ElliCalc

Software Manual

Version 3.5 8.2.2011

CONTENTS

1 Introduction

ElliCalc is an ellipsometric software to extract thickness and optical data from thin, transparent layers on different substrates. ElliCalc uses Ocean Optics microspectrometers.

ElliCalc offers a lot of different options like:

- Simulation and measurement of multilayer systems (weakly absorbing or transparent)
- A powerful software engine in the background (“SCOUT”)
- Additionally: an easy-to-use “internal “ mode for thickness extraction and/or Cauchy dispersion
- A graphical user interface that is very easy to use (recipes)
- Simulation of up to 10 layers (weakly absorbing or transparent)
- Highly accurate thickness measurements between some nanometers up to about 25 µm.
- Extraction of dispersion n(λ) and k(λ), roughness, EMA-fractions and other layer parameters, if using SCOUT add-on (and Cauchy models in internal mode)
- 3D - mapping mode with a motor driven xy(z)-stage (=function of position)
- Online/multipoint measurements (=function of time)
- Remote control via OLE-commands from external software
- Video
- Combination with reflectometry (“NanoCalc”)

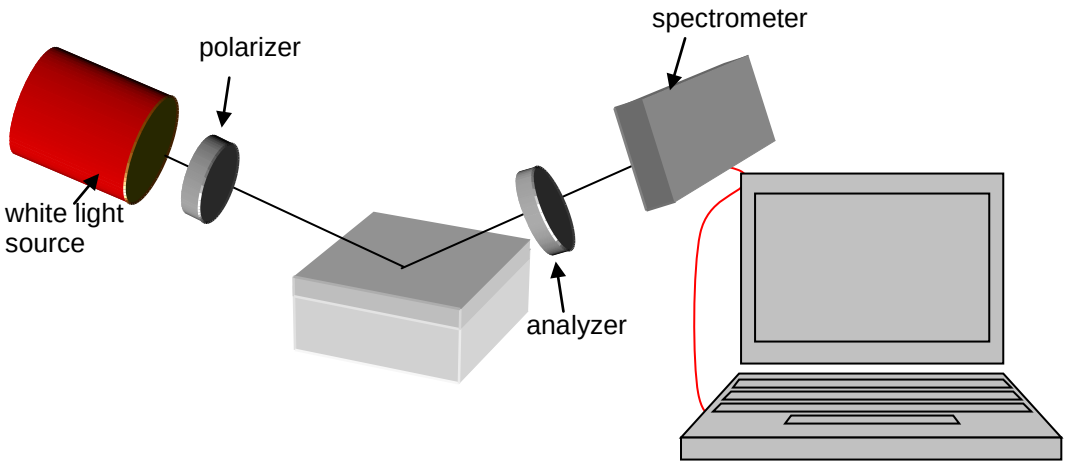
Measurement principle
A thin layer is illuminated with **white** light via a collimating optics and a spectrometer measures the change of polarization (that occurs after reflection) as a function of wavelength. ElliCalc software determines thickness (and optical parameters) of the layer.

The mathematics to extract useful data about the film is quite ambitious, but the user is separated from these problems. The internally measured properties are called “Psi” and “Delta” (in degrees) or sometimes tan(Psi) and cos(Delta). Of course in spectroscopic ellipsometry these 2 properties are measured as a function of wavelength (in contrast to single wavelength ellipsometry)

ElliCalc has 2 different modes of operation:

1. data extraction via an optional software tool called “SCOUT”. This SCOUT software is very powerful and works more or less in the background. SCOUT is able to handle very complicated dispersion curves, but needs some experience with optical modeling. ElliCalc acts as a user interface to simplify the data extraction process. Even without deep understanding of the underlying physics it is possible to measure complex layer systems by using a recipe concept. A layer recipe has to be loaded and the rest is a “one-button-solution” (of course there must be an expert in the beginning to establish this recipe. Ask your software supplier…)
2. data extraction by ElliCalc itself (without SCOUT). In this “internal mode” it is very easy to extract thicknesses and –to some extent- dispersion values without optical modeling. Recipes may be used, but even without recipes it is extremely simple to get results. This “internal mode” does not need an expert, but it is not as powerful as the “SCOUT mode”.

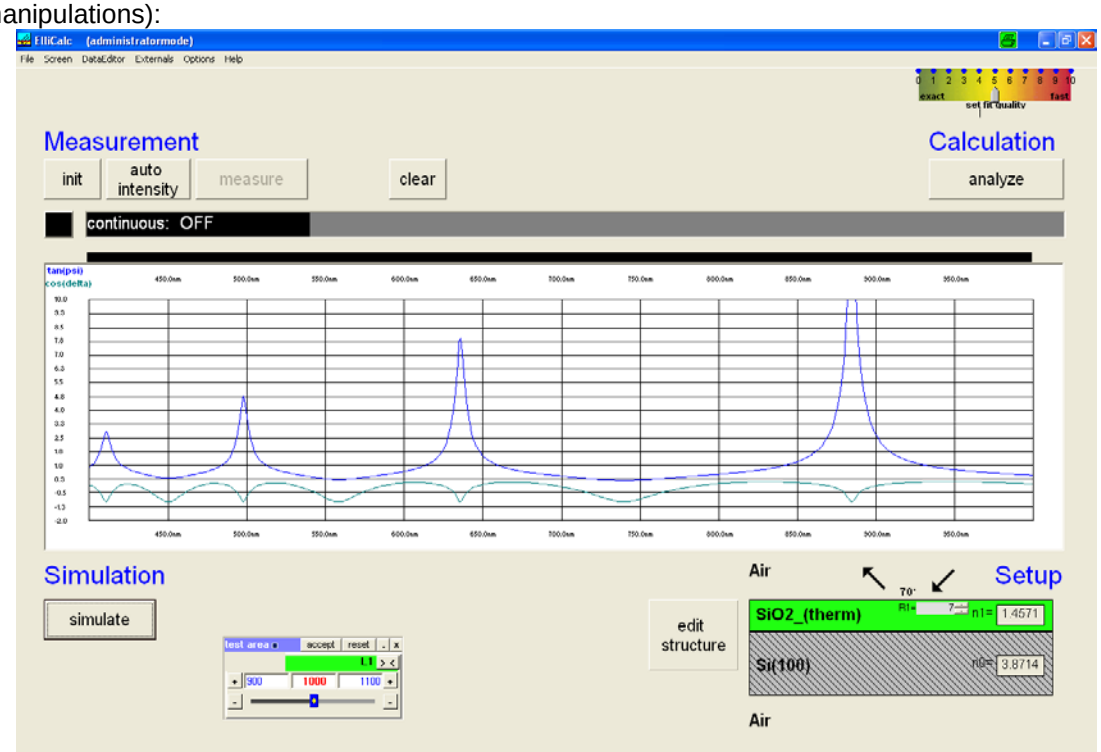
1.1 Measurement setup



A broadband white light source is focused on a thin layer under oblique incidence. The incoming light is polarized by a “polarizer”, the reflected light is analyzed by an other polarizer, the so called “analyzer”. The intensity as a function of wavelength is measured by a spectrometer, a PC extracts the wanted information.

1.2 Measurement signal

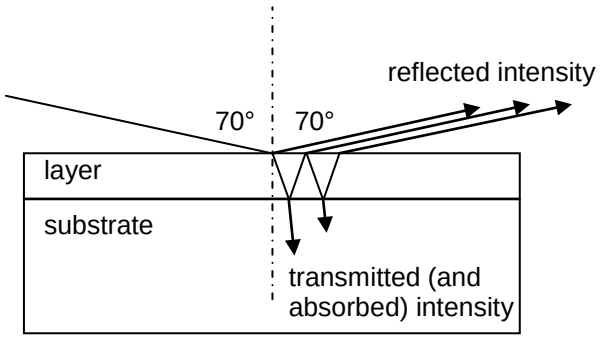
The typical modulated signal of such a spectroscopic thin film measurement might look like this (after some data manipulations):



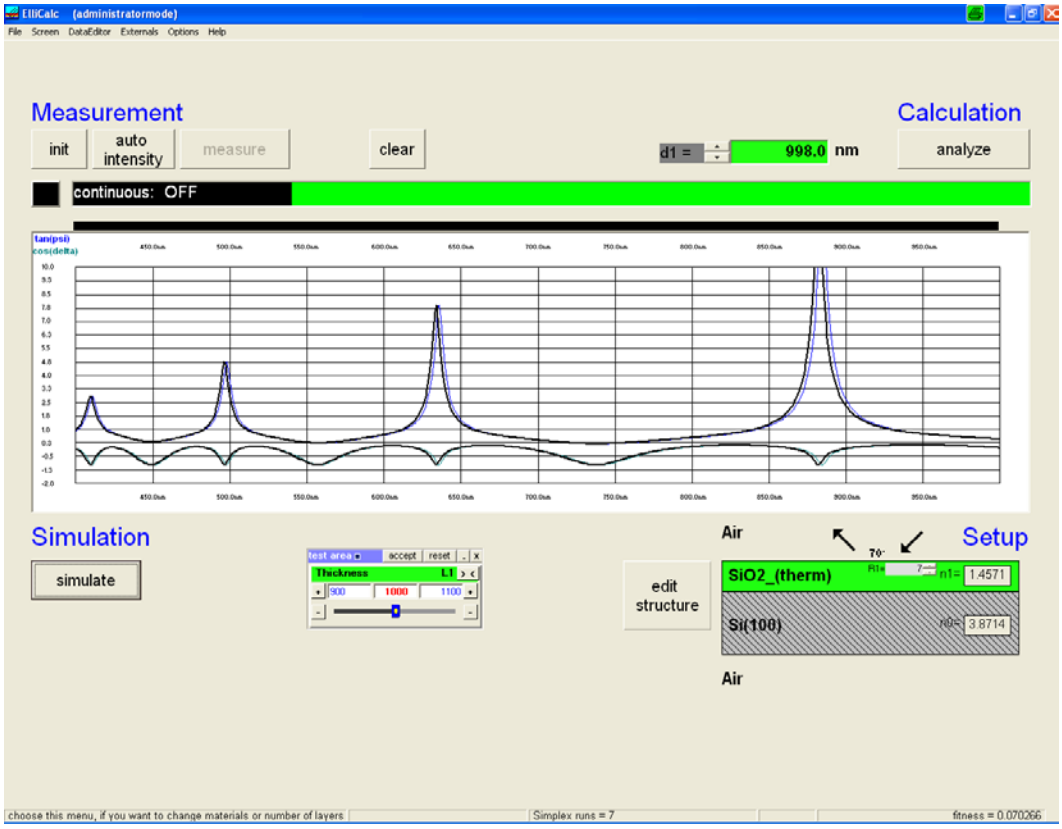
On the screen you see two different curves (Ψ/Δor $\tan(\Psi)$ and $\cos(\Delta)$ as a function of wavelength. ElliCalc uses these signals to extract thicknesses and optical data for this (SiO_2) layer on Si.

1.3 Physical principle

The measurement principle of ElliCalc is the well-known fact of oblique **reflection** and **interference** of light in thin layers. Light is reflected (and normally transmitted), resulting in different phase shifts and different intensities for different wavelengths. Ellipsometry measures the change of phases and intensities between vertically and horizontally oriented light and calculates different layer parameters like dispersion or thickness.



After some calculations ElliCalc will show a result (here: 998 nm) nm as the best fit to the experimental data (blue and magenta curves=measured signals, black curves = theoretical curves):



2 Installation

ElliCalc (and SCOUT) is delivered on a CD-ROM.
Insert the CD-ROM in your CD-ROM drive, use Microsoft Explorer to run „ElliCalc-Setup.exe “. Do not call “ElliCalc.exe” at this level, if you happen to find it in some subdirectory.

ElliCalc will ask you for a directory (and propose a directory „c:\programs\ElliCalc“).
If you prefer other names, change this to "c:\MyPrograms\ElliCalc” or any convenient directory name).
Reboot the PC after installation.
Deinstallation:
If you want to deinstall ElliCalc from your computer, go to „system control“, „software“ and deinstall ElliCalc. Do **NOT** just delete it because ElliCalc adds some files to your windows\system directory !! Always de-install the software properly.

3 Product support

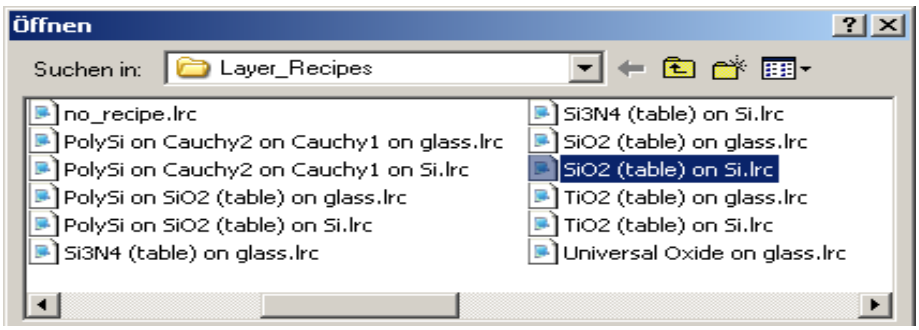
Please contact your local distributor for product support. Here you can find additional information:
www.OceanOptics.de

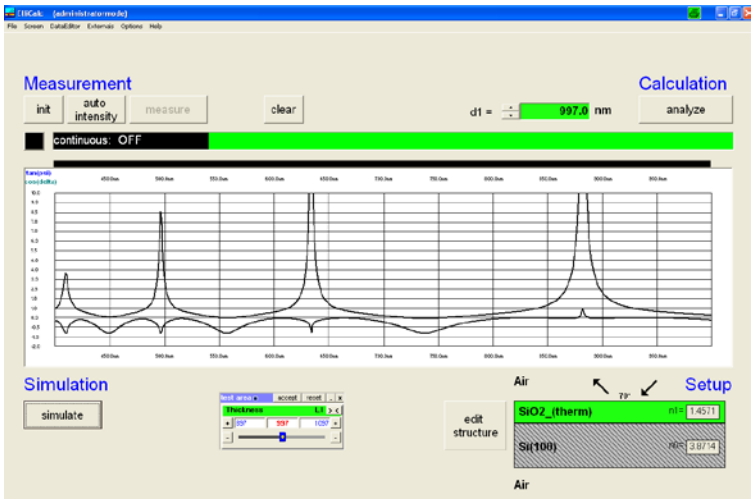
4 Getting started

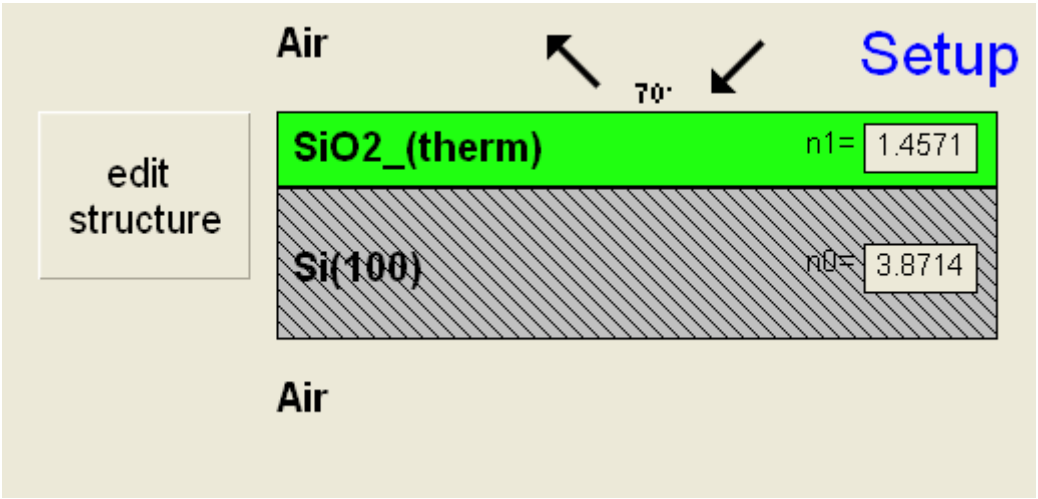
After installation of your hardware and software you should be ready to make your first measurements.

An example:

1. For the first steps it is a good idea to use a special "step wafer" with different oxide thicknesses. You can use this wafer to check the correct functionality of the ellipsometer. Please ask your hardware supplier for information about step wafers.
   Otherwise use a really well known sample with good optical properties (not rough, homogenous, simple layer structure, like SiO_2 on Si). Put the wafer on the stage.
2. Choose a room without too much light, avoid full sunlight and reflections (you might run into problems with stray light).
3. Load a layer recipe (via "files/load layer recipe") corresponding to your sample, e.g. "SiO2 on Si.lrc". Then the structure in Setup picture shows a correct layer system
4. Then put your wafer in the middle of the chuck and switch on your power supply and lamps
5. Start ElliCalc.exe (there should be no warnings or error messages) and wait unil all messages "please wait" have disappeared.
6. click on the button „init"and wait unil all wait and progress messages have disappeared.
7. Now the ellipsometer motors are initialized. There is no absolute need to press the button "auto intensity", as this action has been performed by "init" (but are allowed to do it….)
8. Now press the button "continuous", you should see a live signal. Try to maximize this signal by using the height adjustment and the tilt adjustment of your stage. In case that these 2 adjustments were considerable: press "auto intensity" to optimize the integration time again.
9. Now click on the button "init" and wait for some seconds. The motors of the ellipsometer will move to their starting positions.
10. Click on the black button "continuous". The button turns to red and you should see an intensity signal on the screen. Manually adjust the height of your stage to maximize this signal. Click on the (red) button "continuous" again to stop this mode.
11. Click on the button "auto intensity". The integrations times are chosen automatically so that the maximum signal height is about 75% of the maximum to avoid saturation. If you change your sample now or later and the new sample has a different reflectivity you have to press the button "auto intensity" again. If the new sample is of the same type as before this is not necessary but advisable.
12. Now click the button "measure". The measurement will take some seconds.
13. Now you see the measured data with the typical interference wiggles.
14. Then click on the button „analyze" and wait for the result. You should get meaningful results.




Measurement
Calculation
init
auto intensity
measure
clear
d1 =
997.0
nm
analyze
continuous: OFF
Simulation
simulate
edit structure
Air
70°
Setup
SiO2_(therm)
n1=
1.4571
Si(100)
n0=
3.8714
Air

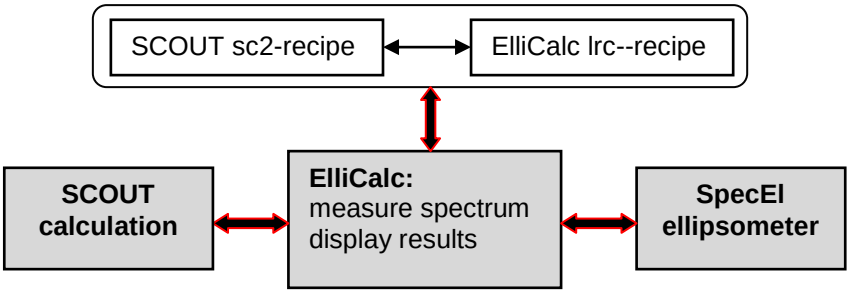

Air
70°
Setup
edit structure
SiO2_(therm)
n1=
1.4571
Si(100)
n0=
3.8714
Air

5 User modes of ElliCalc

ElliCalc has two different user modes, the "SCOUT-mode" and the "ElliCalc internal mode". At the moment the "SCOUT-mode" is the normal mode, the "internal mode" can only extract thicknesses and Cauchy dispersion
The "SCOUT-mode" requires that another software, called "SCOUT" is installed on this PC, the "internal mode" only uses ElliCalc.

