NanoCalc

Software Manual

Version 4   10.3.2014

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1   Introduction

NanoCalc is a software to extract thickness and optical parameters of thin, transparent layers on different substrates. NanoCalc uses Ocean Optics microspectrometers.

NanoCalc offers a lot of different options like:
- Simulation and measurement of multilayer systems (weakly absorbing or transparent)
- An easy-to-use "internal " mode for thickness extraction
- Optional: A powerful software engine in the background ("SCOUT")
- A graphical user interface that is very easy to use (recipes)
- Simulation of up to 10 layers (including 1 thick layer)
- Highly accurate thickness measurements between some nanometers up to about 250 μm
- Extraction of dispersion $n(\lambda)$ and $k(\lambda)$, roughness, EMA-fractions and other layer parameters, if using SCOUT add-on and Cauchy models in internal mode
- Use of reference systems
- 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 ellipsometry ("ElliCalc")

It is possible to measure in **reflection mode** (e.g. SiO_2-layer on silicon) and in **transmission mode** (e.g. Ti_2O_3 layer on a transparent BK7 glass).

Measurement principle
A thin layer is vertically illuminated with **white** light via a fiber and the spectrometer measures the reflected (or transmitted) light as a function of wavelength. NanoCalc software determines thickness of the layer.

NanoCalc 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. NanoCalc 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 NanoCalc 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
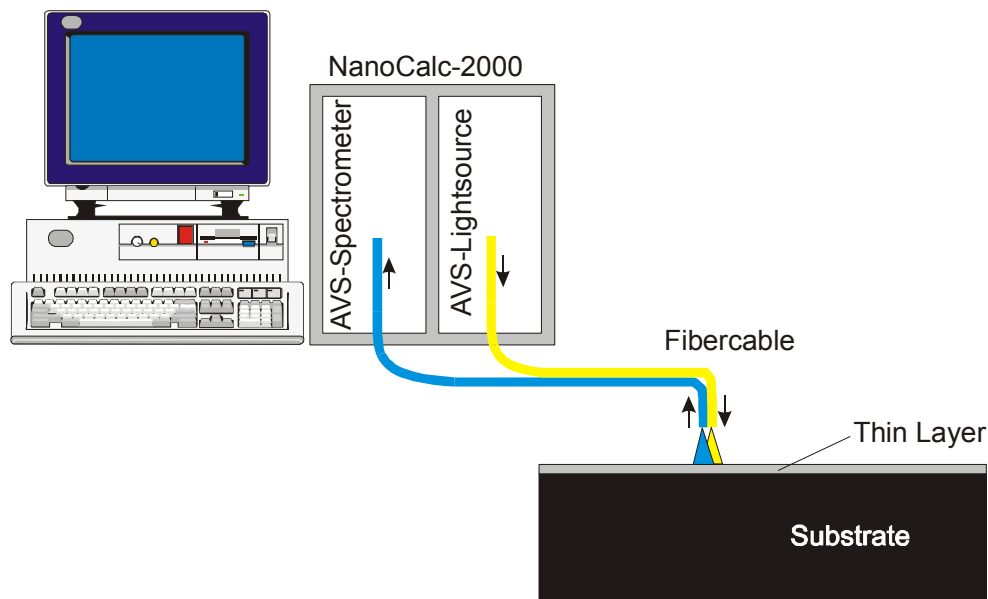
A broadband white light source is reflected by a thin layer under vertical incidence (after a calibration measurement). The reflected intensity as a function of wavelength is measured by a spectrometer, a PC extracts the wanted information.

