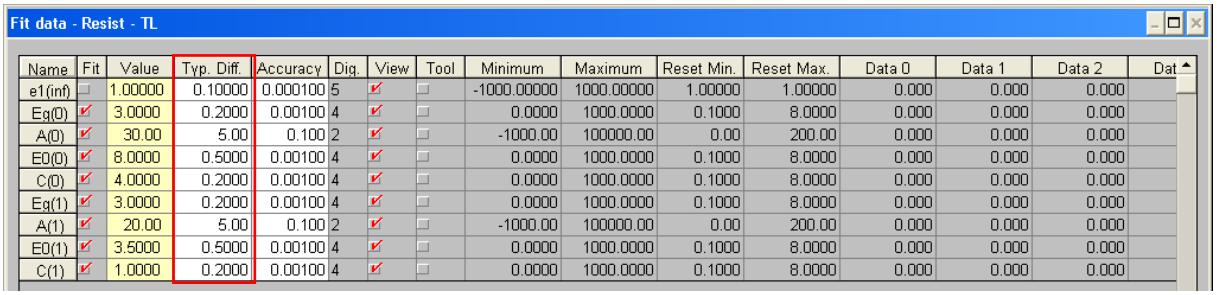
The combination of both oscillators is already quite similar to the “shifted interval fit” results:



Step 6) Fitting the Tauc-Lorentz layer (Oscillator 1 +2) to the "shifted interval fit" results

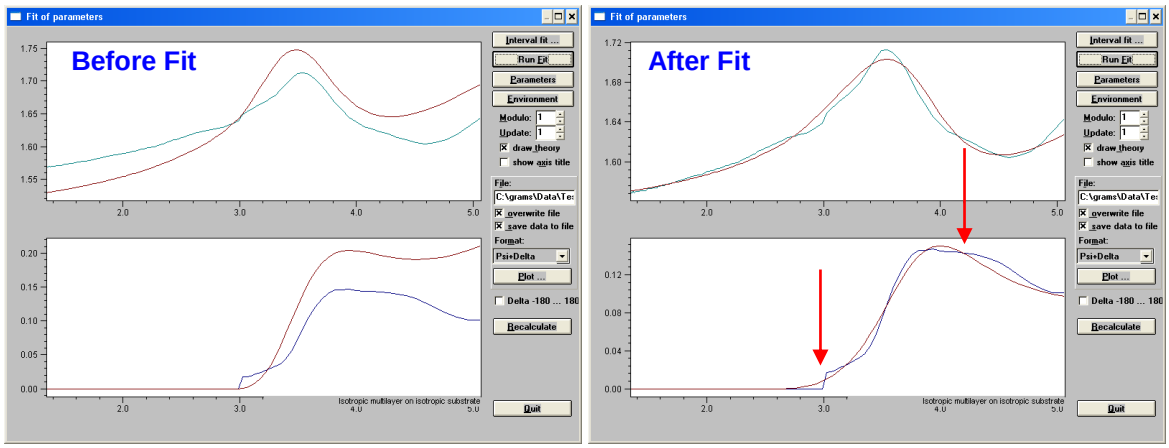
When the start parameters were found the "typical differences" are set to reasonable values to ensure a good fit progress.

Press "Fit >>>" in the "Resist - TL" Tauc-Lorentz oscillator window. Select the typical differences as shown in the screenshot:



Name	Fit	Value	Typ. Diff.	Accuracy	Dig.	View	Tool	Minimum	Maximum	Reset Min.	Reset Max.	Data 0	Data 1	Data 2	Dat
e1(inf)		1.00000	0.10000	0.000100	5			-1000.00000	1000.00000	1.00000	1.00000	0.000	0.000	0.000	
Eg(0)		3.0000	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
A(0)		30.00	5.00	0.100	2			-1000.00	100000.00	0.00	200.00	0.000	0.000	0.000	
E0(0)		8.0000	0.5000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
C(0)		4.0000	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
Eg(1)		3.0000	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
A(1)		20.00	5.00	0.100	2			-1000.00	100000.00	0.00	200.00	0.000	0.000	0.000	
E0(1)		3.5000	0.5000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
C(1)		1.0000	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	

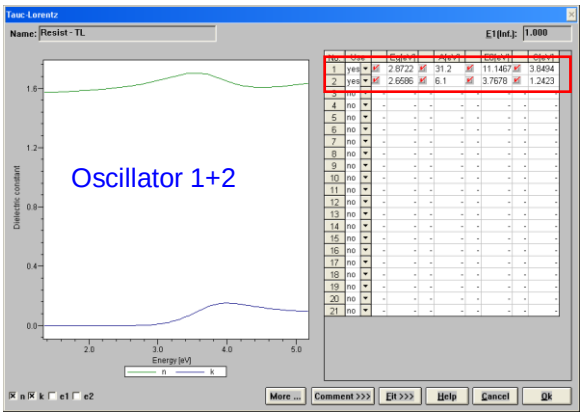
The window can be closed and the fitting window is opened and the fit procedure is initiated. After the fitting, there are still some deviations visible, which are indicated by the red arrows.