5.1 SCOUT mode

ElliCalc works as a graphical user interface for a sophisticated film software **"SCOUT"** working in the background**.**
The whole process is necessarily driven by recipes**.**

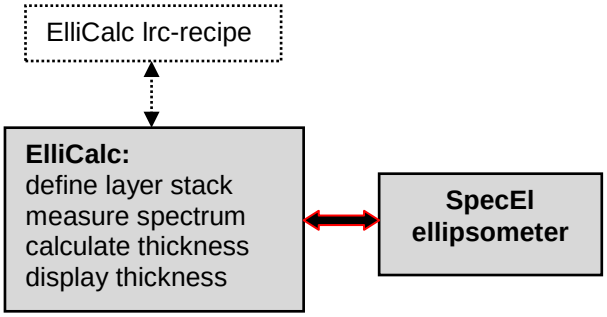


- within ElliCalc you have to load a **"recipe"**, e.g. "SiO2 on Si.lrc". This ASCII-readable recipe contains a link to a SCOUT recipe like "SiO2 on Si.sc2". All necessary layer informations are contained in this SCOUT recipe and are read by ElliCalc, but only for display purposes.
- ElliCalc now controls the hardware, measures the sample and sends the measured Psi/Delta-values to SCOUT (via a file EC_Data.xy in directory "ElliCalc\Internal_Files").
- SCOUT does the calculation of all parameters
- the results are given back to ElliCalc via OLE-connection. The main fit parameters (thickness, refraction, absorption, roughness and EMA-fractions) are displayed by ElliCalc, as well as all other SCOUT fit parameters.

This SCOUT mode relies totally on good SCOUT recipes. So there must be someone (you or the administrator or OceanOptics) in the background being familiar with the details and the physics of SCOUT. The advantage is a "one-button-ellipsometry" for the user and an enormous calculation power !

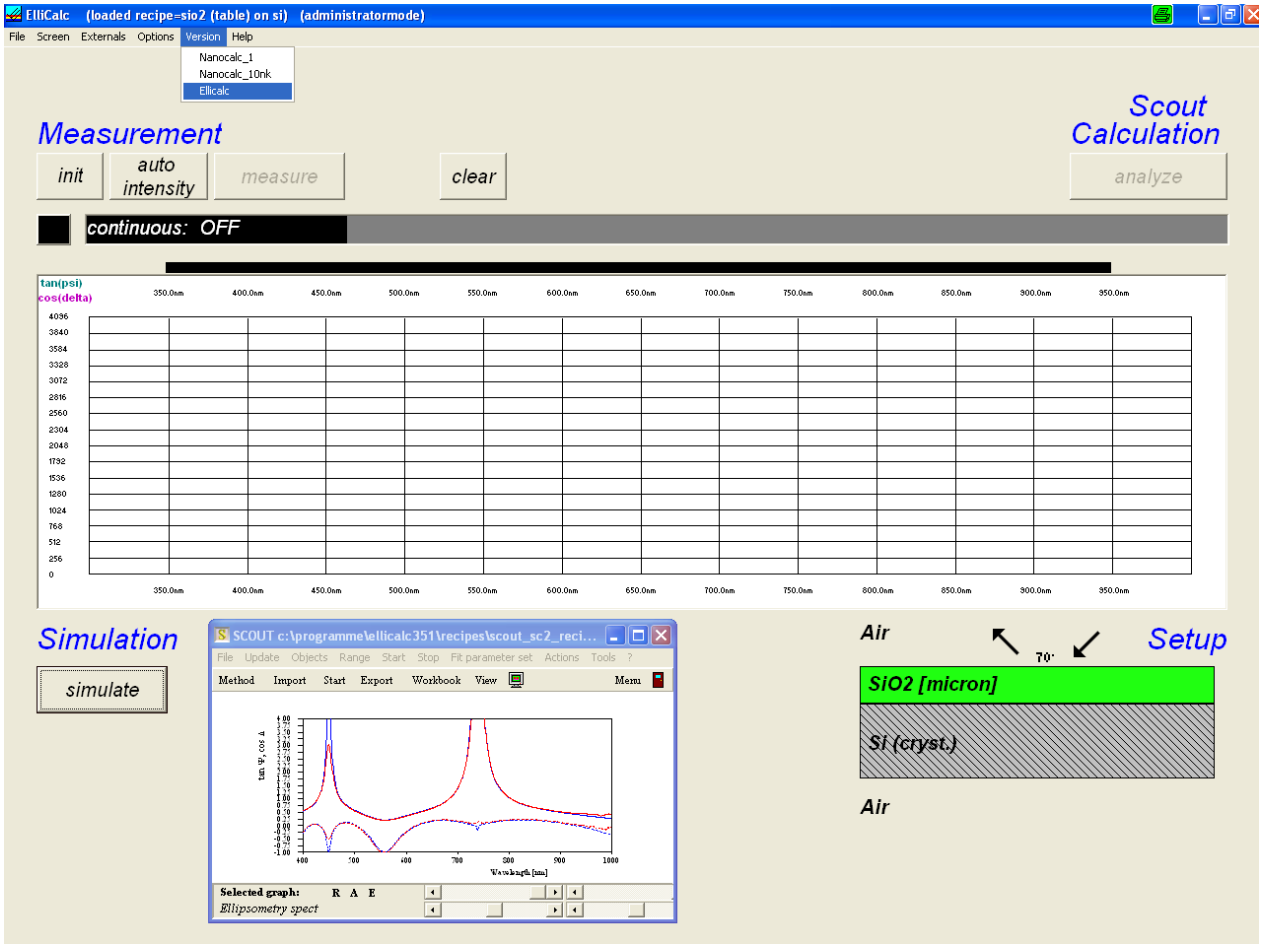
5.2 Internal mode

In this internal mode the user can create own layer stacks and does not need the external SCOUT software at all. There is no need to work with recipes, but is is recommended. BUT: At the moment only thickness values and a Cauchy dispersion can be extracted.



5.3 Combiversion with NanoCalc

If you bought a combiversion ElliCalc + NanoCalc (= ellipsometry and reflectometry) you will see an extra menu “version”. Here you can switch from one application to the other.

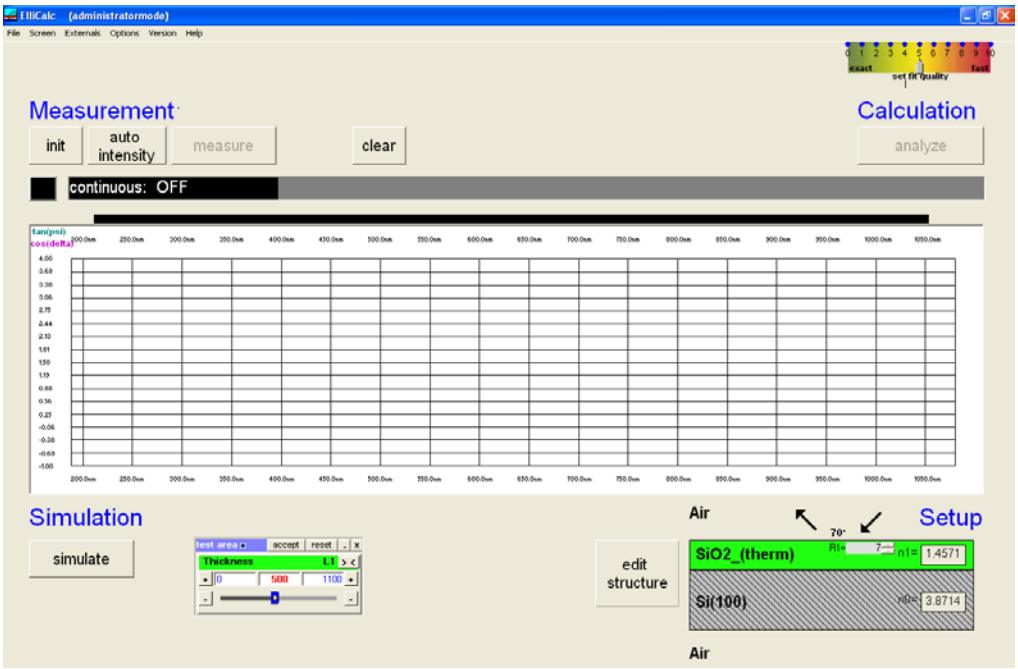


5.4 List of all menus and buttons

Main menu	Sub-menu	SCOUT mode	Internal mode
FILES menu	Load Scout layer recipe	x	x
	Load ElliCalc layer recipe		
	Save as layer recipe		x
	Change layer recipe	x	
	Export raw data	x	x
	Import raw data	x	x
	Show all results	x	
	Exit	x	x
SCREEN menu	Spectrometer data	x	X
	Limits	x	x
	Dispersion	x	x
	Psi/Delta or tan(Psi)/cos(Delta)	x	
EXTERNALS	Mapping	x	x
	Analyze mapped data	x	x
	Online/multipoint	x	x
	Analyze online data	x	x
	RS232	x	x
	Video camera	x	x
	Show plot	x	x
OPTIONS	Change buttons	x	x
	Roughness	(x)	x
	Special modes		x
	Fit parameters		x
	Some setups ElliCalc (motor steps)	x	x
	Some setups SCOUT (stoptime)	x	
	Some setups (change colors)	x	x
VERSION	NanoCalc_1	x	x
	NanoCalc_10nk	x	x
HELP	Contents	x	x
	About	x	x
EDITSTRUCTURE			x

6 Basic features of ElliCalc

6.1 Init



This button performs 2 tasks:

- initialize the motors for polarizer and analyzer (e.g. end positions)
- automatically set the integration times to good values (so there is no need to press “auto intensity” directly after an init procedure). But: If you change the stage height you should apply “auto intensity”

hint:
If you change your sample you may run into saturation of the spectrometer = a (nearly) horizontal part in some of the measured curves near to the upper limit of the plot.

6.2 Auto intensity

This option automatically adjusts integration times.

This button has to be pressed if you use a completely different sample (each sample has a different reflectivity, so a different integration time). Normaly the “init button” already has performed such an auto intensity procedure.
If your sample is of the same type as your last sample (=has nearly the same reflectivity) it is not necessary to press this button.

AutoIntensity tries to get 75% of the maximum allowed value. You can change this value by manually editing the file “thinfilm.ini”

6.3 Simulate

This routine simulates a spectrum.

- in SCOUT-mode: from the .sc2-layer recipe data within SCOUT
- in ElliCalc internal mode: from the data in EditStructure (identical to the data in Thinfilm.ini-file)

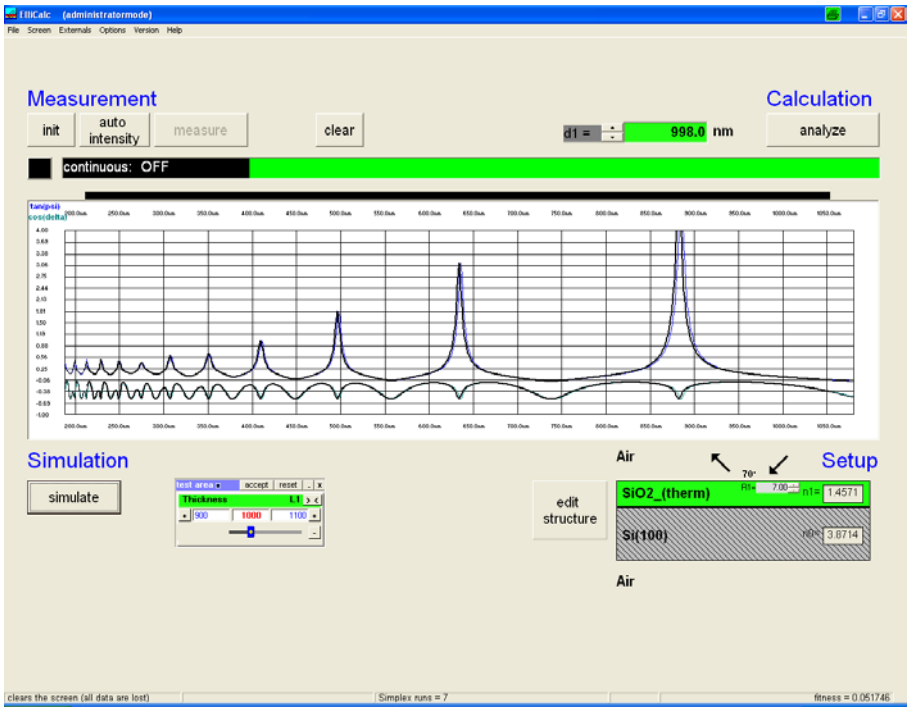
Hint:
If you want to have a short check which structure is simulated at the moment, put the mouse cursor over the appropriate layer for some seconds and you see the layer thickness.
OR:
Leave your mouse cursor for some seconds over the button SIMULATE and look at the text in the status bar.

6.4 Measure

This routine measures the ellipsometric spectra of your test device.

If you use a double spectrometer, you had to adjust the crossover wavelength. Below this wavelength the data are collected from channel A ("master spectrometer"), above this wavelength they are collected from channel B ("slave spectrometer").

6.5 Analyze



This routine analyzes a spectrum (either simulated or measured) within the data extraction limits.

- In SCOUT-mode: SCOUT is doing the calculations. The structure that is simulated may only be changed within SCOUT.
- In ElliCalc's internal mode: ElliCalc is doing the calculations (only thickness and Cauchy parameters at the moment)

Hint:
To have a short check which structure is simulated at the moment, put the mouse cursor over the appropriate layer for some seconds and you see the layer thickness.
OR:
Leave your mouse cursor for some seconds over the button SIMULATE and look at the text in the status bar.

6.6 Continuous mode

The continuous button switches between continuous mode (=red button) and “stop continuous” (button =black). Then there will be a continuous measurement of the signal (necessary to adjust the height and tilt of your stage !!)
All others buttons of ElliCalc are disabled until you finish the continuous mode.

6.7 Fitness

Any extraction of parameters is accompanied by a value of "fitness". This is the sum of the mean square deviations between measured and simulated curve (normalized to the range of extraction). The fitness is a rough guide whether your thickness value is "good" or not.

In the file “Thinfilm.ini” you will find 3 entries in section [fit]:
Failure_RedLevel=1
Failure_YellowLevel=0.1
RYG_LevelsAreDisplayed=False
If you change the variable RYG_LevelsAreDisplayed from “False” to “True” (in main menu “Fitparameters”), the usual rainbow pattern on the screen will disappear and a simple color will show up.

- If the fitness is below Failure_YellowLevel=0.1 you will see a GREEN color.
- If the fitness is between Failure_YellowLevel=0.1 and Failure_RedLevel=1 you will see a YELLOW color.
- If the fitness is above Failure_RedLevel=0.1 you will see a RED color

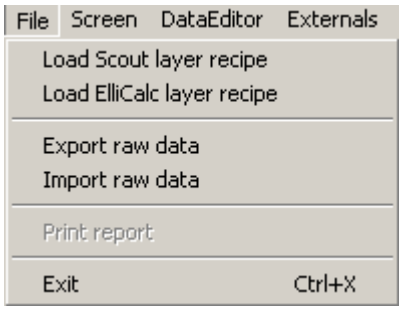
Attention:
If you measure very thick layers (with a good correlation between maxima positions, but bad correlation between signal heights) you may end up with high values of fitness, but nevertheless the thickness results may be o.k.

7 Detailed features of ElliCalc

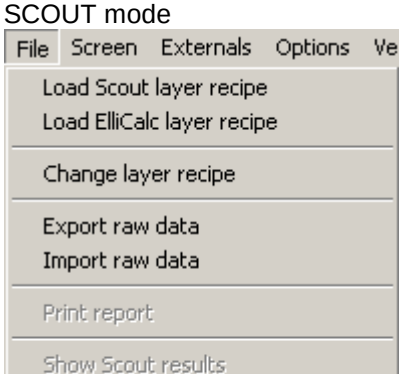
In this chapter the most common commands and menus of ElliCalc are decribed.
Special commands and menus for “SCOUT mode” and for ElliCalc’s “internal mode” are decribed in later chapters.

7.1 Main menu “File”

Internal mode



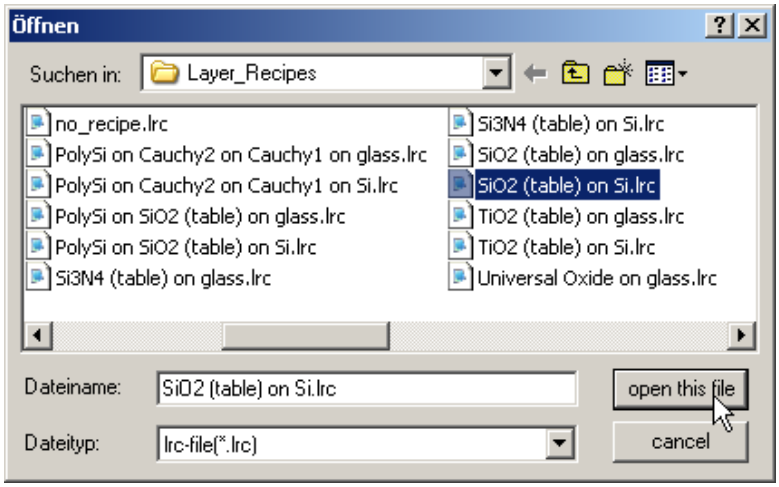
SCOUT mode



7.1.1 Load layer recipe

This routine loads a layer recipe that has been saved earlier (extension: .lrc). Do not change the extension .lrc.
In SCOUT mode you may either load another SCOUT recipe (“load Scout layer recipe”) or you may switch to ElliCalcs internal mode (“Load Ellicalc layer recipe”). See the screenshots above.
In SCOUT mode all buttons captions are in *italic*, otherwise in normal.

It is assumed that all .lrc-files are in the default directory “ElliCalc\recipes\layer_recipes”, but you can change the directory path to any other directory on your PC (provided that you did not use "UseLastFile-names_EC=False" in section [Filenames_EC] in Thinfilm.ini).



There is a section [Scout] in this layer recipe with an entry for "Scout_Recipename_EC". This entry is a **link** to the corresponding SCOUT .sc2-recipe in the directory "c:\programs\scout\scout_sc2_recipes" (or similar directory name).
If this linked .sc2-recipe is existent, SCOUT will be used for calculations = “SCOUT mode”. If this link is empty, ElliCalc will calculate without SCOUT = “internal mode” (at the moment only for thicknesses and Cauchy parameters!)

Example for SCOUT-mode (in ellipsometry):

```
[Scout]
Scout_DirPath=c:\programs\scout
ScoutStopTime=15
Scout_RecipeName_NC=
Scout_RecipeName_EC=SiO2 (table) on Si.sc2
```

Example for ElliCalc internal mode:

```
[Scout]
Scout_DirPath=c:\programs\scout
ScoutStopTime=15
Scout_RecipeName_NC=
Scout_RecipeName_EC=
```

The *.lrc-file is an ASCII file that contains most parameters of the software, but NO measured or simulated values of psi/delta (or tan(psi) /cos(delta)) as a function of the wavelength.
If you load a recipe you will not see any curve on the screen, but a change in the setup or the limits.