1.2 Measurement signal

The typical modulated signal of such a spectroscopic thin film measurement might look like this (after some data manipulations):
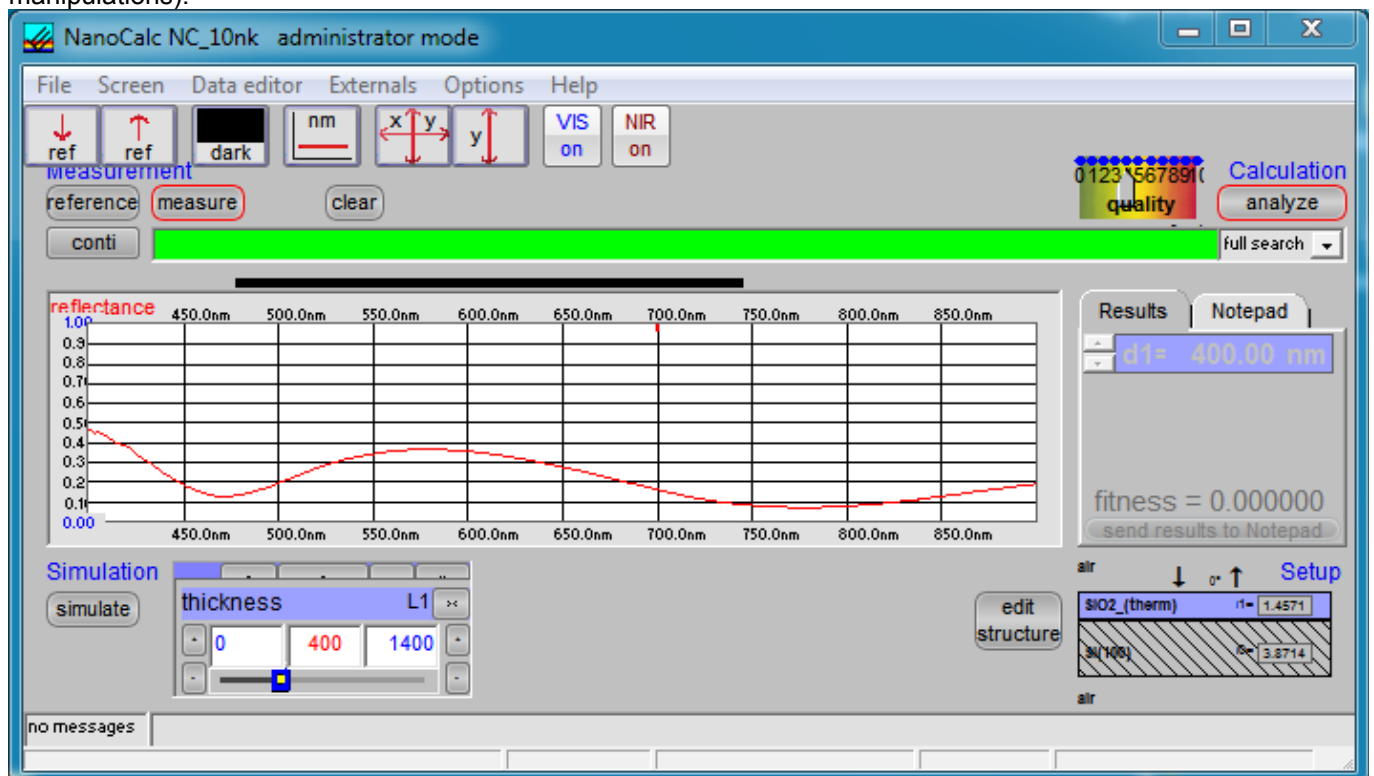
NanoCalc uses this signal to extract thickness (eventually also dispersion) for this (SiO_2) layer on Si.

1.3 Physical principle

The measurement principle of NanoCalc is the well-known fact of **interference** of light in thin layers. Light is reflected (and transmitted), resulting in phase shifts and superposition of amplitudes and finally adding up to different intensities for different wavelengths (=different colors). You see these colors in every-day-life, if you observe the colors of thin oil films on water or if you carefully observe the colored anti-reflective coating on lenses of cameras or binoculars.
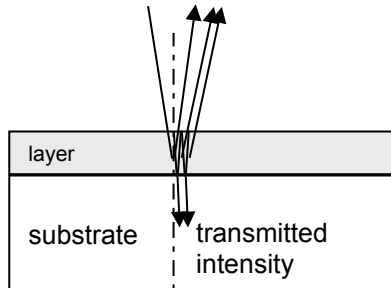
information:
in reality: nearly vertical incidence