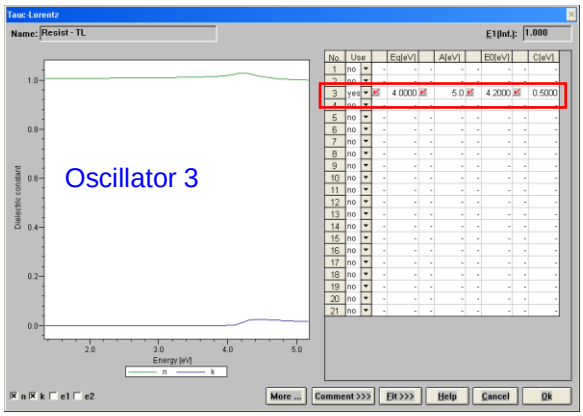


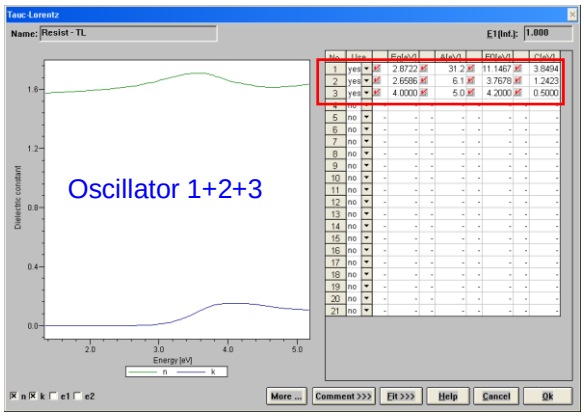
The deviation around 3.0 eV is likey an artifact by the "shifted interval fit procedure". It will be neglected.

The structure at 4.0 eV seems to be an additional oscillator.

Step 7) Introduction of a third oscillator into the Tauc-Lorentz layer at around 4.0 eV



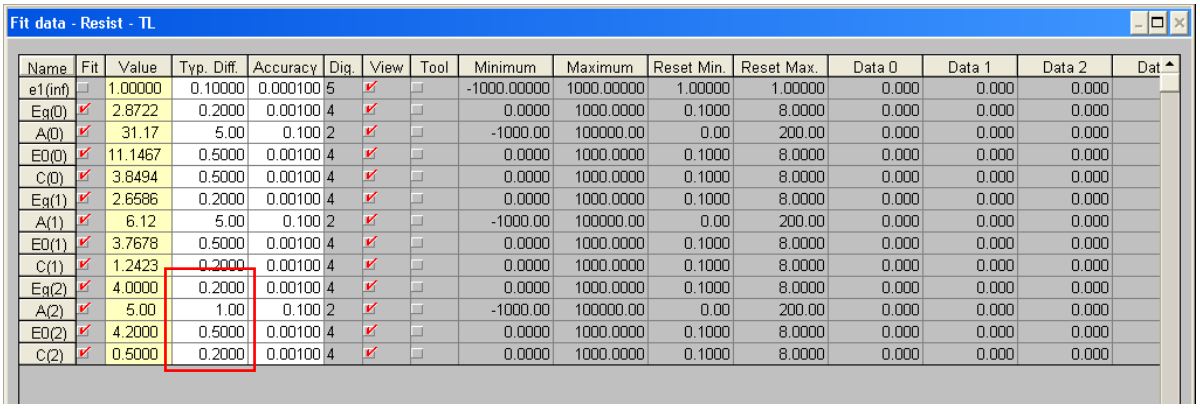




Step 8) Fitting the Tauc-Lorentz layer (Oscillator 1+2+3) to the "shifted interval fit" results

When the start parameters were found the "typical differences" for oscillator 3 are set to reasonable values to ensure a good fit progress.

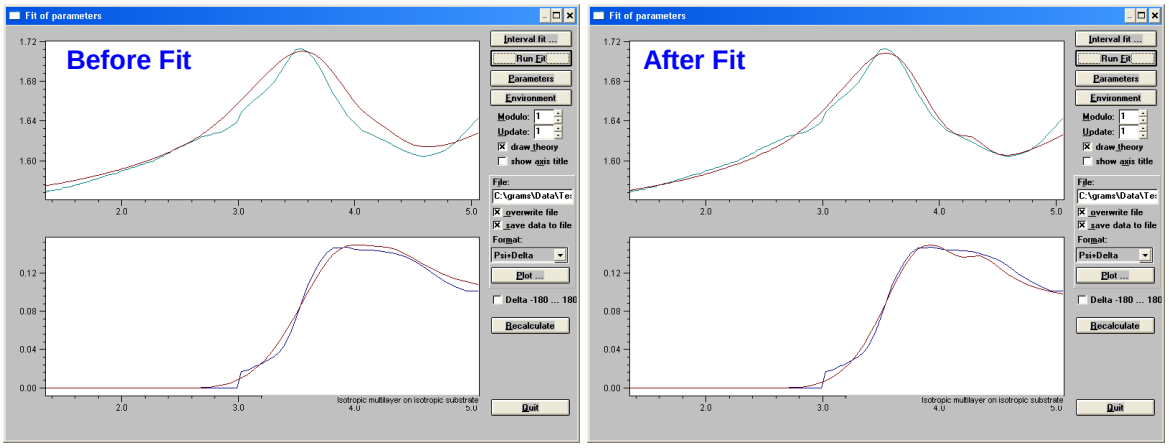
Press "Fit >>>" in the "Resist - TL" Tauc-Lorentz oscillator window. Select the typical differences as shown in the screenshot:



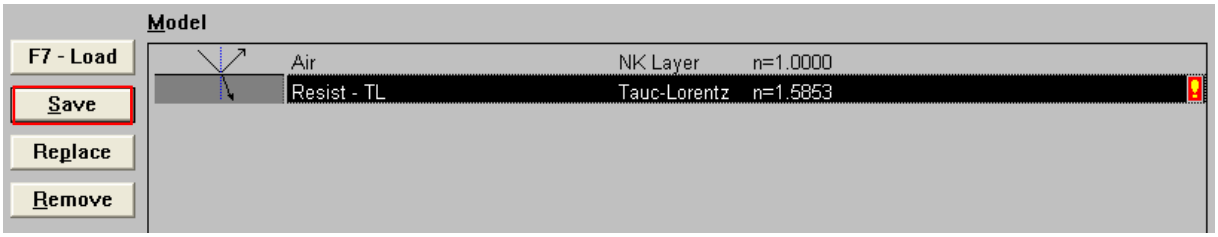
Name	Fit	Value	Typ. Diff.	Accuracy	Dig.	View	Tool	Minimum	Maximum	Reset Min.	Reset Max.	Data 0	Data 1	Data 2	Dat
e1(inf)		1.00000	0.10000	0.000100	5			-1000.00000	1000.00000	1.00000	1.00000	0.000	0.000	0.000	
Eg(0)		2.8722	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
A(0)		31.17	5.00	0.100	2			-1000.00	100000.00	0.00	200.00	0.000	0.000	0.000	
E0(0)		11.1467	0.5000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
C(0)		3.8494	0.5000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
Eg(1)		2.6586	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
A(1)		6.12	5.00	0.100	2			-1000.00	100000.00	0.00	200.00	0.000	0.000	0.000	
E0(1)		3.7678	0.5000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
C(1)		1.2423	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
Eg(2)		4.0000	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
A(2)		5.00	1.00	0.100	2			-1000.00	100000.00	0.00	200.00	0.000	0.000	0.000	
E0(2)		4.2000	0.5000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	
C(2)		0.5000	0.2000	0.00100	4			0.0000	1000.0000	0.1000	8.0000	0.000	0.000	0.000	

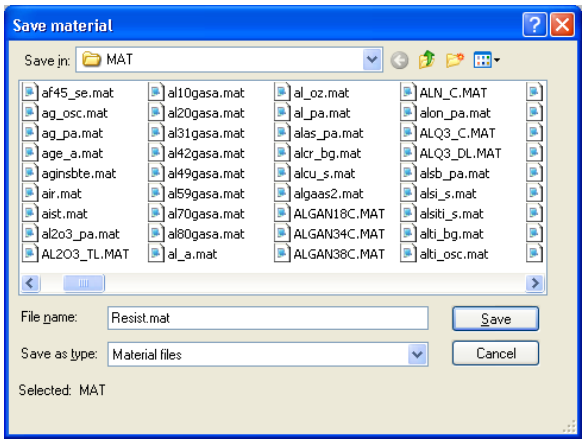
The window can be closed and the fitting window is opened and the fit procedure is initiated.

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.



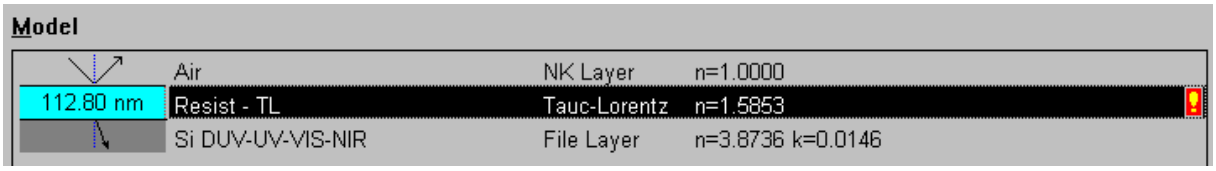


The layer is saved in c:\grams\mat directory using the filename “Resist.mat”. When it is saved the material library is updated and the new material is available.

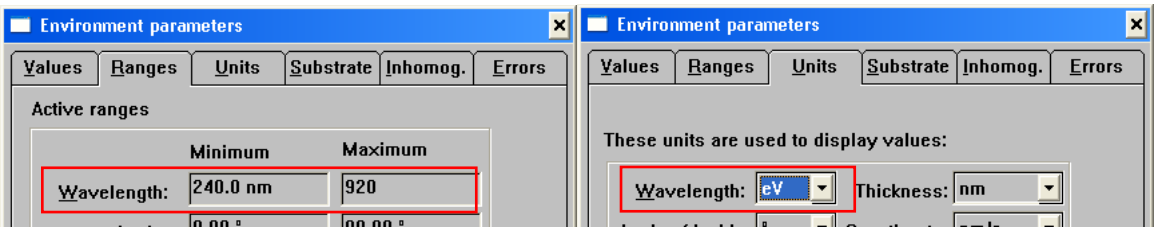
If the update is not done automatically it must be initiated manually: select the “Dir” icon from the icon bar and press “OK”.