7.1.2 Import raw data

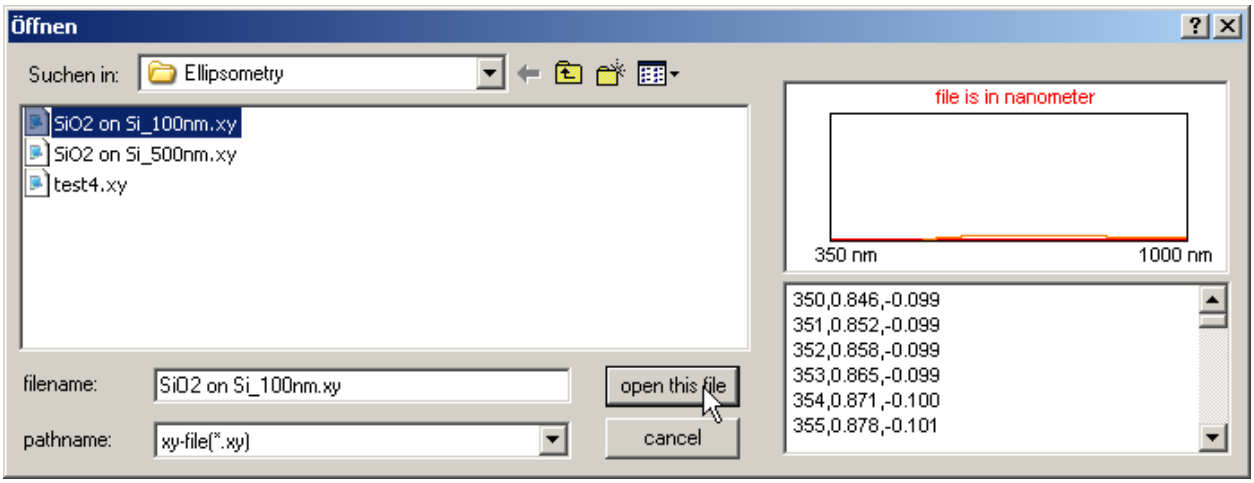
(internal mode and SCOUT mode)
You are asked for an import- directory. The imported values are displayed in blue (=similar to measured values). The scale of the screen is not adjusted.

7.1.3 Export raw data

(internal mode and SCOUT mode)
If a curve was produced by simulation or measurement it may be exported as ASCC-file (“raw data”). This file has a very simple structure: (lambda, tan(Psi), cos(Delta)

```
350,0.796,0.064
351,0.780,0.050
352,0.764,0.034
353,0.749,0.014
354,0.736,-0.009
355,0.722,-0.035
356,0.710,-0.064
357,0.697,-0.096
```

You are asked for a directory to save this file. Please use the default directory \RawData_Files\Ellipsometry



7.1.4 Print report

This routine allows you to enter some user data (names of operator, of sample and so on), shows a preview and prints on the Windows standard printer. Changing the printer is possible only within Windows itself.
Entering of user data: you may also change the names of the labels (empty labels: this line is not shown on the final print). In the preview window you may zoom in and out. After pressing the print button you have the chance to change some printer options.

If you want to get a printout of the complete screen or parts of it:
It is recommended to use a hardcopy program to print the different parts of the software with enough options to change colors, resolution etc.
We recommend a shareware ”HC.EXE” (http://www.sw4you.de and on the CD-ROM in : tools\general), which will include a small button in every (!) window of your system near to the close button.

For online-users: we recommend to buy the OPTION ElliCalc-Online for printouts of Multipoint Measurement, Result-Windows with Statistic Data’s and Excel-Connection.

7.1.5 Show all results

See chapter “Special features for SCOUT mode”

7.1.6 Exit

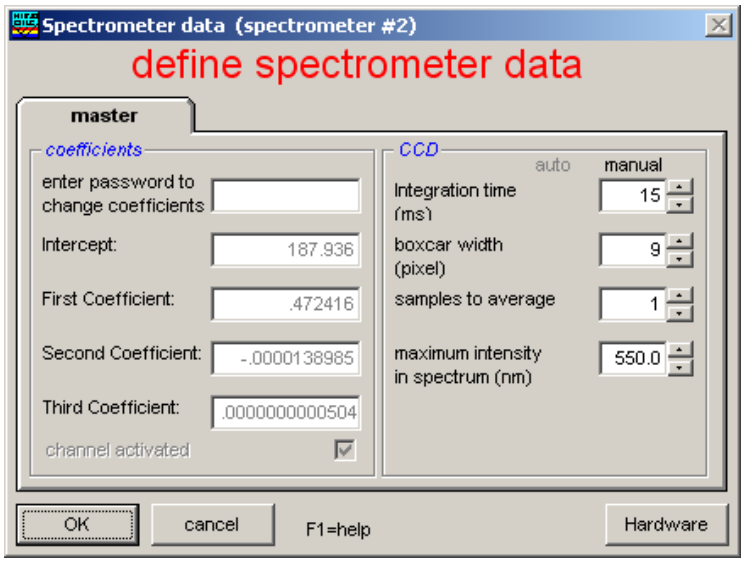
This routine exits ElliCalc and SCOUT and closes all windows. All important data have been written to the Thinfilm.ini -file before and will be reloaded in the next run.
Important warning:
Do NOT close SCOUT separately !!! This would break the OLE-connection between SCOUT and ElliCalc. The only way to restore this connection is to exit ElliCalc and restart the software !

7.1.7 Function keys

If you click on the button **F1**, you get access to help functions.

7.2 Main menu “Screen”

7.2.1 Spectrometer data



The 4 spectrometer coefficients are displayed for information purposes. They are automatically set by the Thinfilm.ini file which is specific for each single system.

Changing these values will screw up the system and is therefore password protected and only accessible for technical service.

For calibration purposes you may change these values (with a password and only within several percent deviation from your original values).

physical meaning:
These 4 numbers are the coefficients in a formula that shows the dependence between wavelength (in nanometers) and pixel number of your spectrometer according to the following formula:

$$\lambda = I + C_1 \cdot P + C_2 \cdot P^2 + C_3 \cdot P^3$$

with:
I = intercept
C_1 = first coefficient
C_2 = second coefficient
C_3 = third coefficient
P = pixel number

Hint: Ask your hardware supplier if you have the impression that it might be necessary to recalibrate the spectrometer (a red HeNe-laser should show 632.8 nm)

7.2.1.1 Integration time

Whenever you change this value, it is written to disk (in file “Thinfilm.ini”) and will be used as a startup value.

How to change integration time:
1. method = “auto intensity” button (or “init” button !): This method starts with the lowest available integration times for different positions of the polarizer and checks the resulting spectra (every 10 nm) to find an optimum integration time. The software will try to achieve a maximum signal of 75 % of the total range and will try to avoid saturation. The absolute value of the integration time will depend very much on the reflectivities of your reference materials, your substrate material and your layer material.

2. method = use the menu "options/spectrometer data" and and enter a value. Be careful: this may lead to bad results ...

You may check the value of integration time at any time without entering the menu OPTIONS: Put your mouse cursor over the button MEASURE and wait for about 2 seconds: a small window will pop up to inform you about integration time, samples to average and boxcar width.
These values correspond to the channel A ("master spectrometer") if you use a double spectrometer.

7.2.1.2 Boxcar width

physical meaning:
The OceanOptics spectrometer is able to average over some pixels to increase signal/noise-ratio.
A boxcar width of 1 pixel means no averaging at all (which is an ideal situation and would correspond to a very narrow fiber). This has to be used if you want to measure very thick layers (like 50 micrometers of resist)
A boxcar width of 5 pixels means an averaging over 2 pixels on the left side and 2 pixels on the right side (= 5 pixels altogether). This averaging routine is shifted from the left side of the simulated spectrum to the right side with a step size of 1 pixel only. Values of 5-9 are recommended if you want to measure films in the range of 1 micrometer or less as you get a better signal-to-noise ratio.

hint:
You may check boxcar width at any instance without entering the menu OPTIONS: Put your mouse cursor over the button REFERENCE or MEASURE and wait for about 2 seconds: a small window will pop up to inform you about integration time, samples to average and boxcar width.
These values correspond to the **channel A** spectrometer if you use a double spectrometer.

7.2.1.3 Samples to average

Whenever you change this value, it is written to disk (in file “Thinfilm.ini”) and will be used as a startup value.

physical meaning:
The Ocean Optics /spectrometer is able to average over some runs to increase signal/noise-ratio.

Tips:
Try to use small values for Samples To Average while keeping the lamp intensity as high as possible (to get short measuring times). This is especially important in mapping mode.

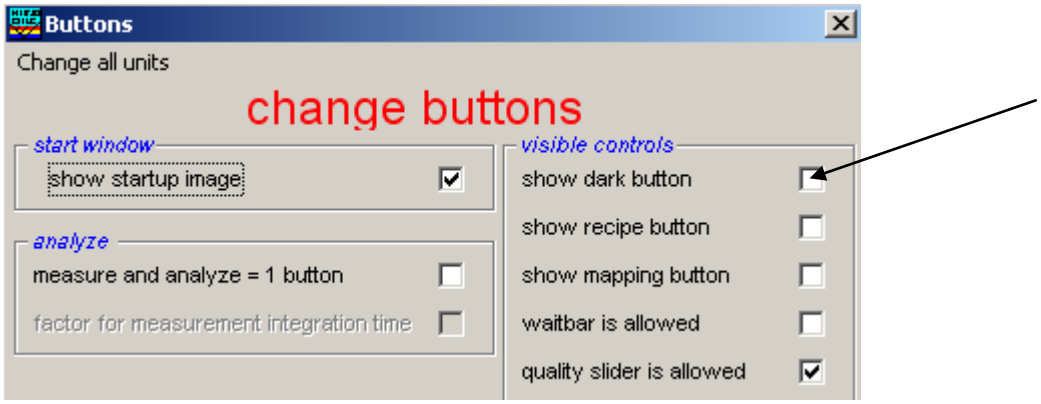
You may check Samples To Average at any instance without entering the menu OPTIONS: Put your mouse cursor over the button MEASURE and wait for about 2 seconds: a small window will pop up to inform you about integration time, samples to average and boxcar width.

7.2.1.4 Internal correct for dark

If you choose this option, dark current is corrected automatically (see button “measure”).

The Ocean Optics Spectrometer is able to measure the dynamic dark current internally within a couple of pixels that are NOT irradiated by external light, and is correcting dynamically.

7.2.1.5 Dark button



If you choose this option, dark current is corrected mathematically. This is only necessary if you can't protect your system against ambient light or stray light.

7.2.1.6 Maximum intensity

This value describes the maximum intensity in the spectrum of your (halogen ?) lamp.

This value helps ElliCalc to achieve an automatic adjustment of the integration time within the limits of the screen (=without saturation)

If you use a double spectrometer there are TWO such wavelengths corresponding to the different lamps and the different sensitivities of the two spectrometers.

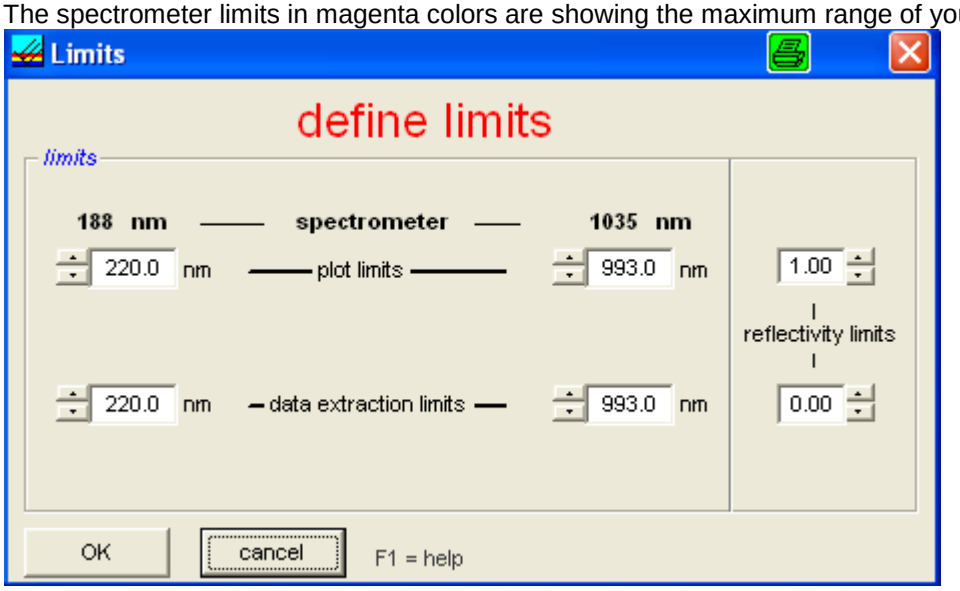
If you use a double spectrometer with different sensitivity regions, e.g. 200-600 nm for channel A ("master spectrometer") and 500-1100 nm for channel B ("slave spectrometer"), ElliCalc **joins** the 2 spectra to get a single spectrum (200-1100 nm). The wavelength where the two overlapping spectra are joined is called "crossover wavelength". (any value is possible, 550 nm would be a good choice in this case).

7.2.1.7 Crossover wavelength

If you use a double spectrometer with different sensitivity regions, e.g. 200-600 nm for channel A ("master spectrometer") and 500-1100 nm for channel B ("slave spectrometer"), ElliCalc joins the 2 spectra to get a single spectrum (200-1100 nm). The wavelength where the two overlapping spectra are joined is called "crossover wavelength". (any value is possible, 550 nm would be a good choice in this case).

7.2.2 Limits

The spectrometer limits in magenta colors are showing the maximum range of your specific system.



7.2.2.1 Plot limits

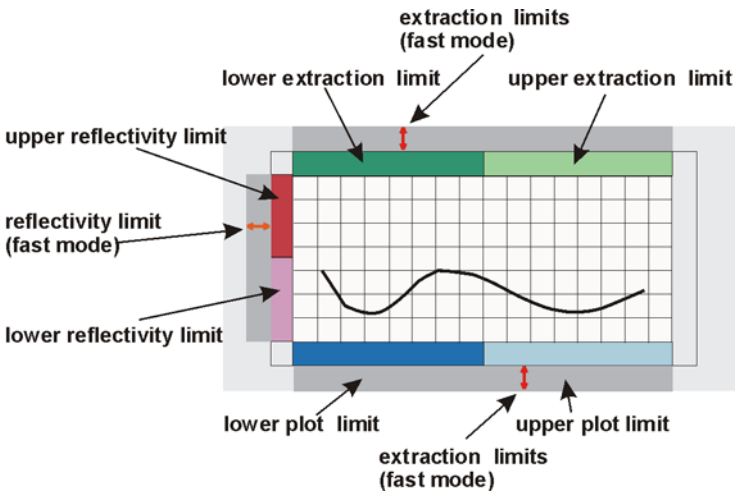
The plot limits are the left and right side of the plot on your screen and coincide with limits of measurement.

The adjustable values of the plot limits depend on the grating in your Ocean Optics spectrometer and are noted in the calibration sheet of your system.

The plot limits may be changed within ElliCalc in steps of 1 nm.

1. normal mode to change the limits:
   open the menu “spectrometer data \ limits” and enter numbers or use the up-down arrows
2. fast and rough method to change the limits:
   If you click in the field near the LOWER numbers you may change the plot limits without entering the menu option/limits:
   If you click in the **LEFT** half with your LEFT mouse button you will decrease the lower plot limit.
   If you click in the **LEFT** half with your RIGHT mouse button you will increase the lower plot limit.
   If you click in the **RIGHT** half with your LEFT mouse button you will decrease the lower plot limit.
   If you click in the **RIGHT** half with your RIGHT mouse button you will increase the lower plot limit.
   The same feature applies to plot limits and reflectivity limits.

3. fast and precise method to change the limits:
   If you move your mouse very near to the lower part of the plot window (but still in the grey part) you will see a little vertical arrow and the value of the wavelength is displayed. If you now click with the left mouse button, you are able to change the lower plot limit (right mouse button=upper plot limit). The same applies to the other 2 grey zones = extraction and reflectivity limits (see picture)



4. Zoom
   You may zoom by dragging the mouse from one point to another within the plot area.
   If you click with the right mouse button a small popup window will appear with the chance to undo this zoom.
   You can also change the plot limits back to the full range (according to your spectrometer limitations).
   You can also set the current plot limits as a standard or return to a previously set standard.

ATTENTION:
Tto be consistent with data handling, ALL materials files contain n and k data between 150 nm and 1100 nm. Usually only *parts* of these data are measured data (e.g. between 206 nm and 840 nm or between 300 nm and 1100 nm). If you simulate, the valid part of the curve is shown in *black* while the rest is shown in g*rey* (and you get a message).
Extraction limits are restricted to the range of valid n and k data.

7.2.2.2 Extraction limits

These limits cannot be larger than the plot limits. Try to use a large extraction range as long as your signal is “good”.

1. normal mode to change the limits:
   open the menu “spectrometer data \ limits” and enter numbers or use the up-down arrows

2. fast and rough method to change the limits:
   If you click in the field near the UPPER numbers you may change the extraction limits without entering the menu “spectrometer data \ limits”.
   If you click in the **LEFT** half with your LEFT mouse button you will decrease the lower extraction limit.
   If you click in the **LEFT** half with your RIGHT mouse button you will decrease the lower extraction limit.
   If you click in the **RIGHT** half with your LEFT mouse button you will decrease the lower extraction limit.

If you click in the **RIGHT** half with your RIGHT mouse button you will decrease the lower extraction limit. The same feature applies to plot limits and reflectivity limits.

3. Fast and precise method to change the limits:
   If you move your mouse very near to the upper part of the plot window (but still in the grey part) you will see a little vertical arrow and the value of the wavelength is displayed. If you now click with the left mouse button, you are able to change the lower extraction limit (right mouse button=upper extraction limit)

ATTENTION:
To be consistent with data handling, ALL materials files contain n and k data between 150 nm and 1100 nm. Usually only *parts* of these data are measured data (e.g. between 206 nm and 840 nm or between 300 nm and 1100 nm).
If you simulate, the valid part of the curve is shown in *black* while the rest is shown in g*rey* (and you get a message).
Extraction limits are restricted to the range of valid n and k data.

7.2.2.3 Y limits

To zoom in the plot and to see some more details you may change the Y limits. In most cases you will not need this option.

1. normal mode to change the limits:
   open the menu “spectrometer data \ limits” and enter numbers or use the up-down arrows

2. fast and rough method to change the limits:
   If you click in the field near the LEFT numbers you may change the reflectivity limits without entering the menu option \ limits:
   If you click in the **LOWER** half with your LEFT mouse button you will decrease the lower reflectivity limit.
   If you click in the **LOWER** half with your RIGHT mouse button you will decrease the lower reflectivity limit.
   If you click in the **UPPER** half with your LEFT mouse button you will decrease the lower reflectivity limit.
   If you click in the **UPPER** half with your RIGHT mouse button you will decrease the lower reflectivity limit.
   The same feature applies to plot limits and reflectivity limits.