After some calculations NanoCalc will show a result (here: 400.36 nm) as the best fit to the experimental data (red curve=measured signal, black/gray curve = theoretical curve):
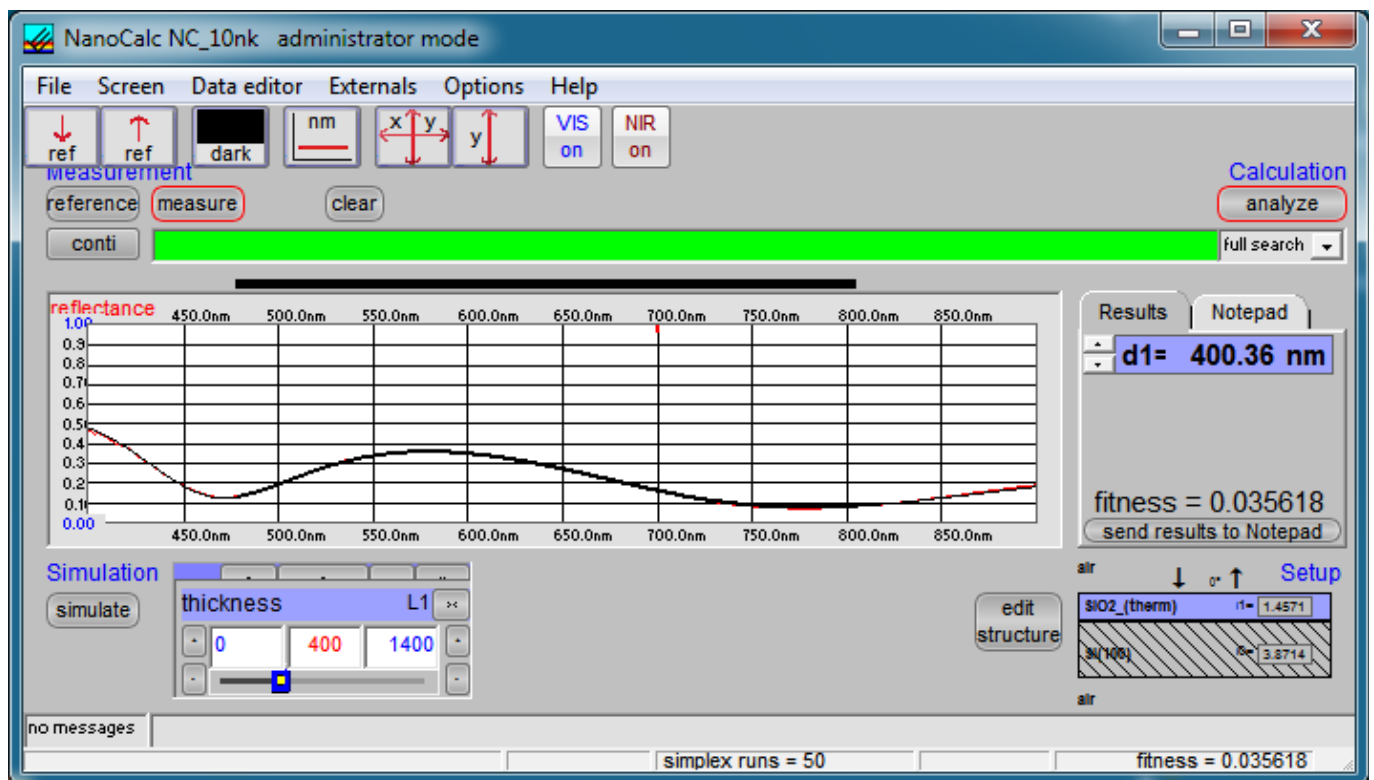
2 Installation

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

NanoCalc will ask you for a directory (and propose a directory „c:\programs\NanoCalc").
If you prefer other names, change this to "c:\MyPrograms\NanoCalc" or any convenient directory name).

Deinstallation:
If you want to deinstall NanoCalc from your computer, go to „system control", „software" and deinstall NanoCalc.
Do **NOT** just delete it because NanoCalc adds some files to your windows\system directory and to the registry !!
Always deinstall the software properly.

3 Product support

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

www.oceanoptics.eu

Thinfilm@oceanoptics.eu

Ocean Optics

4 Getting started

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

First example = without SCOUT-software:

1. You need a blank silicon wafer as a reference and a wafer with a thin layer (e.g. 400 nm SiO_2 on Si). It is a good idea to use a special "step wafer" with different oxide thicknesses as a first test or for calibration purposes. Please ask your hardware supplier for information about step wafers.
   Choose an experimental setup with a fiber or a microscope.
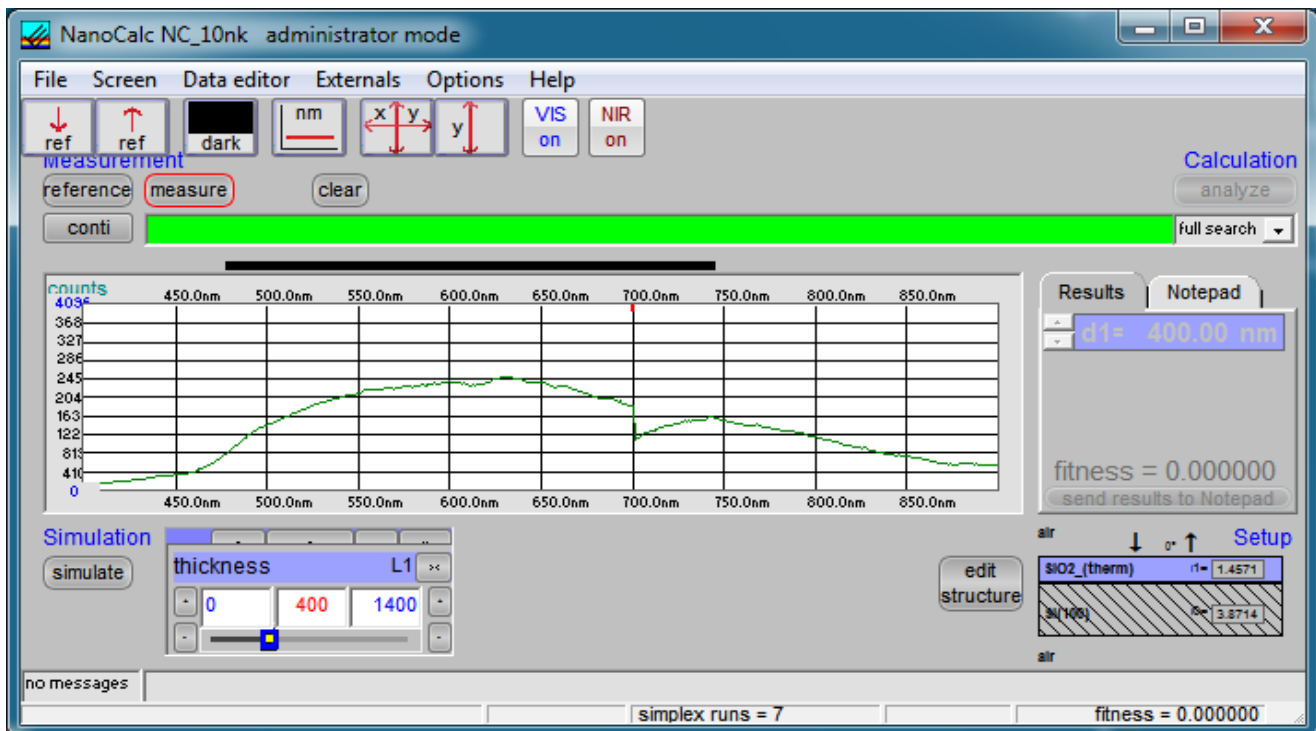
2. Then insert your reference wafer, switch on your lamp, start NanoCalc and click on the button continuous mode ("conti").

   This button turns **RED**. Then click on the button "reference" (this button turns **RED** as well) and now you should see the spectrum of your lamp as it measured repeatedly in short time intervals.

   You should observe a spectral region comparable to the data of your spectrometer (e.g. 250 -1100 nm, depending on your grating). The example above shows a step at 700 nm, because it was a double spectrometer. The decrease of the intensity at low and high wavelengths depends both on the lamp and the spectrometer.

   It is important to use a "good" amplitude of this signal = not too high and not too low. This means:
   a. there should be no saturation of the CCD-detector (=a flat region) in the signal.
   b. try to get a signal height of about 50-90% of the scale height for oxide samples (or similar) and about 20% for metallic samples. The exact value is of no concern as long as your signal in the measurement of the real sample does not cause saturation.
   There are several possibilities to get a "good" signal amplitude:
   a. increase or decrease integration time (with the buttons ±1 ms or ±10 ms) to adjust the signal between 20-90%.
   b. or adjust the lamp intensity (e.g. NanoCalc-2000-VIS/NIR), if this is possible
   c. adjust the distance of the fiber to your sample (not less than 2-4 mm)

3. Then click on the button „continuous mode" again to turn off the continuous mode. Both buttons turn to **BLACK** again. The last reference measurement is saved internally and you still see it on the screen. From now on there is no need to repeat this reference measurement unless you like to control repeatability etc. BUT: from now on you should not change the lamp intensity or the distance to your sample or a microscope magnification. Your sample should also have the same thickness as the reference sample.