Step 9) Fitting the Tauc-Lorentz layer (Oscillator 1+2+3) to the Ψ, Δ measurement results

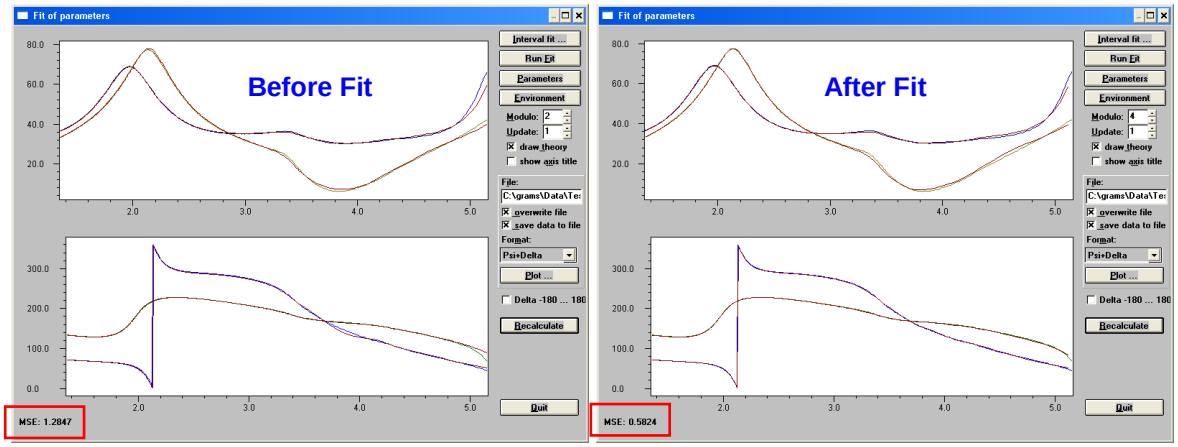
The initial experiment is loaded which contains the Cauchy-Model and the original Ψ, Δ measurements. The Cauchy layer is replaced by the Tauc-Lorentz layer from the material library.



The spectral range is set to 240 to 920 nm. Then the wavelength scale is set from wavelength to photon energy (eV).

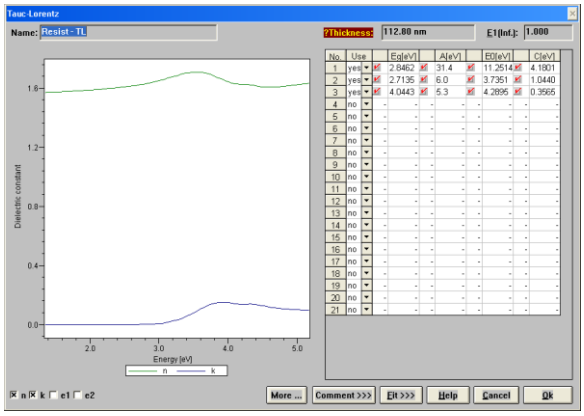


The fitting window is opened and the fit procedure is initiated.



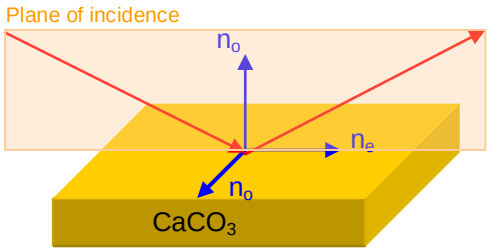
The MSE value finally was improve from 1.28 to 0.58. The model fits the measurement well.

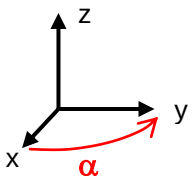
The final dispersion of the Resist film is shown in the following screenshot:



7.3. 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.