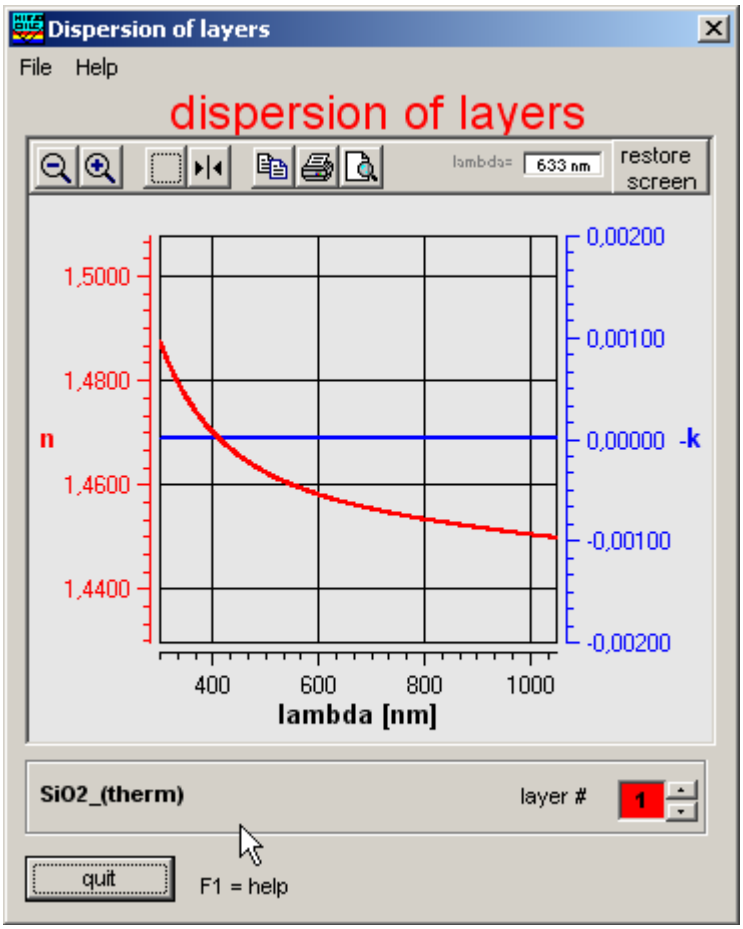
   2. Fast and precise method to change the limits:
      If you move your mouse very near to the left part of the plot window (but still in the grey area) you will see a little horizontal arrow and the value of the wavelength is displayed. If you now click with the left mouse button, you are able to change the lower reflectivity limit (right mouse button=upper reflectivity limit)

7.2.3 Dispersion

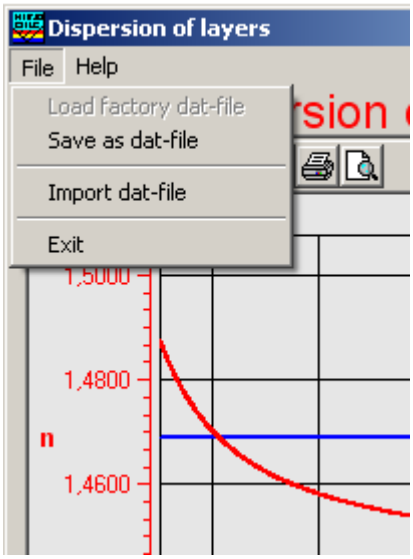
This form shows the refraction index n and the absorption index k (within the plot limits) for different layers. This form is just a tool to control your data, nothing can be really changed in this form.

There are two cursors available for n and k (press the cursor symbol and drag them with the mouse, atrthe beginning they are on top of oneanother)

- You may use 2 cursors (symbol #4). At start time of the cursors both cursors are painted on top of one another, move them with the mouse. The cursor values are shown in blue (= k(λ)) and red (=n(λ))
- You may also zoom in and out and in an area (symbols #1 - #3)



You may also save these dispersion values as a dat-file, but be very careful about the target directory !!

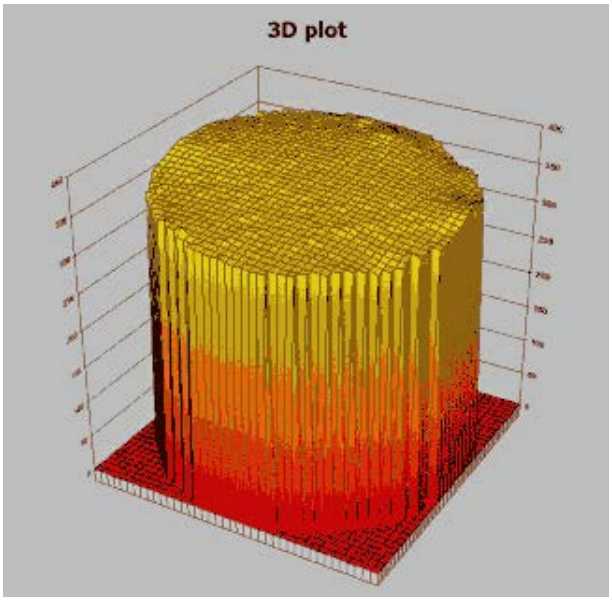


ATTENTION:
To be consistent with data handling, ALL materials files contain n and k data between 150 nm and 1100 nm. Usually only *parts* of these data are measured data (e.g. between 206 nm and 842 nm or between 300 nm and 1100 nm).
If you simulate, the valid part of the curve is shown in *black* while the rest is shown in g*rey* (and you get a message).

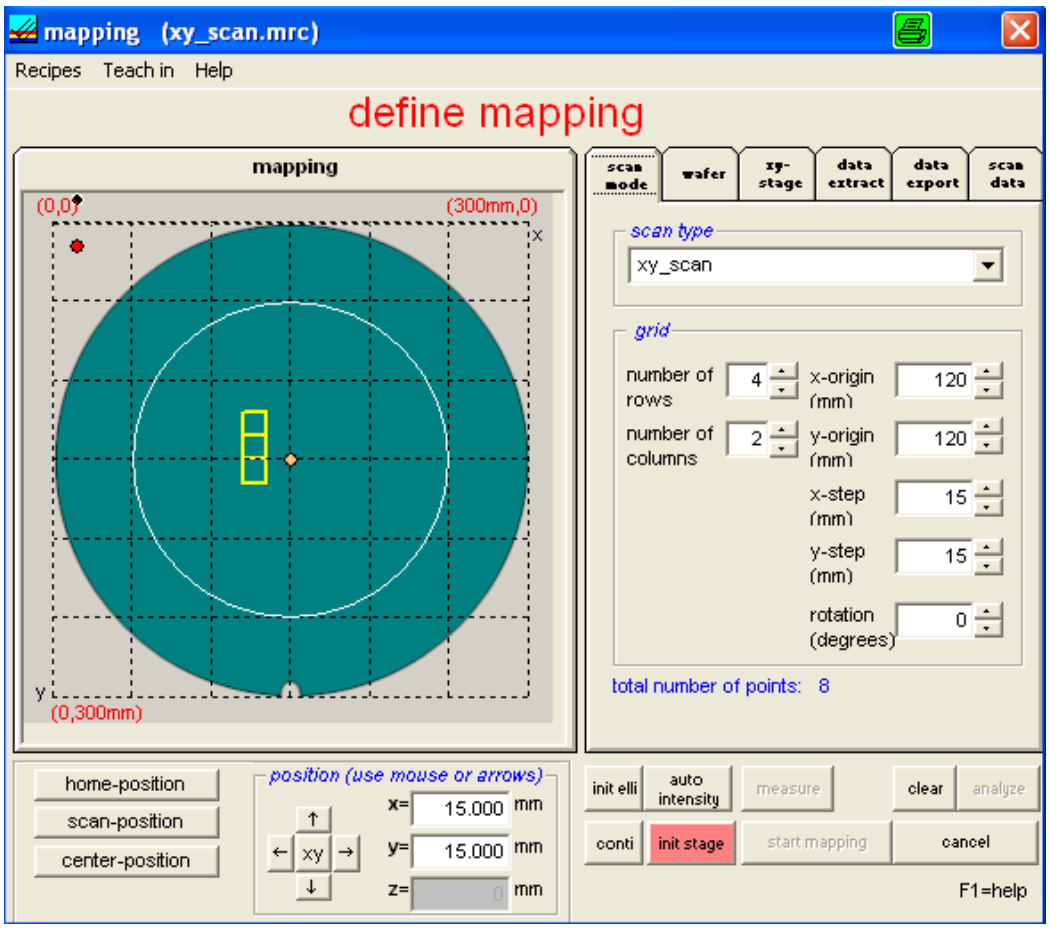
Extraction limits are restricted to the range of valid n and k data.

7.3 Main menu “Externals”

7.3.1 Mapping



You need a mapping-xy-stage and a special mapping add-on software for ElliCalc to measure in mapping mode. In this mode it is possible to measure and display your film parameters as a function of x and y.



main menus of mapping mode

1. menu “Recipes”
   - Save as map recipe
   - Load map recipe

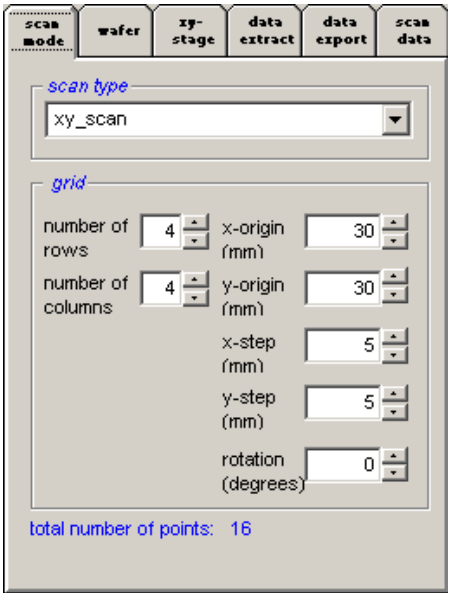
   Here you may save or load ALL the settings you have done in all the various possibilities. It is recommended to save your usual settings in a recipe. It is possible to use a special recipe name like “myownRecipe”. Recipes for mapping will receive the extension “.mrc” and will be saved in menu “Recipes\Map_Recipes”
2. menu “Teach in”

   This will be explained later in the following section
3. menu “help”

   this is the usual access to help functions

main buttons (lower right side)

init stage
you can initialize your ellipsometer (right mouse button=time adjustments possible)
auto intensity
you can adjust the nintegration times automatically (right mouse button=time adjustments possible)
measure
you can take a real (test) measurement with your sample. Thus you can control all settings before you start the mapping
clear
clears the screen
conti
this will make a continuous mode for measurement
analyze
you can analyze the layer parameters your sample. Thus you can control all settings before you start the mapping
initialize stage:
After starting mapping mode you have to initialize the xy-mapping stage first.
Until the xy-mapping stage is initialized the function start mapping is deactivated.
start mapping
this will start the mapping sequence
cancel
leave mapping mode



Scan mode:

a. shape of the wafers:

1. You may use square or round wafers.
2. To use your own design as a background you need to edit the file OwnDesign.bmp within the ElliCalc directory (this is possible with lots of drawing programs, or ask your software supplier for help).

b. wafer size

Wafer size may be changed between 50 mm and 300 mm (= 8"). A grid is shown with a constant grid distance (e.g. 10 mm).

c. scan region

It is possible to change:

- the x and y coordinates of the origin in steps of 0.1 mm
- the number of rows and the number of columns of the scanning grid
  (from 1 to 100)
- the size of the x and y steps (in multiples of 0.1 mm)

The wafer plot shows what you are doing.

d. rotation

here you can rotate the scan region

e. mapping positions

measuring position:

If you press one of the position buttons, the mapping stage will immediately go to this point and a red circle is displayed on the screen. Additionally the coordinates of this point are displayed. If option "measure on each click" in Tab2 is activated, a measurement will be performed.

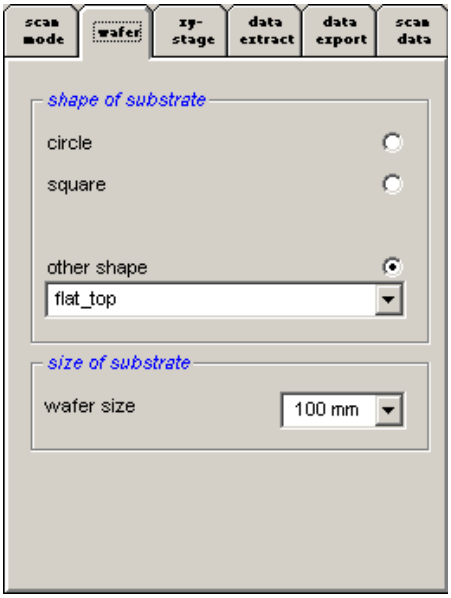
You may reach any point by clicking with the LEFT mouse button or by entering the coordinates and pressing the xy-button.

You may move up and down or left and right by pressing the appropriate arrow buttons. If you press the arrow buttons with the left mouse button the cursor will move in increments of xSteps. If you press the arrow buttons with the right mouse button the cursor will move in smaller increments of xSteps/10

f. position buttons:

1. home position
   Typically this is in the right lower corner of the xy-stage. The hardware of the stage will define this point at the beginning of the mapping experiment (and it can be changed manually in the ini-File in section [mapping], HomepositionX/Y=.... The numbers mean the percentage compared to wafersize (0.05 =5% of wafersize)
2. scan position
   this is the origin of the scanning coordinate system
3. center position
   this is the center of the (round) wafer stage

The wafer plot shows what you are doing.

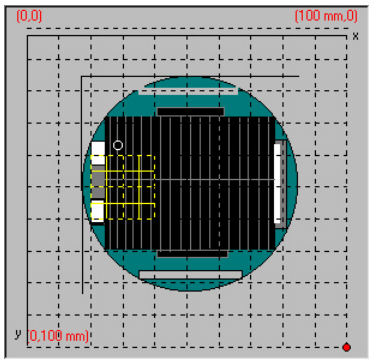


Wafer:

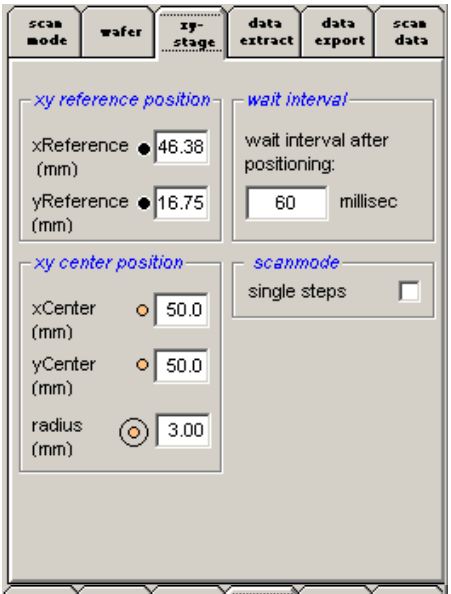
The shape of the substrate may be:

a. circular (between 50 and 300mm)
b. square (between 50 and 300 mm)
c. your own design (change file "OwnDesign.bmp" with any drawing software)

example:



Wafer size may be changed between 50 mm (= 2") and 300 mm (=8"").

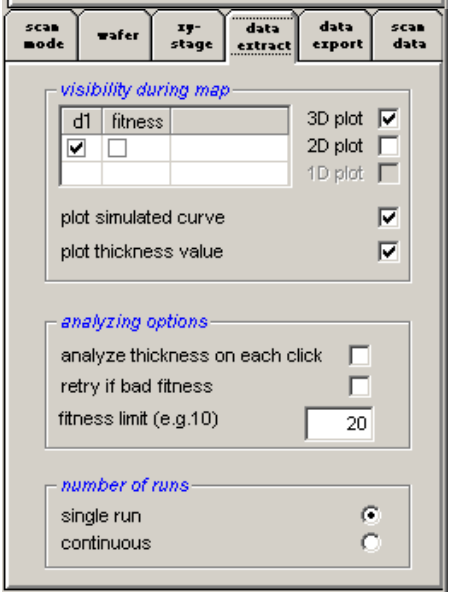


Stage:
Ocean Optics can deliver an xy-stage for 8'' (=300mm).

a. serial port:
The port is used for communication with the mapping-stage. Ask your hardware supplier for details..
To drive the mapping-stage you need one COM-port for xy-stages (or a USB port and a converter).

b**. wait interval:**
After each measurement the scanning may be interrupted for a certain interval of time

c. single step:
If you activate this option each single measurement is waiting for a trigger signal (a keystroke with ENTER key or an external TTL trigger signal which is applied to the spectrometer. Ask your hardware supplier…)



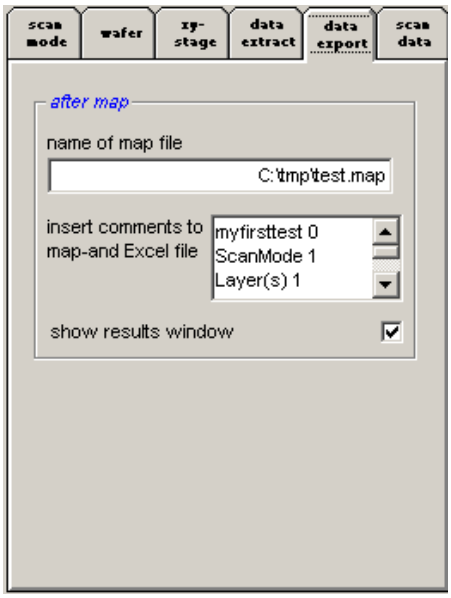
Data extract:

a. plot during map
With this option you choose the layer you want to "extract" = to display.
You cannot choose more than one parameter as only one parameter can be displayed at a time. If you use ElliCalc_10nk you may calculate up to 10 layers (but display ONE of these)

b. analyzing options
Analyze parameters on each left mouse click. This is a very useful feature to make a quick check on film parameter distributions on your wafer (do not forget to activate option "plot value during mapping").
Fitness limit: if your results are completely wrong for some reasons, all measured values with a fitness greater than this fitness limit here will be set to zero. This feature is useful, if dust causes a measurement error during mapping. Without this feature you might get enormous spikes.

c. visible during map
You have the choice between 1D-plots for line scans, 2D-plots and/or 3D-plots.
The 2D-plot and the 3D-plot contain the same data.
A 1D-plot is possible only if you measure along ONE row or column (and not a two-dimensional field.)

d. number of runs
You have the choice between a single run (for real measurement purposes) and a nearly infinite number of runs (=30000) for demonstration purposes.



Data export:
You may choose the following options during a mapping experiment:

1. plot the simulated curve
2. plot parameter value

It is more informative to see the analyzed curve and the calculated parameter value during the simulation, but this is time-consuming. If the mapping takes a longer time it is recommended to switch off these 2 features.

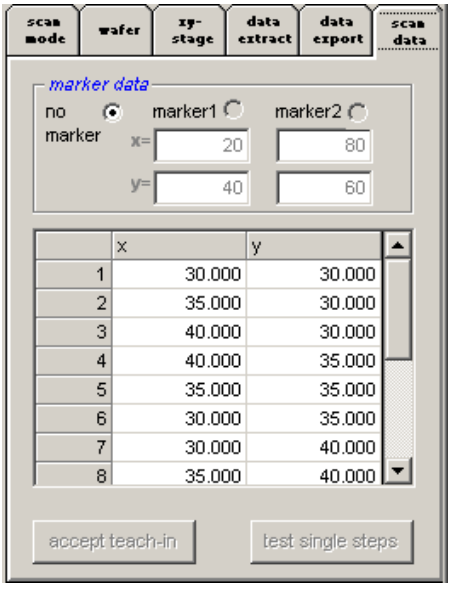
You may choose the following options after a mapping experiment:

1. write data as map-file
2. insert comments in map or Excel-files
3. show results window

1. Write data as map-file
All parameter and fitness data together with some coordinate information are written to a ASCII-file in directory "ElliCalc\data\map_files".
examples can be found in the directory "ElliCalc\data\map_files"

2. insert comments in map or Excel-files
you may enter text like "sample #1, "Paul McCartney" or "myfirsttest".
This text will be a header for your map-files and also for all exported Excel_files

3. show result window
If you accept this option a results window with possibility for Excel export will open after the mapping process.