4. Put your wafer with the thin film onto the stage and press the button „measure". Pay attention not to have dust particles in the region where you measure.
    You should get a spectrum like this (with different numbers of extrema or even no extrema).
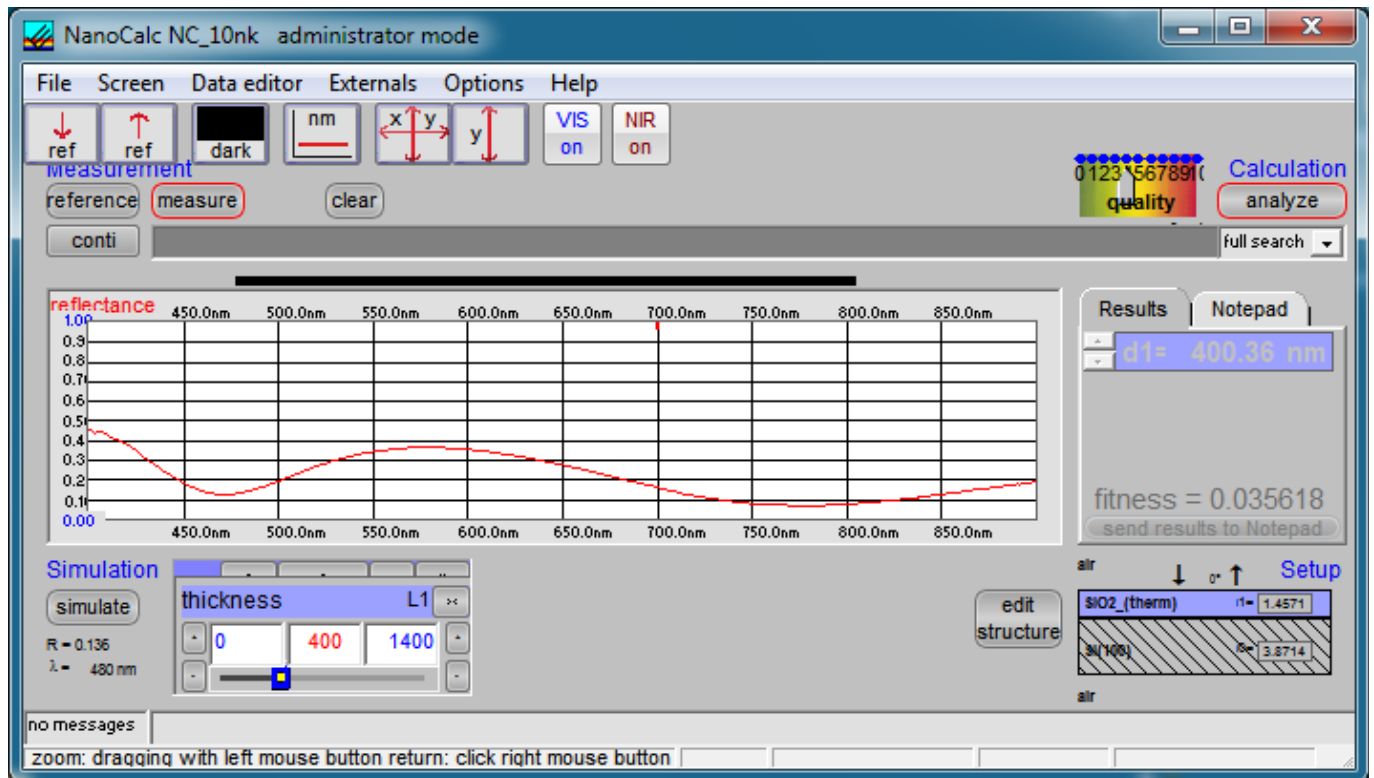
5. Then press the button „edit structure" and choose the correct parameters for your layer setup:
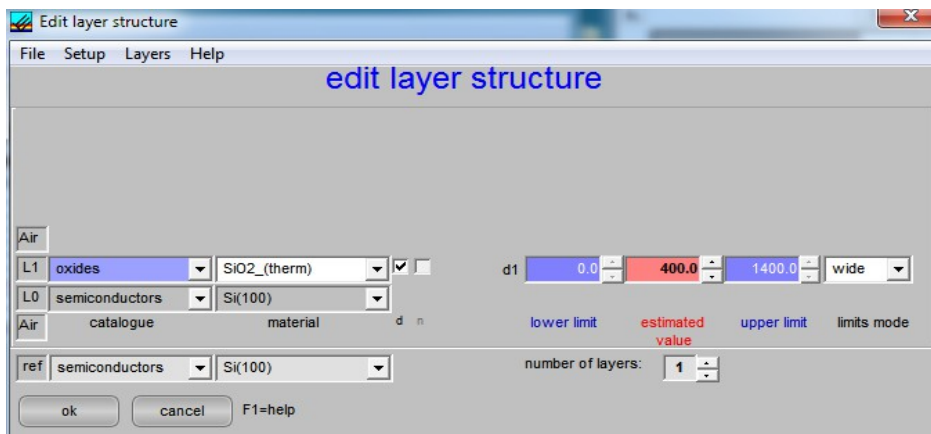
number of layers   = 1
catalogue for substrate= semiconductors
catalogue for layer 1 = oxides
material for substrate = Si
material for layer 1   = SiO2_(therm)
estimated thickness   = 400 nm

It is not important to choose perfect values for thickness and estimation limits at the moment, but the range (wide/narrow/user) should be ok.

When should you use "narrow limits" or "wide limits" or "user limits" ?