n_o : refractive index $n_{ordinary}$

n_e : refractive index $n_{extraordinary}$

α: angle n_e relative to x

θ: Sample stage rotation

Figure: Anisotropic sample and coordinate system

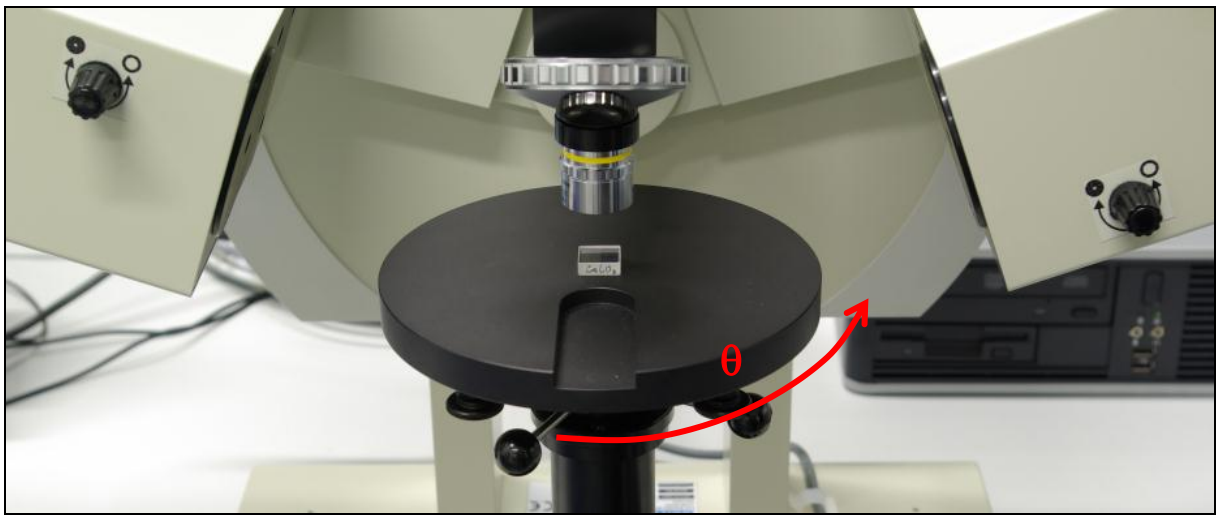


Figure: Sample on rotatable sample stage

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 condition of the rotatable stage are added to the standard measurement dialog for spectroscopic meausurements.

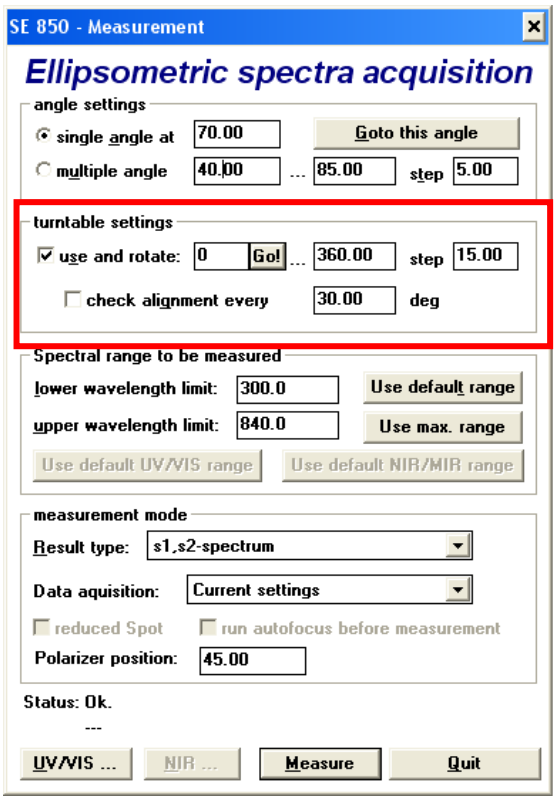
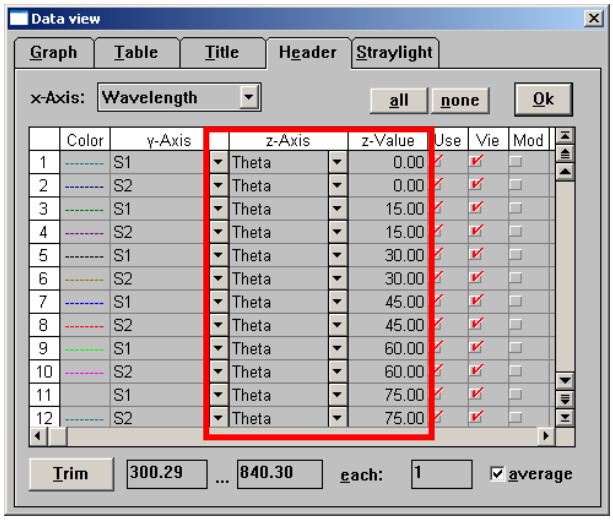


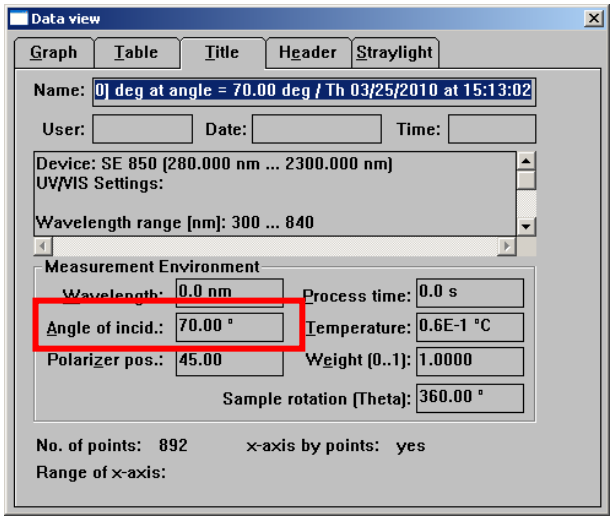
Figure: Measurement dialog with added rotatable stage settings

In the example above the stage is rotated from θ = 0° to 360° every 15°. This results in a set of measurements added as a single dataset to the data section of SPECTRARAY.