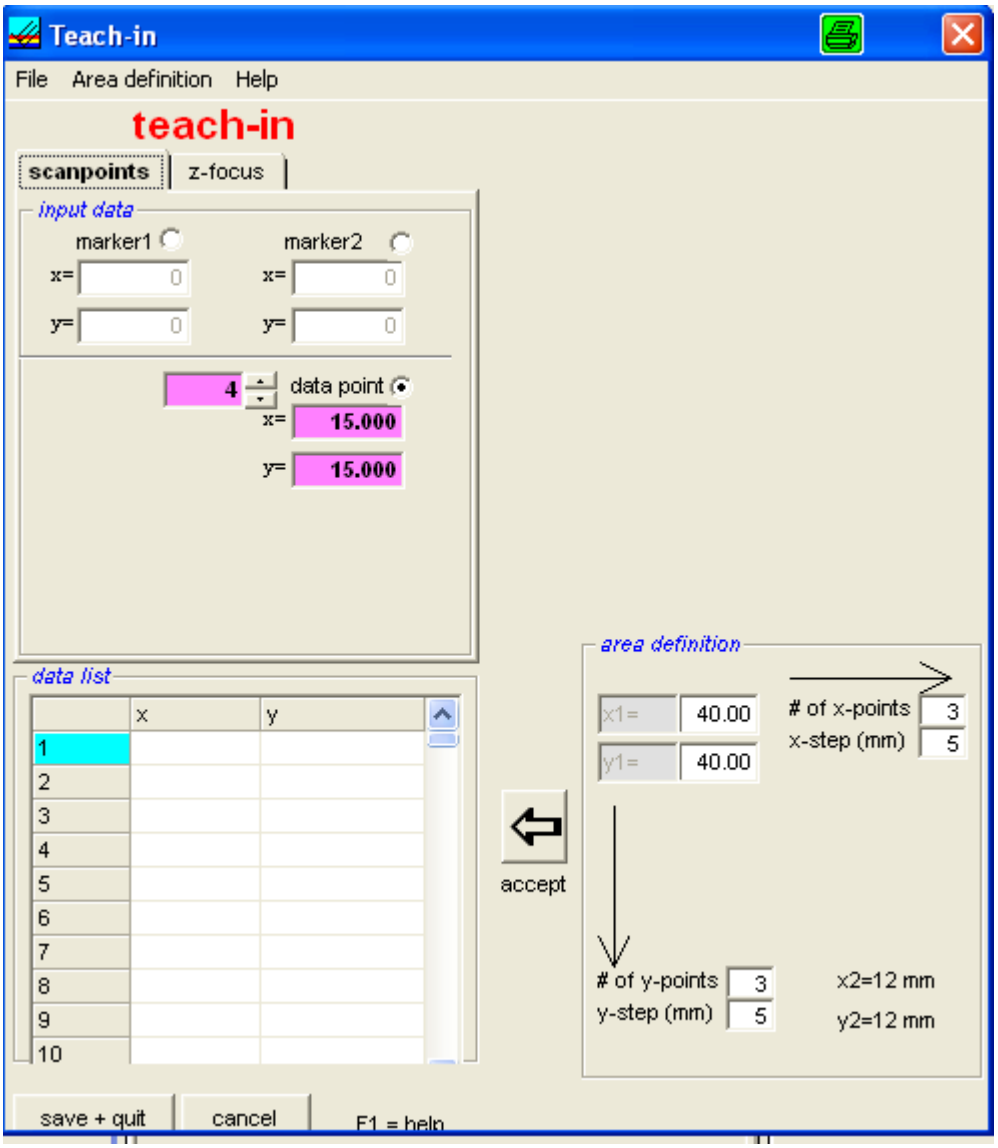


Scan data:
This feature is used in microscope arrangement (e.g. for measuring structured wafers) if you want to hit the xy-positions with higher accuracy.
Usually the wafer or sample will be positioned on the chuck with some mechanical adjustments (like pins on 2 sides of the wafer and adjustment to the wafer flat). This will result in a medium accuracy, but not comparable to fine positioning like in semiconductor photolithography.

How to get a higher accuracy:

1. click on "marker 1":
   The stage will move to this position. If you now look through the microscope you will see a slight deviation between the illuminated spot and the real marker on your wafer.
2. Correct this deviation by moving the stage (use the keyboard arrows: clicking or pressing once = 10 micrometer, SHIFT + clicking or pressing once = 1 millimeter). The red circle on the screen will move slightly off the marker.
3. Repeat step 1 and 2 for marker 2
4. Now the software knows both deviations and is able to calculate what to do: shifting the origin and rotating the scan pattern a little bit. Press the button: "accept teach-in"
5. Control the values of rotation angle and xy-origin
6. Start mapping as usual

Teach in:
Teach in is an interactive tool to write new map-recipes without using text editors to edit the map recipe file.



Now the method with teach-in-mode:

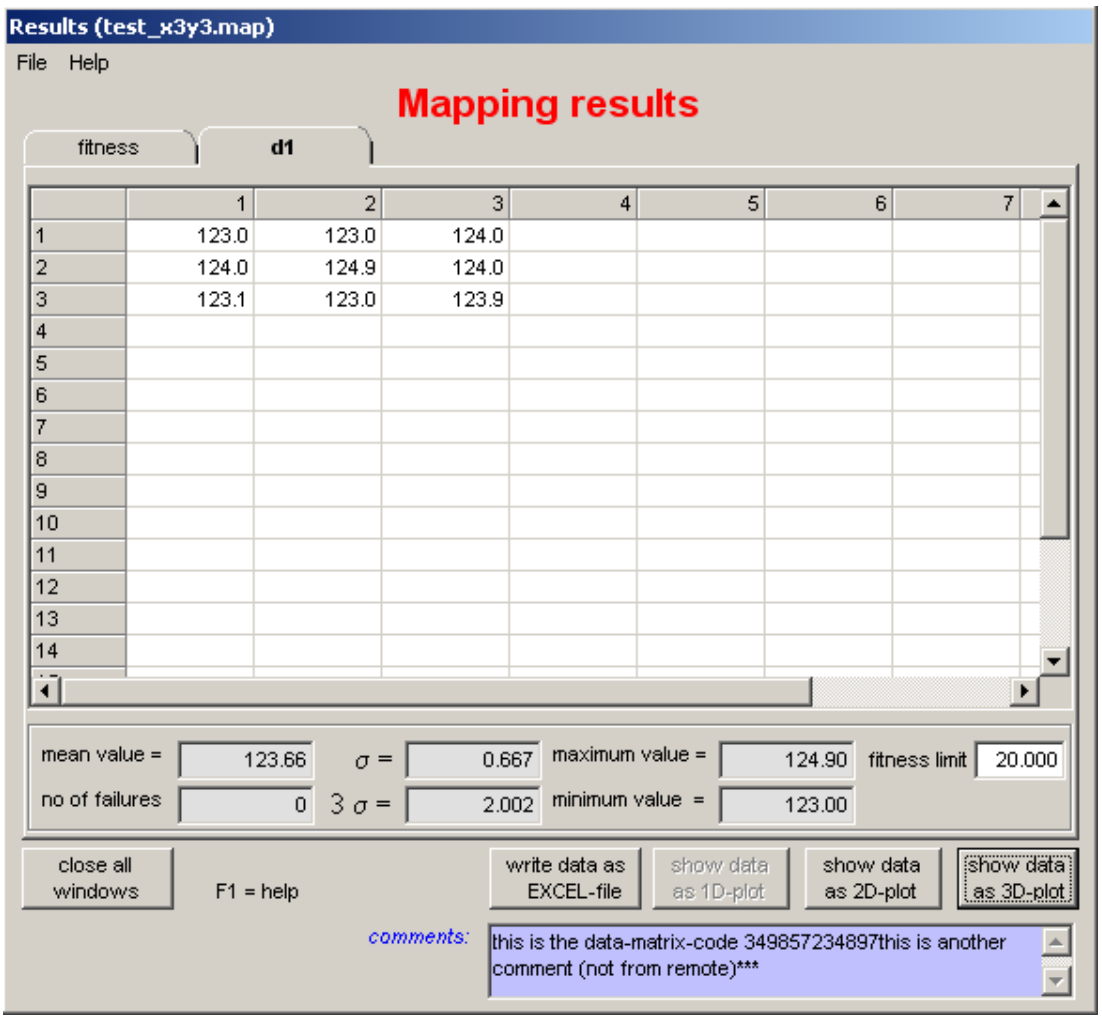
1. Open the mapping window (main menu “map data”) and then the menu “TeachIn”
2. You will see this window:
3. To set the first marker position, click on “marker 1”, then move the measuring position
   with the arrow keys on the keyboard
   or by clicking somewhere in the wafer area
   or by typing values in the text box
4. To set the second marker position, click on “marker 2”, then move the measuring position as before
5. To set the first data point, click on “data”, then move the measuring position as before
6. To set the next data point, click on the up down counter (now it should show the value 2 instead of 1)
   and then move to the measuring position as before
7. Save the new recipe (like test.mrc) with the extension .mrc

It is possible to change any or these values by clicking on the first columns in the appropriate row. Then the stage moves to that position and you are able to change it.

It is NOT possible to interchange or delete rows.

7.3.2 Result List

As soon as the mapping is finished you will see a result list:



On the first page you see the measured thickness values for each layer. In the picture above there was just one layer and 3 x 3 = 9 measured data points. In the last page you can see the associated fitness values for each coordinate. In the text windows below the data window you see mean values, maximum and minimum values and standard deviation σ, the 3σ-value and the number of failures (according to the measured fitness and your fitness limit).
If you did not choose a regular scan pattern, you will see a one-dimensional list.

If you click on the buttons with the numbers in a row or a column you will highlight a certain number of data points (in the picture above column 3 was highlighted). Now you can control these selected values in a one- or two-dimensional plot by pressing the appropriate button in the last row. You may also choose a smaller amount of data by dragging with the mouse (e.g. 2 x 2 = 4 points).

If you press “write data to EXCEL-file” EXCEL will be opened (if installed on your PC) and the data will be transferred to a spreadsheet.
With “close all windows” you will return to NanoCalc main window and all mapping windows will be closed.

If you enter a value for “fitness limit” and press ENTER, the screen will be updated and all cells with a higher fitness than your limit will be plotted in red (cells in grey show that this point was outside the wafer).

7.3.3 Analyze mapped data

This feature helps to analyze mapped data that have been measured earlier.

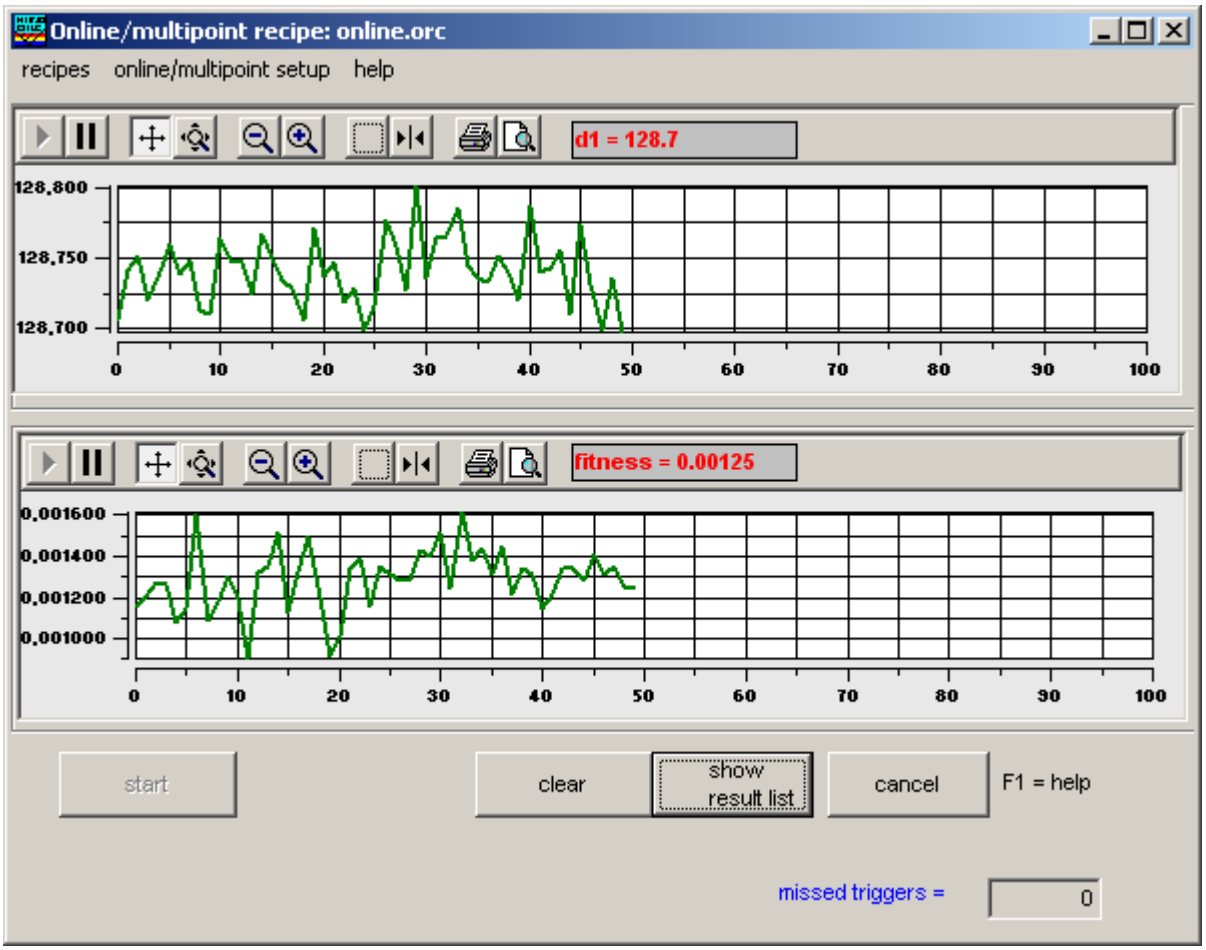
You are asked for a file name (extension .map) in directory ElliCalc\data\map_files. Then the results window is opened and you may inspect your data, plot the data or export them to Microsoft Excel.

7.3.4 Structure of .map-file

The first 2 lines are comments, the file format is very strict.

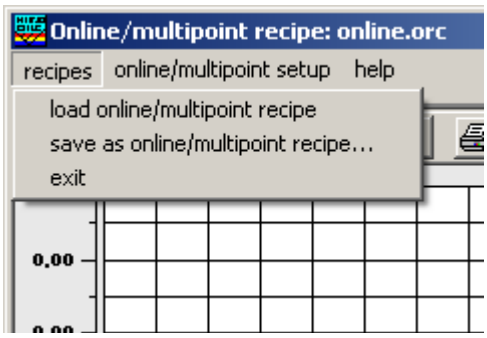
```
test4
user4
***
xy-ScanMode
1 Layer(s)
1 Layer(s)ToExtract
2 Row(s)
2 Col(s)
4 total points

5 xStep
5 yStep
***
IndexNo, row, col, x, y, fitness, d1
1, 1, 1, 30.000, 30.000, 0.048, 132.880717
2, 1, 2, 35.000, 30.000, 0.048, 132.806642
3, 2, 1, 35.000, 35.000, 0.048, 132.918102
4, 2, 2, 30.000, 35.000, 0.048, 132.858514
```

7.3.5 Online/multipoint measurements



load online recipe:
The online setup window contains lots of input data, so usually you will want to use an online recipe to do that job for you.

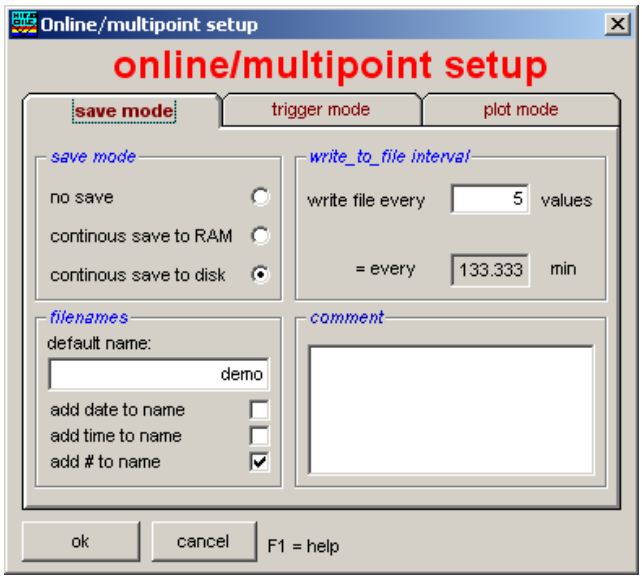
You will be asked for a file name (usually in directory "ElliCalc\recipes\online_recipes"). After loading this file nothing happens except new parameters in setup, like different y-axis or other trigger parameters.



save as online/multipoint recipe:
The online setup window contains lots of input data, so usually you will want to use an online recipe to do that job for you.
If you changed some setup parameters you can save them as a new online recipe.
You will be asked for a new file name (usually in directory "ElliCalc\recipes\online_recipes").

online/multipoint setup:
Depending on the switch "show setup first" in menu "online\setup" the setup window for online measurements is shown at first or not. If you want to rename your files at the beginning of each measurement cycle it is recommended to open the setup window first.

The setup window contains lots of input data, so usually you will want to use an online recipe to do that job for you.



Save mode:
In this first part of online setup you can choose:

a. Option "save mode"

1. Do not save the online data
   all data are lost and only visible on screen
2. save online data to RAM
   At the end of the run you may observe and analyze your data in the results window
3. save online data to disk
   according to option "write_to_file_interval" all data are written to file in smaller portions with filenames that are determined in option "filenames"

b. Option "filenames"

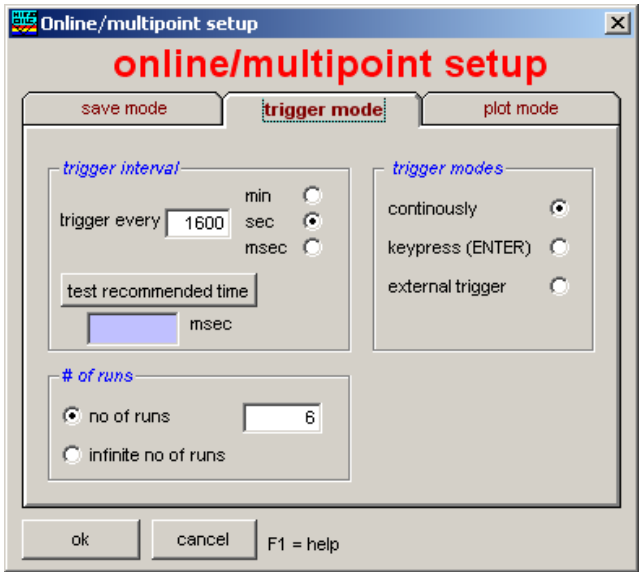
1. Choose a name like "series 1" or "test4" or alike
2. Choose one or more options "add….." example: a filename might look like: test156.onl

c. Option "trigger interval"

You might want to save the value (not the file !) every trigger, but for some reasons you might want to save only every third trigger.

d. Option "write_to_file_interval"

You might want to save the file (not the value !) every trigger, but for some reasons you might want to save only every third trigger.