- if you have GOOD knowledge about the thickness of your layer (within about 50-100 nm), choose "narrow limits"
- if you have less knowledge about the thickness of your layer (but layer thickness should be LESS than about 5 micrometers in thickness), choose "wide limits"
- if you have no knowledge about the thickness of your layer (but layer thickness should be MORE than about 5 micrometers in thickness), choose "user limits" and guess the limits

6. After changing the layer structure please check the spectral <u>extraction range</u> (the black bar above the curves) again. Use a smaller range for a thicker layer (and shifted more to VIS/NIR), and a range as wide as possible for thin layers, e.g. 250 - 1100nm.
7. Press the button „analyze". The result for the thickness of the oxide is shown in the upper right text window.
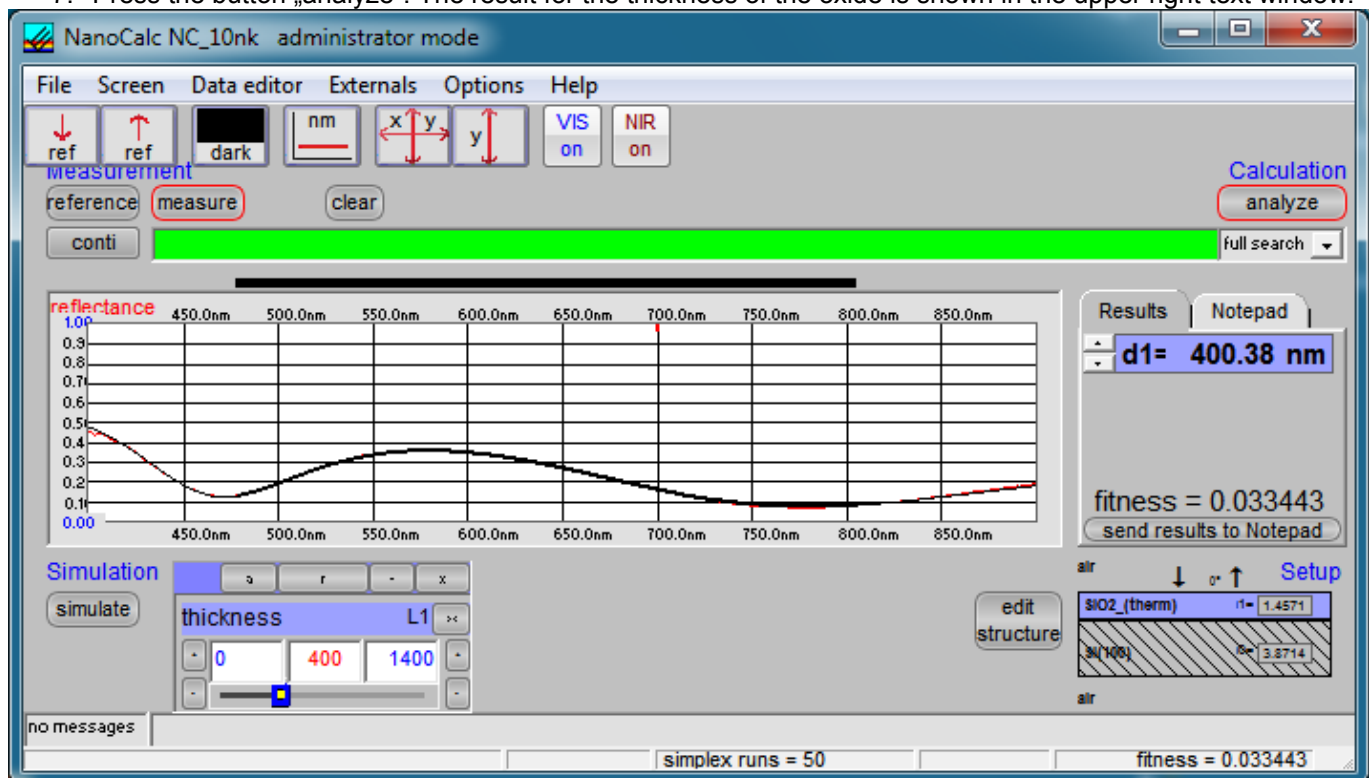
Second example = with SCOUT-software:
Now it is assumed that you own the SCOUT software and want to use this powerful tool for extracting data. This mode does not work, if SCOUT is not installed on your PC !
1. Get a reference spectrum in the same way as described above in steps 1 – 3

2. Now load an appropriate recipe with the menu "File\Load Scout recipe". You will be asked for the name of the recipe. In the case of an oxidized silicon wafer we use the recipe: "Cauchy on Si.lrc" which is in the list of delivered recipes. This recipe contains a Cauchy model for the dispersion n(λ) of SiO2 and will also deliver the oxide thickness.
After loading this recipe you can see the layer structure. The button EditStructure is no longer available. All details of the layer system and all extraction limits etc are contained in the SCOUT recipe and can only be modified within SCOUT (which needs some knowledge of optics and some experience with the SCOUT software)