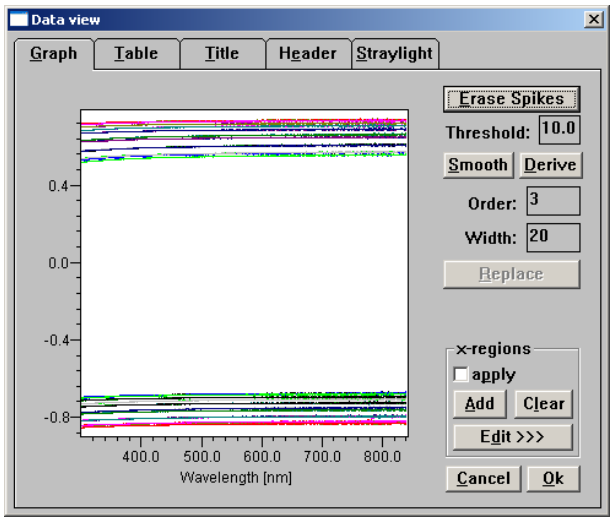
The Tab “Header” section shows the individual spectra for each angle θ.



The angle of incidence is shown in the tab “Title”.

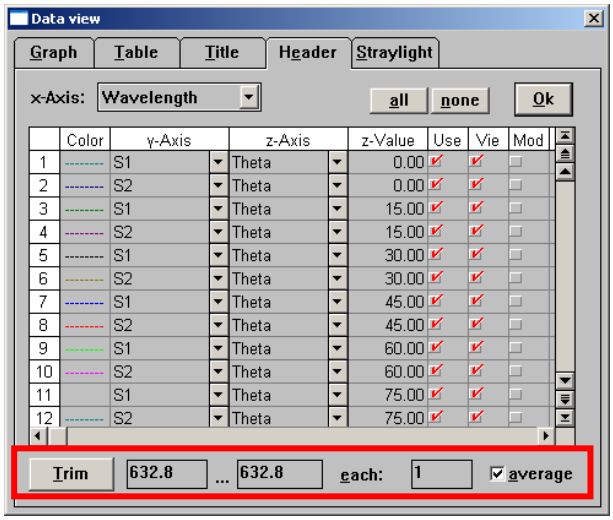


The Tab “Graph” section shows all measurements:

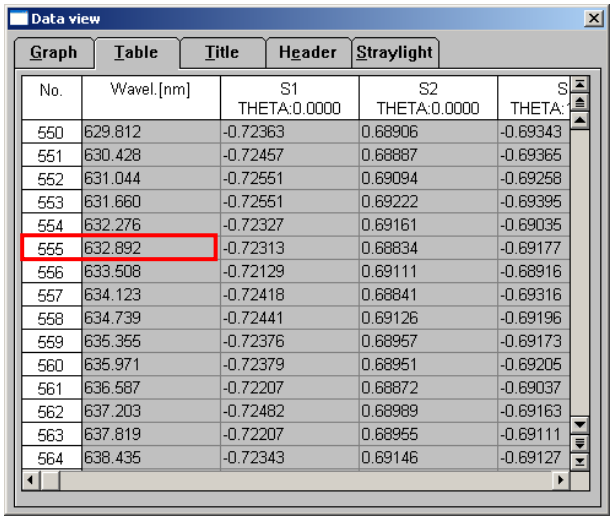


The different spectra taken at different sample rotation angles θ show distinct deviations as a result from the anisotropy of the $CaCO_3$ substrate. The spectra show a parallel shift to each other, so the observation at a single wavelength instead of the full spectra will be sufficient. Now the s1, s2 values for e.g. 632.8 nm (any other wavelength is possible as well) as a function of the sample rotation angle θ are extracted from these spectroscopic measurements.

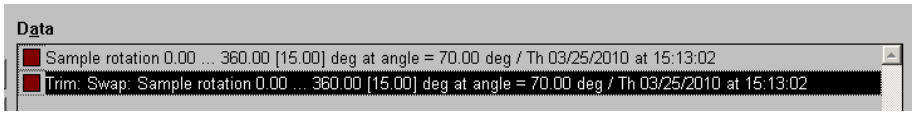
This is done by using the “Trim” function which can be found in the Tab “Header” section. The same wavelength value 632.8 is selected for both “min.” and “max.” numerical entry boxes.



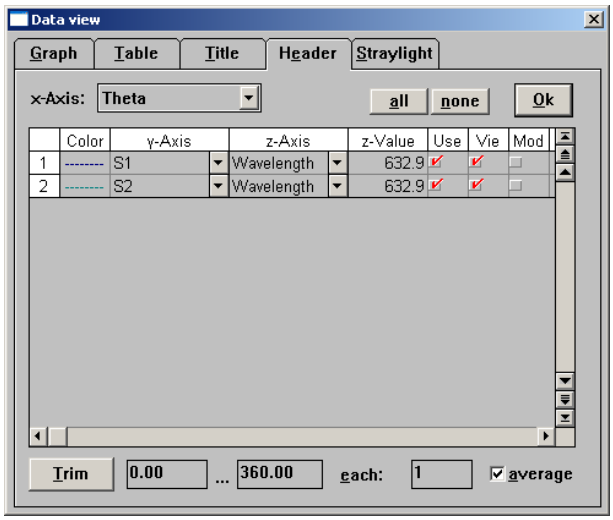
The results will be given for the wavelength which is closest to the selected value which will be rounded to 632.9 nm in this example.