Trigger:
In this second part of online setup you can choose:

a. option "trigger mode"

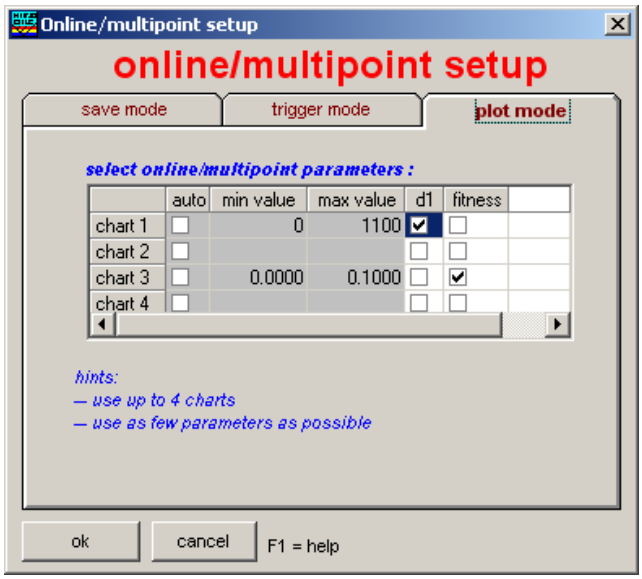
You can trigger continuously by adjusting the appropriate software parameters like trigger interval.
you can trigger externally with a TTL-signal to your spectrometer. Please consult your hardware supplier…

b. option "trigger interval"

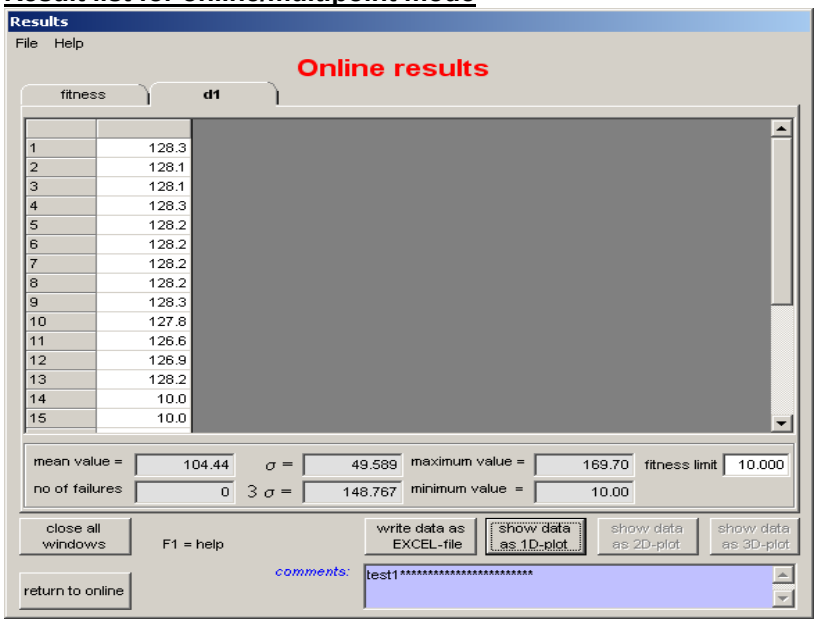
Here you choose the time interval between two software triggers. Pay attention on the correct unit.
You may test the trigger interval empirically with "test recommended time". Add some safety margins.

c. option “number of runs”

You might want to run a certain number of data points only or (nearly) infinitely. Attention: “infinite” means about 999999 data points.



Result list for online/multipoint mode



On the first page you see the measured thickness values for each layer. In the picture above there 5 measured data points. In the last page you can see the associated fitness values for each measurement. In

the text windows below the data window you see mean values, maximum and minimum values and standard deviation σ, the 3σ-value and the number of failures (according to the measured fitness and your fitness limit).

If you press “write data to EXCEL-file” the data are transferred to an .xls-file (Excel need not be installed on this PC).
If you press this Excel-button together with the SHIFT-key the text will switch to “write data as csv-file” and such a csv-file will be generated instead of an .xls-file.

With “close all windows” you will return to ElliCalc main window and all online windows will be closed.

7.3.6 Analyze online/multipoint data

This feature helps to analyze online/ multipoint data that have been measured earlier.

You are asked for a file name (extension: .onl) in directory ElliCalc\data\online_files. Then the results window is opened and you may inspect your data, plot the data or export them to Microsoft Excel.

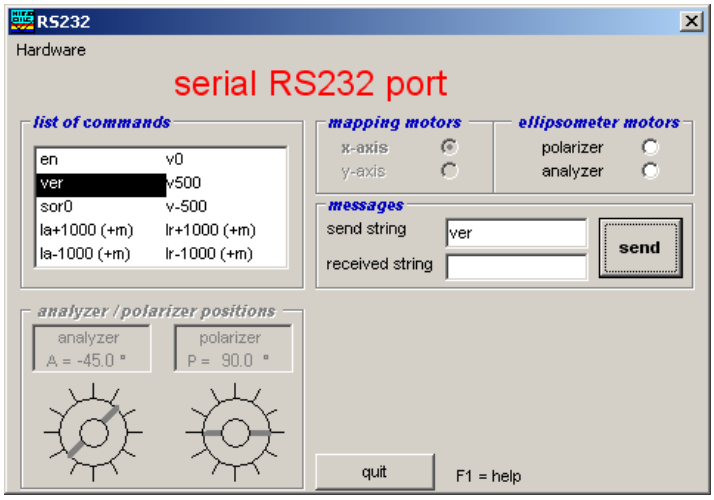
7.3.7 Structure of .onl-file

The first line is a comment, the file format is very strict.

```
test1
***
55 total points
***
triggercounter, time, fitness, d1
1, 10:35:19, 0.010, 128.3
2, 10:35:19, 0.010, 128.1
3, 10:35:20, 0.014, 128.1
4, 10:35:20, 0.009, 128.3
5, 10:35:21, 0.008, 128.2
```

7.3.8 RS232

If you own an xy-stage or any other arrangement with Faulhaber motors you may use this menu to drive the motors and to test their behaviour. You find a list of commands on the left side, for more information please consult the motor manuals.

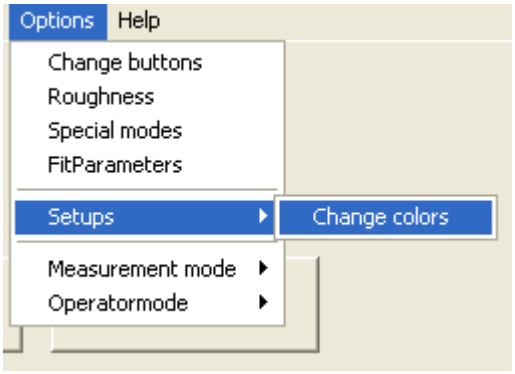


You may open and close each virtual port separately. If you send the signal "ver" the motors of the xy-stage should answer (more precise: this command is "1ver" for motor1 and "2ver" for motor2). Ask your hardware supplier for the motor numbers.

7.3.9 Vision system

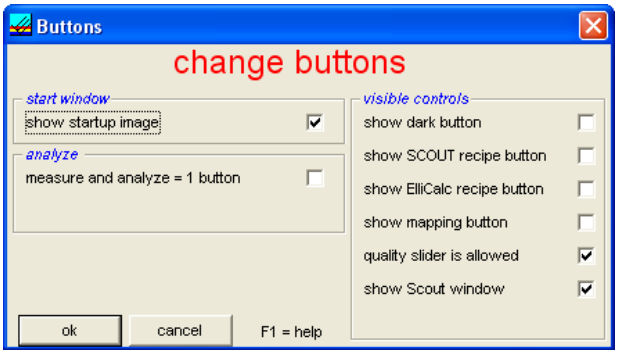
If you own a vision system with an IDS uEye-camera you may turn on the camera with this menu

7.4 Main menu “Options”

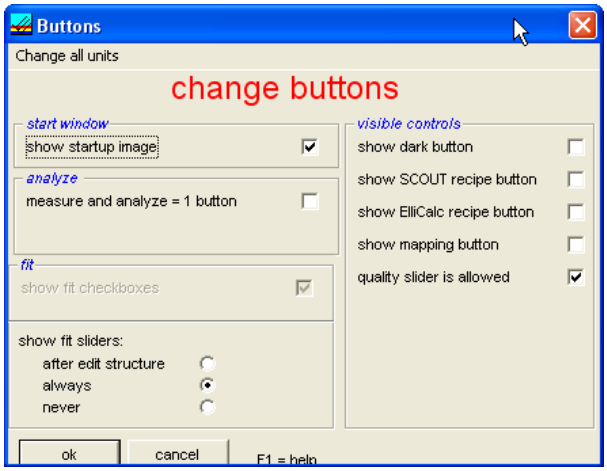


7.4.1 Change buttons

with SCOUT



witout SCOUT = internal mode



In this window you can make visible or invisible:

- The startup image:
  The picture will disappear after some seconds or you might “click it away”

- measure and analyze-button:
  to combine the functions to the measure and the analyze button

- show fit checkboxes (in internal mode of ElliCalc only):
  in the menu Edit Structure there are some fit checkboxes that can be made visible or not. In the current software version only thickness and n and k (for Cauchy models) are activated
- show fit sliders (in internal mode of ElliCalc only):
  you may use fit sliders to check for variations of thickness, n or k

- show dark button:
  to measure any dark current separately
- show SCOUT recipe button:
  it is not necessary to see the SCOUT window, but for experienced users this might be helpful

- show ElliCalc recipe button:
  to make it easier to load recipes
- show mapping button:
  to make it easier to use mapping
- quality slider is allowed
  With this feature it is possible to set the speed (or the precision of the fit) for each individual measurement

7.4.2 Fit parameters

In the 1st Tab “General” you may change the time for simulation = the number of Simplex fits. A longer time usually means more precise data (up to some limit…)
In the 2nd Tab “Traffic lights” you may change the fitness values for the trafficlight = good/medium/bad

7.4.3 Some setups

7.4.3.1 ElliCalc setups

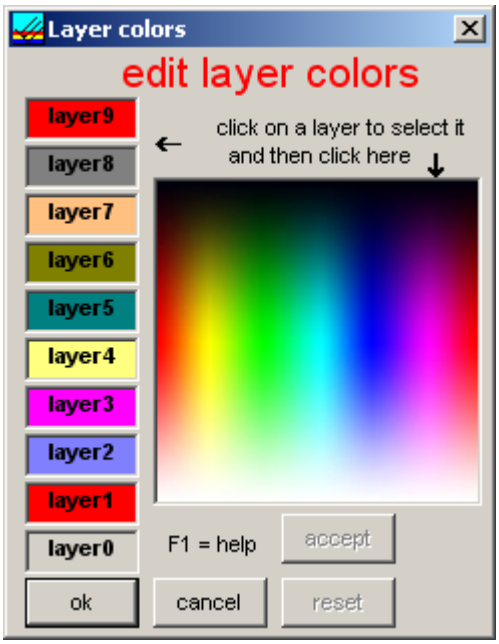
Here you can change:

- Number of polarizer steps
  Typically ElliCalc uses 18 steps per revolution of the polarizer = a measurement every 20°. This is good for most purposes. If you use less steps (e.g. only 9 steps) you might loose presicion (but you may try, it’s faster…)
- Analyzer angle
  Normally this value is 45°. BUT: if you have measured your signal and see that the mean value of Psi is totally different from 45° (e.g. around 15°) then reset the analyzer angle to this mean Psi-value (15°) and repeat the whole mesurement. This will increase the quality of your data and is especially useful for thin layers

7.4.3.2 Change colors

In this menu you may change the colors of your layers in the layer stack. It is just an optical effect and has nothing to do with calculations.

First click on the layer area on the left side. Then move the mouse over the large colored area and click if the color pleases you. Then press OK



7.4.4 Operator mode

NanoCalc can be used in administrator or operator mode.

7.4.4.1 administrator mode

In user mode certain restrictions apply: e.g. the user is not allowed to edit the structure or to change the parameters of the spectrometer.
The default password to come back to administrator mode is: ”**admin**”. This password can be changed arbitrarily, there are no severe restrictions concerning passwords. Please use letters and numbers only.

7.4.4.2 administrator mode

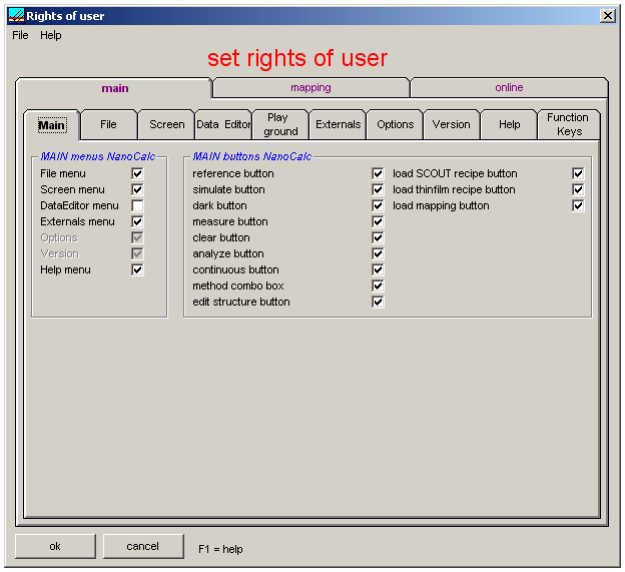
In administrator mode no restrictions apply.
This mode is reserved for the administrator of the system.

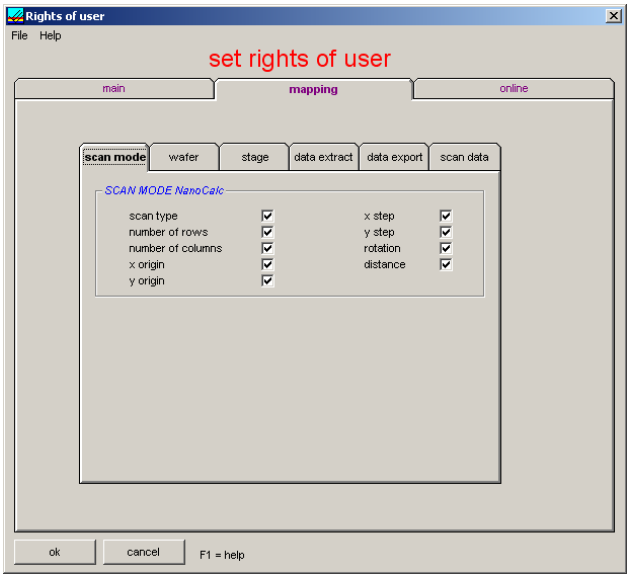
The default password to come back to administrator mode is: ”**admin**”. This password can be changed arbitrarily, there are no severe restrictions concerning passwords. Please use letters and numbers only.

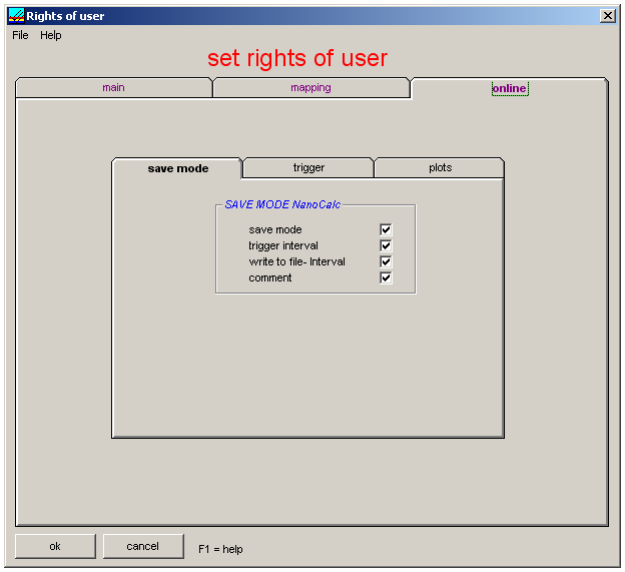
The administrator may define the options that will work for a standard user. To get this Rights of User - window just click ”administrator mode”.

7.4.4.3 Rights of user

The administrator may set the rights for the user for nearly every single feature of the software.







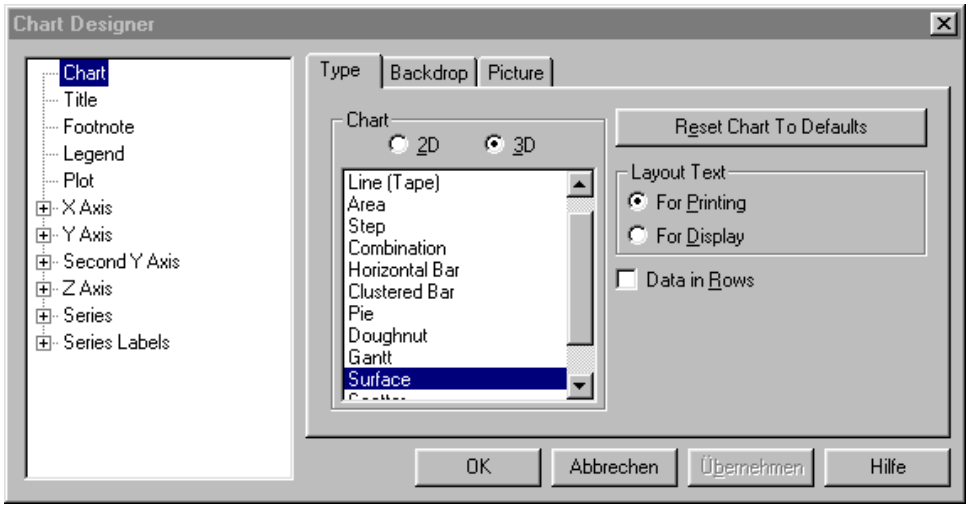
7.4.5 Remote control

There is a very powerful **OLE** remote control as well.
Ask your software supplier...

7.5 Main menu “Version”

This menu is visible only if you own a “combiversion” = a combined version of NanoCalc and ElliCalc. You may switch to the other application

7.6 Chart and chartdesigner

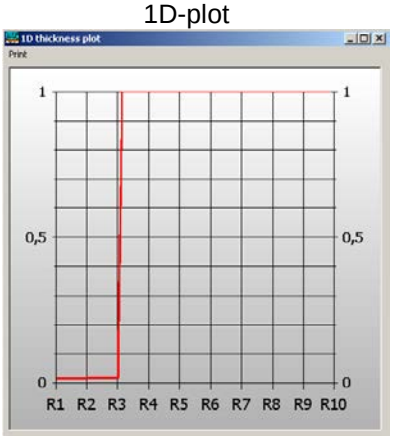


If you produced a 1D-plot or 2Dplot or 3D-plot you may change nearly ALL parameters of the plot by clicking with the RIGHT mouse button

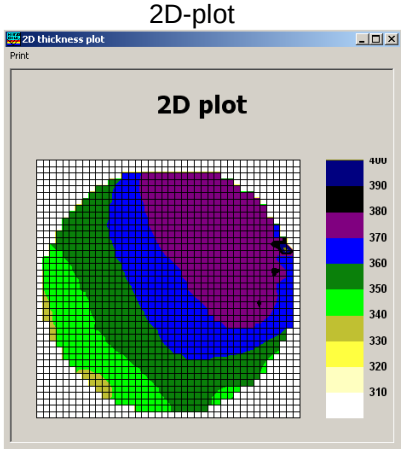
Hint:
To change the view position: keep CTRL button pressed and move the mouse at the same time.

For further information see VCFI5.hlp in the help directory of your ElliCalc installation.

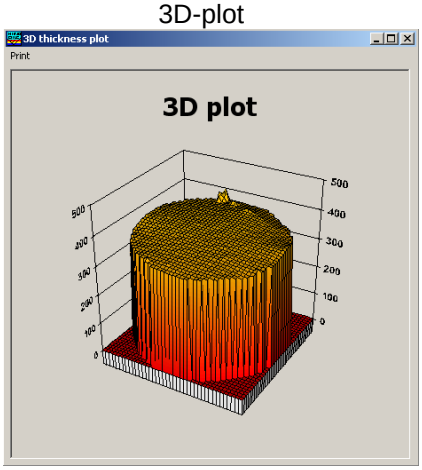
1D-plot



2D-plot



3D-plot



During mapping it is possible to produce 1D-plots, 2D-plots and 3D-plots.
These plot types can be changed interactively after the mapping was finished. Click on the plot with right mouse button to get access to the "chart designer“.