3. Now press the button „analyze". The result for the thickness and the refraction index of the oxide is shown in the upper right text window. (comment: the thickness values for measurements with and without SCOUT are slightly different because a Cauchy model is not the same dispersion as table values)

5   User modes of NanoCalc

NanoCalc has two different user modes, the "SCOUT-mode" and the "NanoCalc internal mode". At the moment the "internal mode" is the normal mode, the "SCOUT mode" may be used, but an extra SCOUT software has to be purchased.

5.1   SCOUT mode

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

```
┌────────────────────────────────────────────────────────┐
│  ┌──────────────────────┐        ┌──────────────────────┐│
│  │ SCOUT sc2-recipe     │◄──────►│ NanoCalc lrc-recipe  ││
│  └──────────────────────┘        └──────────────────────┘│
└────────────────────────────────────────────────────────┘
                                        ▲
                                        ▼
┌──────────────────┐        ┌──────────────────────┐        ┌──────────────────┐
│     SCOUT        │◄──────►│ NanoCalc:            │◄──────►│  reflectometer   │
│  calculation     │        │ measure spectrum     │        │                  │
│                  │        │ display results      │        │                  │
└──────────────────┘        └──────────────────────┘        └──────────────────┘
```
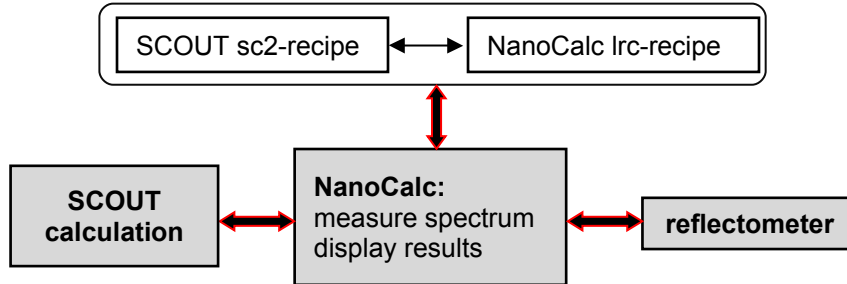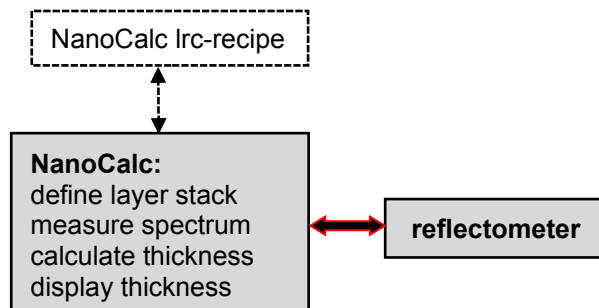
- within NanoCalc you have to load a **"recipe"**, e.g. "SiO2 on Si.lrc". This ASCII-readable recipe contains a link to a SCOUT recipe like "SiO2 on Si.sc2". All necessary layer information is contained in this SCOUT recipe and is read by NanoCalc, but only for display purposes.
- NanoCalc now controls the hardware, measures the sample and sends the measured reflectivity-values to SCOUT (via a file NC_Data.xy in directory "NanoCalc\Internal_Files").
- SCOUT does the calculation of all parameters
- the results are given back to NanoCalc via OLE-connection. The main fit parameters (thickness, refraction, absorption, roughness and EMA-fractions) are displayed by NanoCalc, 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-reflectometry" for the user and an enormous calculation power !

5.2   Internal mode

In this (normal) 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 values of Cauchy models can be extracted.

```
        ┌──────────────────────────┐
        ┆ NanoCalc lrc-recipe      ┆
        └──────────────────────────┘
                    ▲
                    ▼
        ┌──────────────────────┐        ┌──────────────────┐
        │ NanoCalc:            │◄──────►│  reflectometer   │
        │ define layer stack   │        │                  │
        │ measure spectrum     │        │                  │
        │ calculate thickness  │        │                  │
        │ display thickness    │        │                  │
        └──────────────────────┘        └──────────────────┘
```