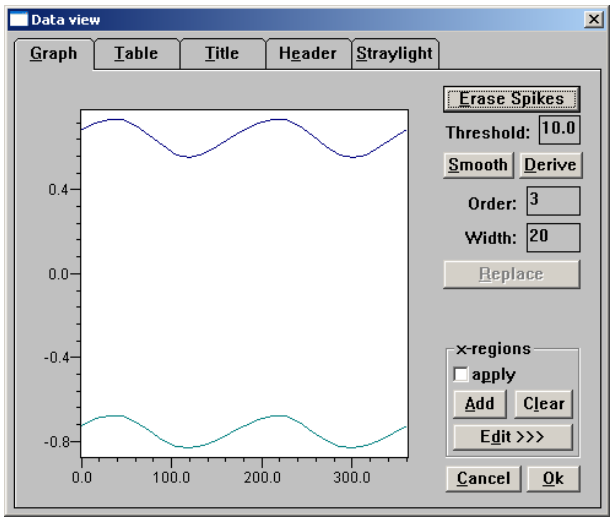


When “Trim” is pressed a new dataset is created containing s1,s2 at 632.9 nm as a function of the rotation angle θ indicated by “Swap” in the name of the dataset.



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

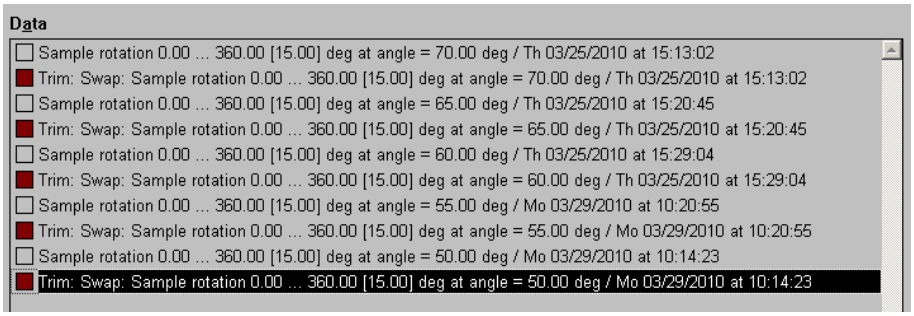




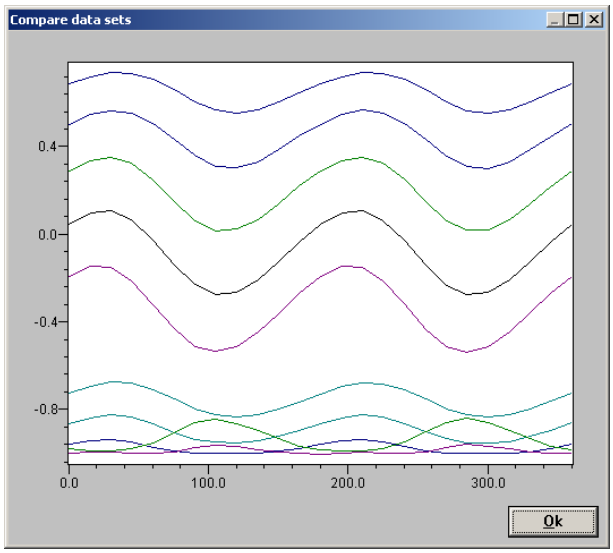
s1 s2

θ

These measurements are now performed between Φ=50° and 70° (steps: 5°) angle of incidence.



The spectra are shown in the following plot.



Modeling of $CaCO_3$:

The anisotropic sample is described using the biaxial anisotropic layer. Due to the fact that $CaCO_3$ is uniaxial anisotropic two of the three axes must have the same dispersion.

$CaCO_3$ is transparent as 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 Cauchy dispersion using “N0” as the only fitting parameter . The final model appears as follows (Cauchy is used here):