8 Special features for “SCOUT mode”

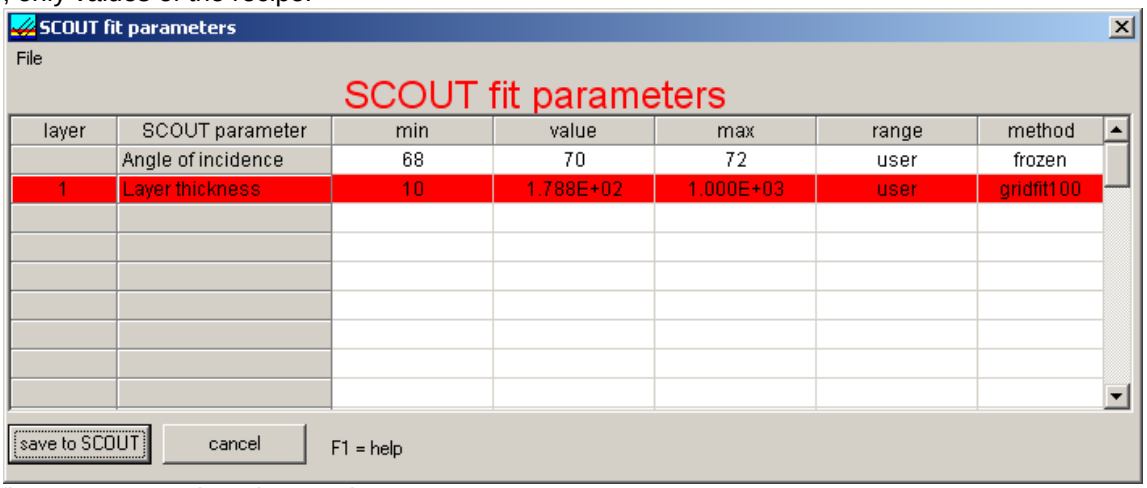
8.1 Main menu “File”

8.1.1 Change layer recipe

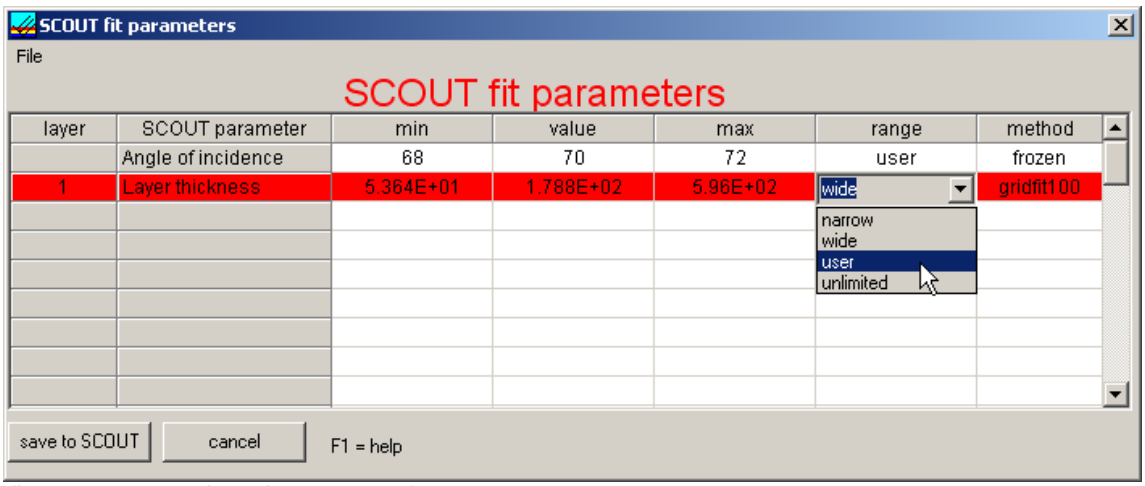
If you load a (.lrc)-recipe containing a link to a SCOUT .sc2-recipe and measure your sample, SCOUT will analyze in the background and the results will be displayed in the graphical user interface of ElliCalc. The layer stack and all layer parameters are defined within SCOUT and are extracted by SCOUT. ElliCalc is only a user interface. There are lots of data in ElliCalc's internal .lrc-recipe, but most of them are not important in this context: SCOUT is the "master".

With "change layer recipe" you may change some of the layer and fit parameters of SCOUT (but not all). Your changes are NOT permanently saved to the SCOUT recipe on the harddisk, only to the running SCOUT instance. If you are convinced that your changes are good enough you may also save them permanently (at the moment only via Scout itself).

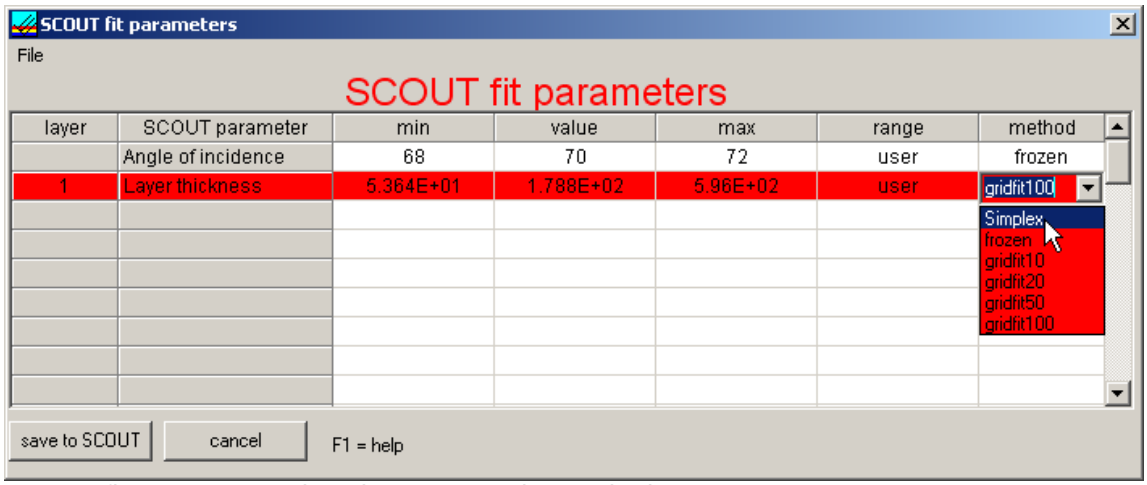
To switch to a completely new recipe you have to load another .lrc-recipe with a different SCOUT .sc2-recipe (do NOT use SCOUT directly !). With "change layer recipe" it is not possible to change the layer structure, only values of the recipe.



SCOUT fit parameters: Changing a value



SCOUT fit parameters: Changing a range for parameters



SCOUT fit parameters: Changing an extraction method

8.2 Main menu “Screen”

8.2.1 Psi/Delta or tan(Psi)/cos(Delta)

Here you may switch between a display in Psi/Delta or in tan(Psi)/cos(Delta), whichever you prefer. The data transfer to SCOUT (via a file EC_data.xy in Internal_Files) is done in tan(Psi)/cos(Delta)

8.3 Main menu “Options”

8.3.1 Some setups

Scout stoptime in seconds.
You may enter a number (in sec) to stop SCOUT calculations independent of the quality of the data. This is equivalent to the above mentioned slider in menu “Fit parameters” / Tab1

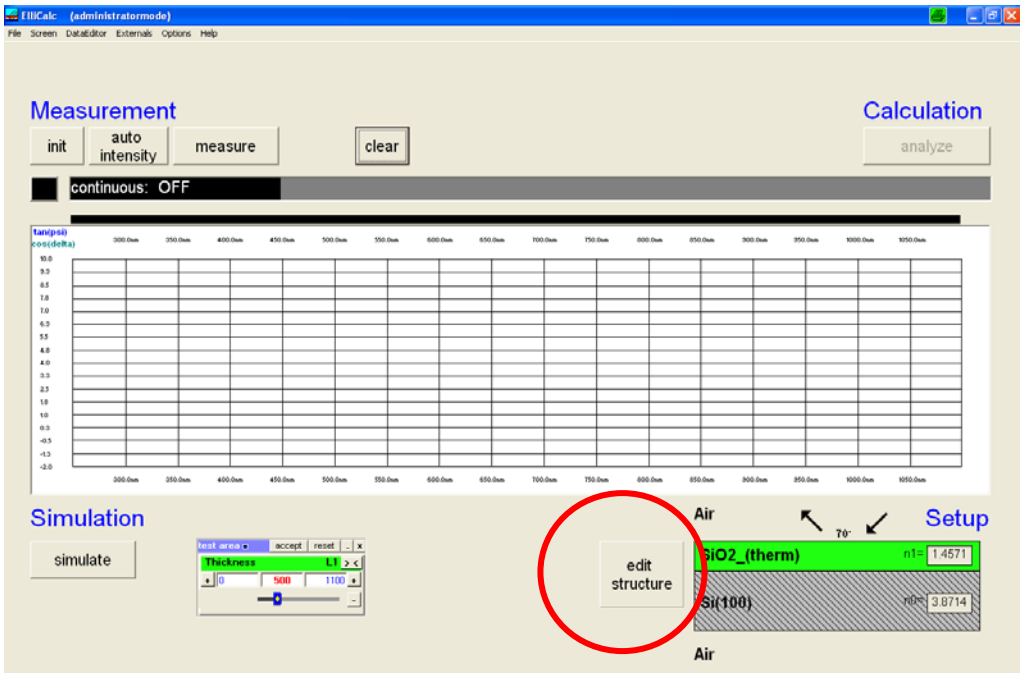
9 Special features for “internal mode”

This internal mode can only extract thicknesses in layer stacks, so this is much more restricted than “SCOUT mode”. You do not need the SCOUT software and it may be faster than SCOUT in simple cases.

To reach this mode you have to use a lrc-recipe without an internal link to a SCOUT .sc2-recipe. There are different possibilities to do do this:

- Press SHIFT+CTRL+F12
- Or: load a special .lrc-recipe, called “no_recipe.lrc”
- Or: edit any .lrc-recipe manually: just remove the name of the .sc2-recipe after “Scout_FileName_EC=name.sc2” in section [Scout]. Be careful with this manual editing, make a safety copy! Finally the line should read: “Scout_FileName_EC=”

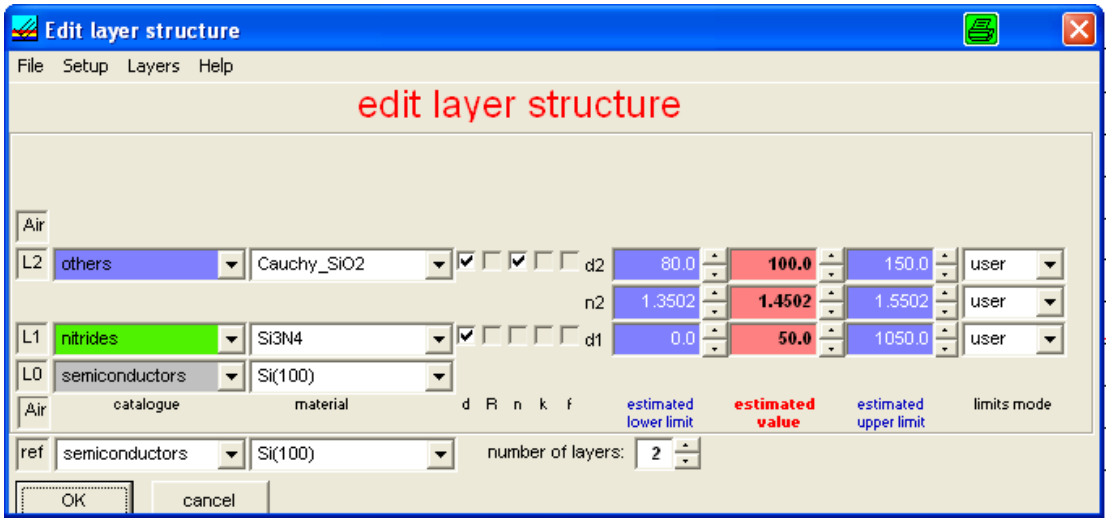
After this change, you will see a new button “EditStructure”, which allows you to edit your own layer stack.



9.1 EditStructure button

You will see this button and this window only if you do not use a SCOUT recipe = if you use ElliCalc’s internal mode. You get good results, but only for the extraction of thicknesses (not dispersion)
In this menu “edit layer structure” you have to define your own layer structure

9.1.1 General



The full menu EditStructure is only available if you do not use SCOUT.

In the menu EditStructure you may enter:

1. The type of catalogue like:
   oxides
   nitrides
   semiconductors
   .....

2. The type of material within one specified catalogue, like „oxides“:
   SiO_2
   CuO
   TiO_2
   ......

3. The number of layers (in the present version: 1 to10)

4. The thickness of all layers in nanometers. This value is regarded as an EXACT value for simulations and as a GUESS for analyzing measured spectra. Whether this guess is used (or not) will depend on the measurement mode.

5. A lower and an upper limit of the thickness. These values are NOT used in simulations. Whether these limits are used for measuring purposes (or not) will depend on the measurement mode.

6. An option „fixed“:
   If you press this option, the lower and upper limits are fixed to the value of the thickness of the layer. Such a layer is regarded as „well known“.Of course it does not make sense to use three fixed layers, there is nothing left to analyze.

7. An option „narrow limits“
   If you press this option the lower and higher limits are set to about 80-100 nm below and above the value of the thickness. This is equivalent to having a FAIRLY GOOD KNOWLEDGE of the thickness

8. An option „wide limits“
   If you press this option the lower and upper limits are set to a wider range. This range depends on the

settings of the menu EditStructureSetup and may be set to:
-- well defined values like: lower limit=200 nm and upper limit=800 nm
(with any thickness value between 200 and 800 nm)
-- constant range like lower limit=thickness-100 nm and upper limit=thickness+100 nm
Thus the search region is restricted to a rather wide, but more or less "reasonable" range. Of course you may also set the limits very narrow, even to a search range of zero.

9. An option „user limits“
If you press this option you may set the lower and upper limit to any value between 0 and 300000 nanometers. These values are equivalent to having absolutely NO KNOWLEDGE of any thickness.

10. A submenu “layers” with lots of commands to delete, insert or switch layers. Especially important is the possibility to include “thick layers” = include the calculation of backside reflections.

9.1.2 Catalogues

In the menu EditStructure you find a row “catalogues” for each layer. You may choose the **TYPE** of material like: glasses, semiconductors, metals etc. In the next row “materials” you may choose the actual material of your layer.
There are different catalogues for photoresists (for different companies like Shipley, MRT and others).
You may add a new catalogue manually or use the menu Edit Refraction Index.

9.1.3 Materials

In the menu EditStructure you find a row “materials” for each layer. You may choose the material itself: Si, GaAs, Ge etc.
In the previous row “catalogues” you first have to choose the TYPE of material of your layer (like “semiconductors”). There are different catalogues for photoresists (for different companies like Shipley, MRT and others).
You may add a new material manually or use the menu Edit Refraction Index.

9.1.4 Thickness

ElliCalc uses values for the thickness between 0 and 300000 nm (=300 micrometers).

9.1.5 Estimates

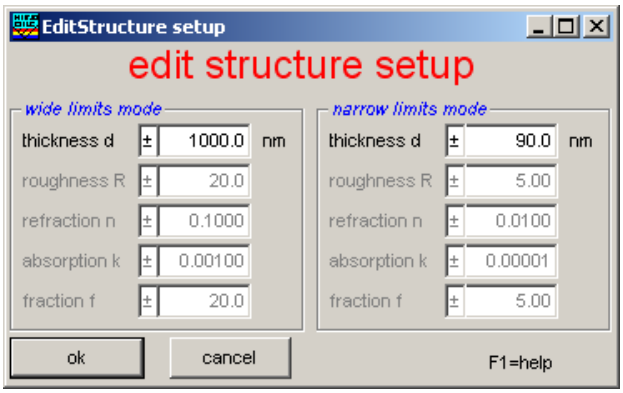
ElliCalc uses a maximum value for the estimates of 300000 nm (=300 micrometers).

In automatic mode it is **NOT** necessary to add values for the upper and lower estimate.
You should give reasonable values for these limits in fitting mode as this influences the time for calculation considerably.

9.1.6 Fixed limits

If you fix a layer you force the upper and lower limit to have the same value as the thickness value. This means that the thickness of a fixed layer is regarded to be “well-known” = exact.

Example: thickness = 500 nm
upper limit = 500 nm
lower limit = 500 nm



9.1.7 Narrow Limits

If you click “narrow limits”, ElliCalc uses rather narrow low and high limits range of about 100 nm above and below your thickness estimate (depending on the material of the layer)

Example1: thickness = 500 nm
upper limit = 600 nm
lower limit = 400 nm
Example2: thickness = 3500 nm
upper limit = 3600 nm
lower limit = 3400 nm

If you need a larger range of limits you have to choose the options WideLimits or UserLimits (up to 300000 nm).

9.1.8 Wide Limits

To use this option you should consult the menu EditStructure \ Setup first:
You have the choice between relative and absolute wide limits
If you choose “relative wide limits” (e.g. ±500 nm and a thickness of 4000 nm), ElliCalc will search between 3500 nm and 4500 nm.

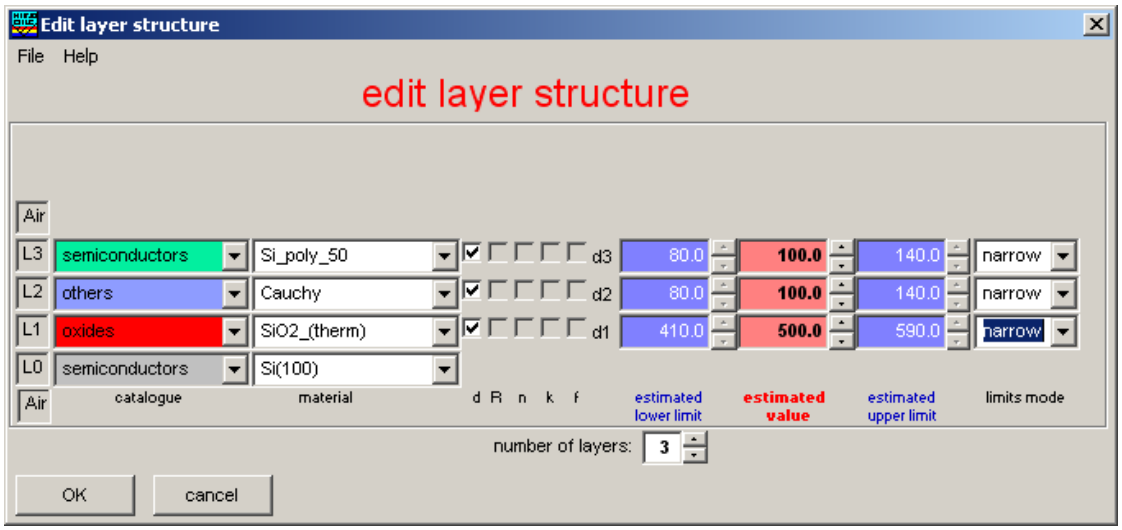
If you choose “absolute wide limits” (e.g. 1500 nm and 6000 nm and a thickness of 4000 nm), ElliCalc will search between 1500 nm and 6000 nm. The value of 4000 nm is of no importance in this case.

9.1.9 User limits

If you click “user limits”, ElliCalc accepts your values for lower and upper limits (up to 300000 nm = 300 micrometers).