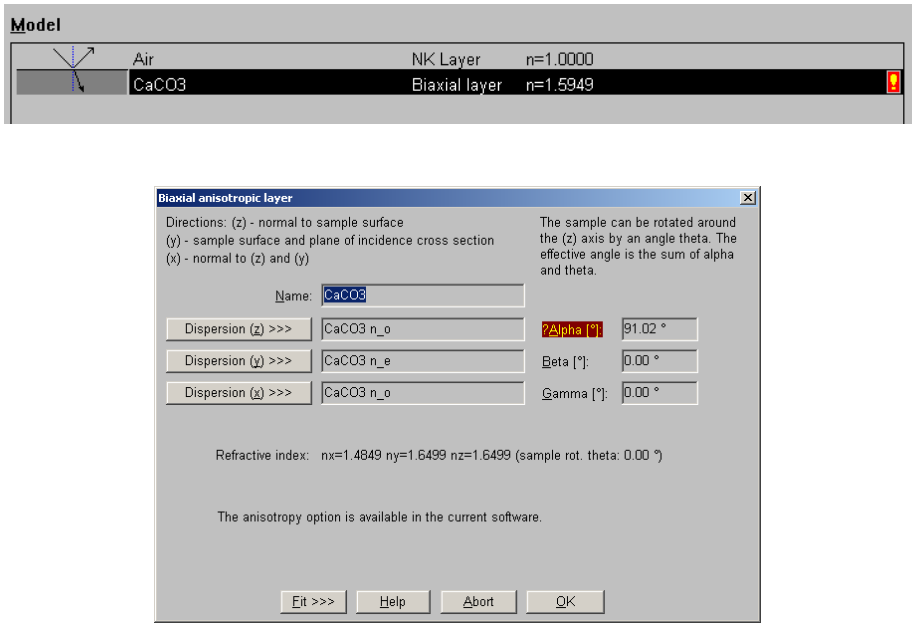


Figure: Biaxial anisotropic layer for a uniaxial CaCO3 with c-axis in surface plane. The rotation angle α is the used as fit parameter. (Here the result is already shown)

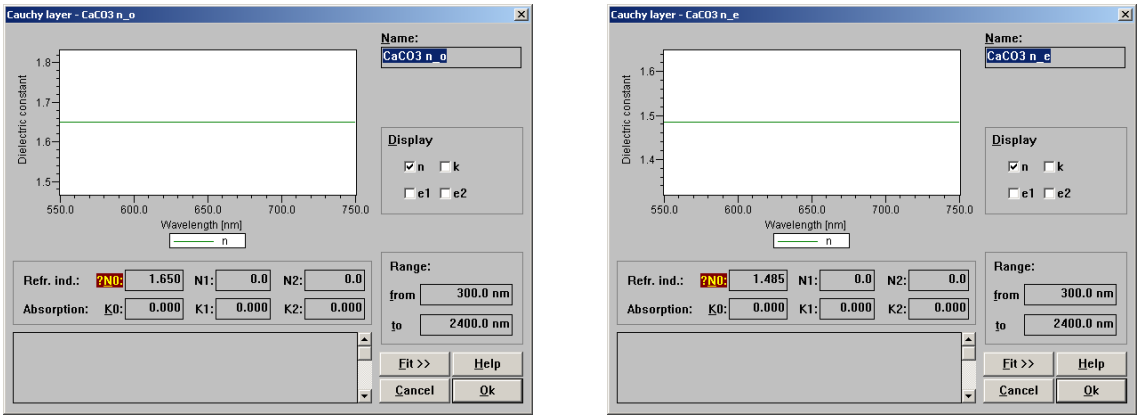
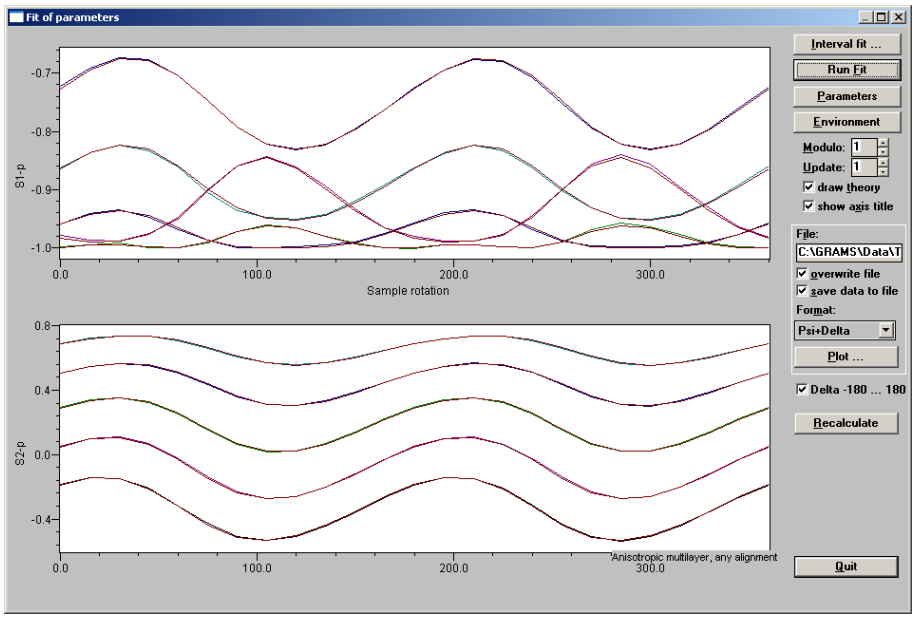


Figure: $CaCO_3$ optical constants described by Cauchy layer with no dispersion. “N1”, “N2” and all k parameter are equal to zero.

The following graph shows the fit window of SPECTRARAY for the correct rotation angle of the sample of α=91°.



For comparison a rotation angle of 10 degrees less (α=81°) is shown. It can bee seen, that the structures are shifted by 10 degrees. So the information of the rotation is included in the phase of the sinusoidal structure.