9.1.10 Number of layers

In its internal mode ElliCalc is doing all simulations with a maximum of 10 layers and am maximum of 12 fit parameters (=thickness and Cauchy).
An example of 3 layers:



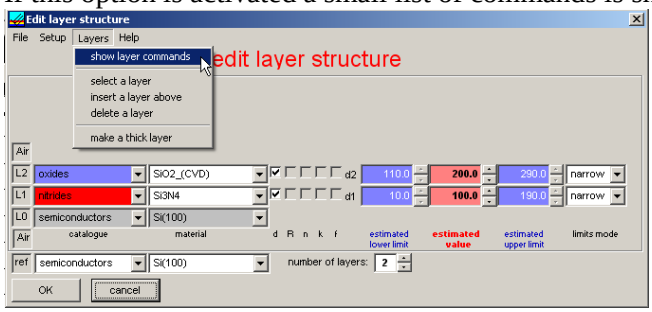
9.1.11 Layer commands

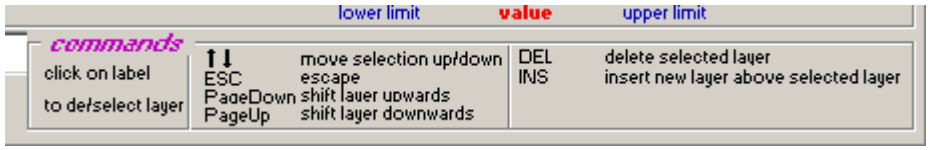
only available in "internal mode"

In menu EditStructure there is a submenu "layers" which helps to insert, remove or shift layers within a stack.

application 1: show layer commands

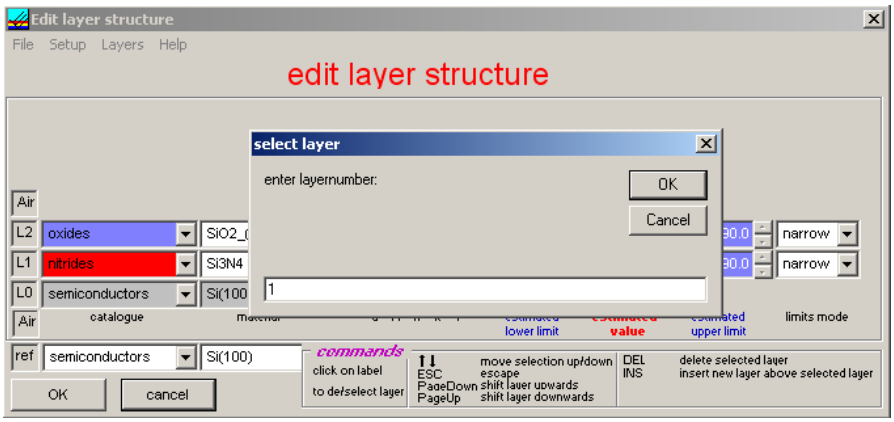
If this option is activated a small list of commands is shown (like PageDown, PageUp, ...)

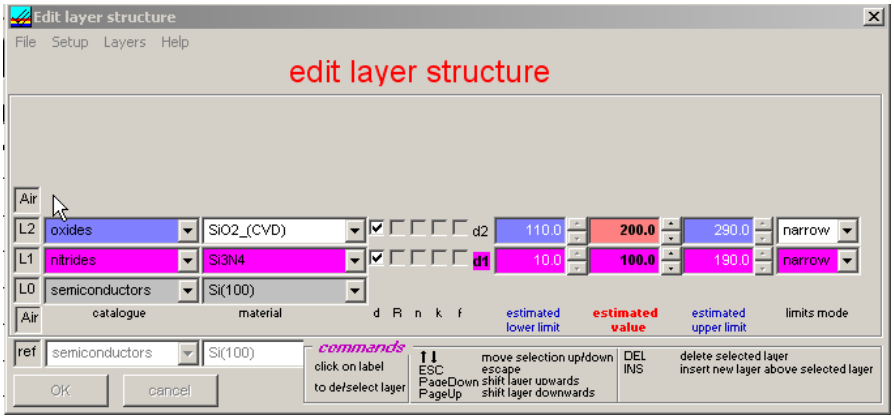




application 2: select a layer

To delete, insert or switch layers you first have to select a layer.
You have 2 possibilities:
a. click on the label of the layer, e.g. L0 with a left mouse click
b. in submenu "layers" there is a command "select a layer"





application 3: delete a layer

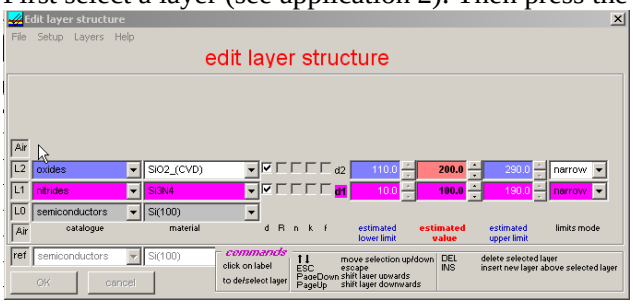
First select the layer that is to be deleted (see application 2). Then press the delete button on your keyboard
Or: select the layer and use the command "delete a layer" in submenu "layers"

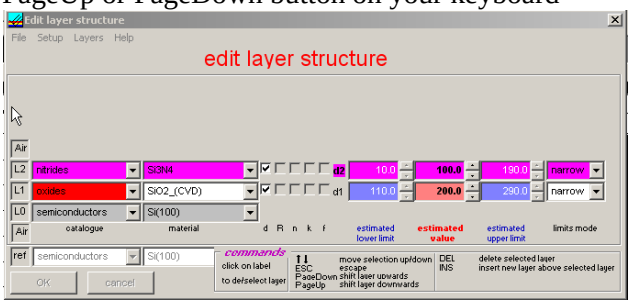
application 4: insert a layer (above another)

First select a layer (see application 2). Then press the insert button on your keyboard
Or: select the layer and use the command "insert a layer above" in submenu "layers"

application 5: switch layers

First select a layer (see application 2). Then press the PageUp or PageDown button on your keyboard





9.2 Main menu “Options”

9.2.1 Roughness

General:

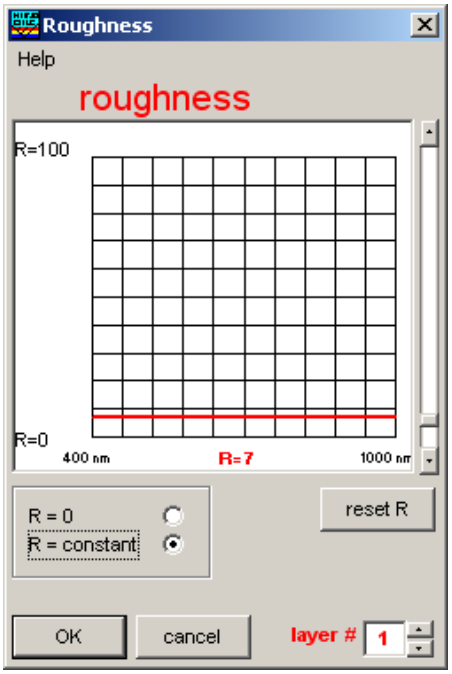
It is quite difficult to measure interference if the substrate or the layers are rough, as the interference patterns get lost.

Example: Roughness is quite common for thick layers like 20 micrometers of photoresist, as the drying process is very critical and the shrinking of the resist does not lead to perfect surfaces.
Roughness is also quite common for technical surfaces like aluminum or brass or steel that are to be covered with protection layers (like DLC=diamond like carbon layers).

Methods:

In ElliCalc internal mode (not in SCOUT mode!) an empirical method is implemented to deal with roughness:

1. **no roughness**
   No roughness is included in the calculation (=default).
2. **constant roughness**
   You will see some textboxes in the setup area which show “R-factors” for each interface. This value means a **percentage** of light that is regarded as lost at this interface. So there is no real physical roughness model. Such a physical model cannot be given as the typical size of the roughness is absolutely unknown. This means that even the scattering mechanism (Mie scattering, Rayleigh scattering etc) is unknown. There are some formulae in the literature but in our case these are not better than the above mentioned method of light loss via some empirical R-Factors.
   An R-factor of R=0 means a perfect surface = no roughness
   An R-factor of R=50 means a loss of 50% light at this interface.
   There is no wavelength dependency of these empirical factors.



In the current version there is no wavelength dependency of these empirical factors.

constant roughness

Attention:

You have to input roughness values in the setup roughness textboxes.

At each interface a certain amount of light is regarded as lost. This percentage has to be input via roughness textboxes in the setup area. These R-factors are not dependent on wavelength.

This algorithm does NOT manipulate measured data, but the measured amplitude might still differ considerably from the simulated amplitudes. This means that the fit procedure might still have problems to find a good solution.

10 Experimental setups and problems

10.1 General

10.1.1 Experimental setup

Ellipsometer setup:

- carefully adjust the height of your stage to get maximized in intensity
- if your samples are not really perfectly plane thin about installing an autocollimator
- try to avoid stray light in the lab
- as your spot size is so small: pay attention on dust particles which may give wrong results

10.1.2 Maximum intensity

This value describes the maximum intensity in the spectrum of your lamp (can be easily checked in “auto intensity” mode).
If you use a double spectrometer there are TWO wavelengths corresponding to the sensitivities of the two spectrometers and your light source.

10.1.3 Polarization

In case of oblique incidence polarization plays an important role. In a vertical arrangement (like NanoCalc) the polarization does not play any role. “angle of incidence” is defined as the angle between the direction of incoming light and an axis vertical to the surface.

10.1.4 Signal to noise ratio

The intensity of your acquired signal depends on:

the adjustment of the lamp (see light source or ElliCalc-2000 manual)
the integration time (see menu options)
the number of averages (see samples to average in menu options)
the diameter of the fiber
the distance between fiber and wafer
the sample itself

Do not extend the extraction limits into regions with a high signal-to-noise-ratio !

10.1.5 Stray light

There is a slight risk to catch stray light from your laboratory lamps. Try to avoid this as much as. External light sources usually change and will produce errors.

10.1.6 Fiber

Your ellipsometer may be equipped with different fibers with core diameters between 50 and 600 micrometers.
The spot size is directly proportional to the fiber diameter, of course the signal intensity decraeses quadratically.
Consult your hardware supplier.

10.1.7 Absorbing media

It is not too easy to measure absorbing media like polycrystalline silicon as their refractive and absorption indices usually depend strongly on preparation conditions.

Try to find good optical models for n(λ) and k(λ).

10.1.8 Passwords

There are several passwords within ElliCalc:

As a start for user mode and administrator mode there is a password “admin”. This password can be changed.
To change intercept, first coefficient and second coefficient and third coefficient (to recalibrate your own spectrometer) there is another password corresponding to the serial number of your Ocean Optics spectrometer. This number is displayed on a separate sheet or on the backside of your spectrometer system. If you could not find this serial number ask your hardware supplier…

10.1.9 Function buttons

If you click on the button **F1**, you get access to help functions.

If you click on the buttons **F2 - F7** different spectra or recipes together with their layer data are loaded for demonstration purposes.

11 Physical explanations

11.1 Refraction index and absorption indices

The refraction index n of a substance is defined as

$$n = \frac{c_{vacuum}}{c_{material}}$$

with c = speed of light

The absorption index k of a substance describes the absorption behavior of materials. Glasses and photoresists have negligible absorption in the visible range.

n and k are a function of the wavelength lambda: n = n(λ). This phenomenon is called „dispersion“.
n(λ) and k(λ) are closely interrelated via the complex dielectric function ε(λ).

11.2 Cauchy coefficients

These coefficients empirically describe dispersion as a function lambda

$$n = n_1 + \frac{n_2}{\lambda^2} + \frac{n_3}{\lambda^4} \qquad k = k_1 + \frac{k_2}{\lambda^2} + \frac{k_3}{\lambda^4}$$

In many cases the 6 Cauchy coefficients are sufficient to describe the spectral behavior of resists, glasses etc. Normally ElliCalc uses „nanometers“ as a unit dimension. If you add your own cauchy parameters in a .dat-file, pay attention on the correct dimension !! It is possible to use other dimensions within the software but not in the .dat-files.

Structure of a .dat-file:

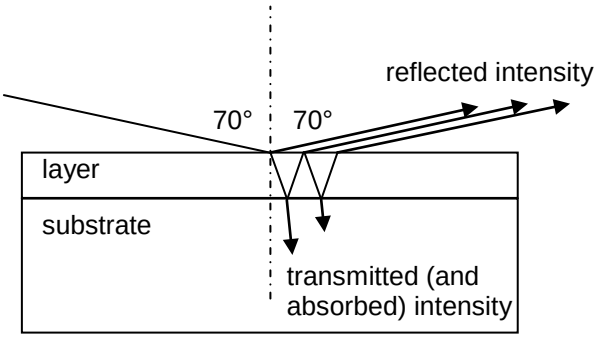
SiO2_(therm)	name of the material
# this is my own comment 1	arbritrary comment (beginning with #)
# this is my own comment 2	
633,1.4570,0	lambda, n and k at 633 nm
150,900	measured data between these limits
Table	(or CAUCHY)
150,1.5510,0	n and k at 150 nm
151,1.5504,0	n and k at 151 nm
152,1.5491,0	n and k at 152 nm
153,1.5477,0	n and k at 153 nm
154,1.5464,0	n and k at 154 nm
and so on.....	

The first lines are not used by the software for calculation.
ATTENTION: Do not use any blanks in the name of the file !
The third line (150,900) means that measured data are measured (=available) between these limits (LowerLimit=150 nm and UpperLimit=900 nm) and all extracted and displayed data (drawn in light Grey instead of black) between 900-1100 nm have NO meaning !!

11.3 Interference

The arrangement in the picture below shows the case of an oblique incidence.

The measurement of ellipsometry of thin films is a good example of an interference problem:



The incoming wave splits up in a reflected and a transmitted wave at each external or internal surface. The amplitudes of these partial waves depend on:

1. angle of incidence (if this angle is >0, then polarization plays an important role)
2. refraction index and absorption index of all layers

Now the superposition of ALL waves (with different phase relations, amplitudes) has to be done. If the layers are thin and flat you have to add **amplitudes** and not **intensities** (see your physics text book). So you may end up with „destructive and constructive interference“: a positive amplitude and a negative amplitude may add up to zero. This is why your measured intensities usually have maxima and minima.

12 Thinfilm.ini

This *.ini-file has to be located in the working directory of ElliCalc and should **NOT** be changed manually.

In emergency cases (= a corrupt file Thinfilm.ini) you may try to overwrite Thinfilm.ini with the default file Thinfilm.ini (on your CD).
ATTENTION: All files from CD-ROMs are write-protected. Click on the file name in Windows Explorer with your right mouse button and remove the write-protection.

Section [UserEdits]

In the file Thinfilm.ini there is a section [UserEdits] very near to the beginning of the file. You may edit the file Thinfilm.ini with any text editor like notepad.exe or wordpad.exe (do not use Microsoft Word or similar programs). These entries are in part only for special customers and special equipment: they are NOT supported !!

Attention: be careful in editing this file ! Make a backup before you edit Thinfilm.ini !!
The section [UserEdits] contains some parameters which cannot be changed within the graphical user interface of ElliCalc because only special users need these features.

```
[UserEdits]
WriteTmpFile=False
WriteRefFile=False
MinimumSearch=False
AllowPixels=True
Plot_During_Online=True
Save_During_Mapping=False
CCD_StartCounts=0
WindowShift=175
AdjustRecipes=False
Special_FFTLayer=-1
Plot_After_FFT=False
YScale_FFTLayer=0
CsvExcelExport=xls
CsvExcelSeparator=;
CsvExcelNumberFormatter=.
ExcelMargins_LRTB=2;2;2;1
UseShutter=False
SpecialLambda=-1
UseClipBoard=True
HideElliCalc=False
StopMappingStage=False
SpectrometerSleepTime=30
```

WriteTmpFile:
if this flag is set to TRUE then ElliCalc will write a temporary file after each measurement. In rare cases the PC together with its network connection may be very slow and it is advisable to set the flag to FALSE. Then it will no longer be possible to use the feature “load last file”
WriteRefFile
if this flag is set to TRUE then ElliCalc will write a file after each reference measurement. In rare cases the PC together with its network connection may be very slow and it is advisable to set the flag to FALSE. Then it will no longer be possible to use the feature “load last reference”
MinimumSearch
this is reserved for a special customer (using antireflective coatings)
AllowPixels
If you disable this feature by setting the flag to FALSE it will not be possible to use the pixel mode. You gain some speed as no recalculation for pixels is done with each measurement.
Plot_During_Online
if you set this flag to FALSE then you gain some speed during online measurements as no plots are shown
Save_During_Mapping

allows to save all spectra during mapping (time-consuming !)
Online_StartCounts
some spectrometers need a certain number of calls to the CCD pixels before they give stable results. If you set this number to any value less than 10 (e.g. Online_StartCounts =5) you will have to wait until 5 dummy measurements have been done. If you use a short integration time it is recommended to use values of 5-10. If you use a longer integration time and you do not want to wait for some seconds it is recommended to set the value to zero (but be aware that the first 1-5 measurements may not be completely correct)
AdjustRecipes
True: the main menu will contain a possibility to change a certain parameter in ALL recipe or ini-files simultaneously
Special_FFTLayer
for NanoCalc and special customer only
if any valid layer number is set to some number <> -1 (=default), the FFT result will be changed to get the thickness result of this special layer and not the total sum of all layers (ask your software supplier for details).
There is also an application to extract the refraction index instead of thickness (ask your software supplier for details).
Plot_After_FFT
for NanoCalc and special customer only
If this variable is set to FALSE only the FFT peak wil be plotted and not the extracted (=simulated) curve
YScale_FFTLayer
for NanoCalc and special customer only
this number gives a zoom factor for the main FFT peak (it can be changed within the software by pressing the + and – buttons)
csvEXcelExport
you may enter csv oder xls (example: csvEXcelExport=csv). Csv is the well-known “comma separated value” format.
csvEXcelSeparator
here you may enter the separator for the csv-format, like “;” oder”,” (example: csvEXcelSeparator=;)
csvExcelNumberFormatter
here you may enter the number formatter for the csv-format, like “,” oder”.” (example: csvExcelNumberFormatter=.)
ExcelMargins_LRTB
To print Excel sheets: this sets Left, Right, Top,Bottom
UseShutter
If you need control over the shutter of the light source (True/False)
SpecialLambda
for NanoCalc and special customer only
UseClipBoard=True
To avoid copying measured data to clipboard
HideElliCalc
To avoid ElliCalc in windows taskline
StopMappingStage
To enable/disable the xy-motors after 1 step
SpectrometerSleepTime
A time in minutes. After this time the spectrometer is asked up to 10 times to “reactivate” it.

13 APPENDIX

13.1 ElliCalc-Quick-Setup

This Appendix helps you step by step to get a first measurement. This description is using the reference stepwafer from OceanOptics, SiO2-Steps on Si-Wafer.

Install the ElliCalc software and AD-Converter (see Appendix A)

Start the computer, the power supply for the motors (black box) and the ellipsometer itself (front side)

Plug-In the USB-Cable (or blue AD-Cable), then install the fibercable between the spectrometer and the lightsource.

Put the sample (step-wafer ?) on the chuck

Start the ElliCalc software (WITH a reflecting sample on the chuck !!)

Load a SCOUT layer recipe that is good for your sample (files\load layer recipe)

Click "init" and wait until this operation is finished (about 15 seconds)

Maximize signal intensity (continuous button) by adjusting stage height

Eventually re-adjust intensity by pressing “auto intensity”

Click "measure"
During the measurement (some seconds) you see the measured raw data and finally the Psi/Delta spectrumFehler! Keine gültige Verknüpfung.A result is displayed in the upper right half of the screen

Now you are ready !!!