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 file		x
	Load Scout layer recipe	x	x
	Load NanoCalc layer recipe	x	x
	Save as file		x
	Save as function key		x
	Save as layer recipe		x
	Save as reference system		x
	Change layer recipe	x	
	Save reference and dark		x
	Load reference and dark		x
	Export raw data	x	x
	Import raw data	x	x
	Show SCOUT results	x	
	Print report	X	x
	Exit	x	x
SCREEN menu	Spectrometer data	x	X
	Limits	x	x
	Dispersion	x	x
	Pixel resolution		x
	Show intensity	x	x
	Psi/Delta/tan(Psi)/cos(Delta)	x	
DATAEDITOR	Edit nk-data	x	x
EXTERNALS	Mapping	x	x
	Analyze mapped data	x	x
	Online/multipoint measurements	x	x
	Analyze online/multipoint data	x	x
	Motor control via 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)	x	x
	Some setups (Scout)	x	
	Some setups (change colors)	x	
	Measurement mode	X	x
	Operator mode(Admin/User/Expertmode	x	x
VERSION	NanoCalc_1	x	x
	NanoCalc_10nk	x	x
	ElliCalc	X	x
HELP	Contents	x	x
	About	x	x

6 Basic features of NanoCalc methods

6.1 Reference
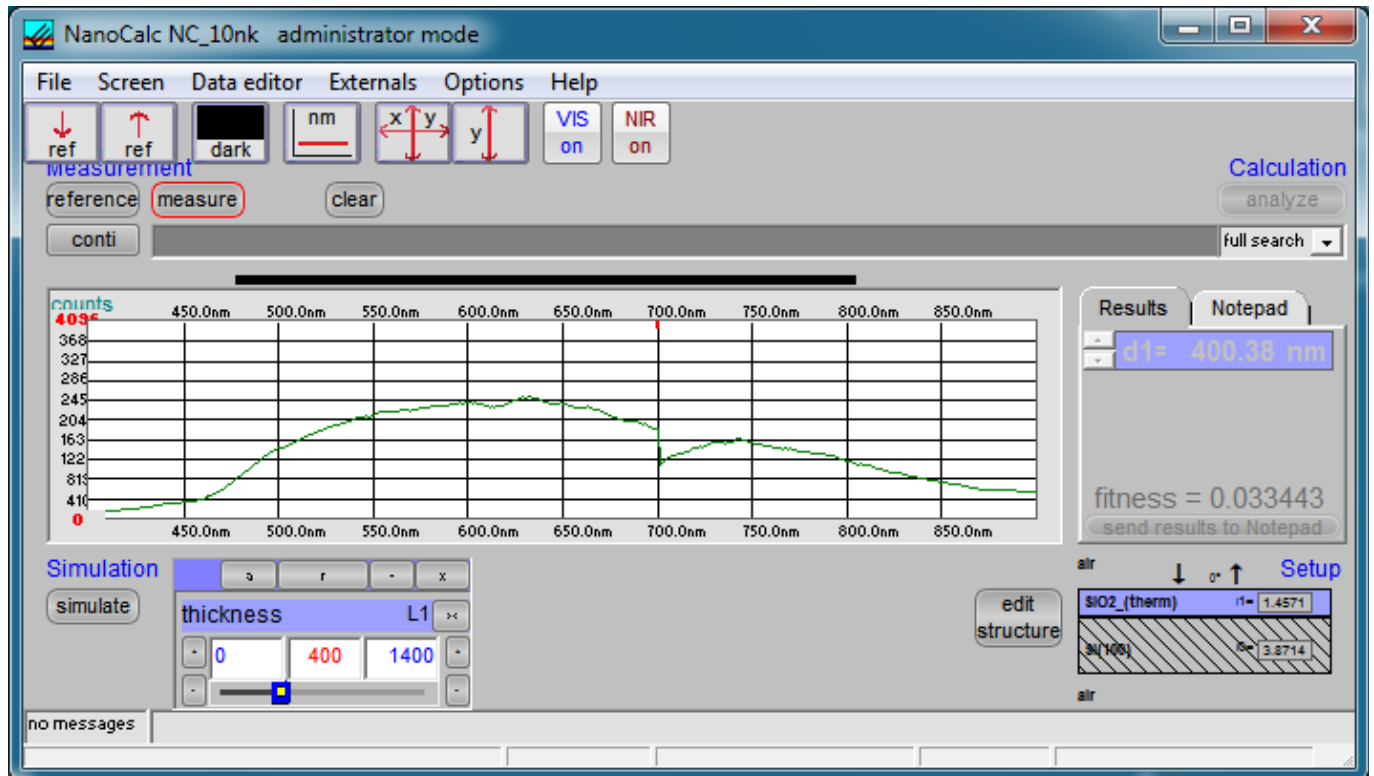
This button measures the reference spectrum and sets internal flags („there is a valid reference spectrum"). This spectrum is valid until you decide to measure it again.

hint:
Pay attention not to run into saturation of the spectrometer ! (= a (nearly) horizontal part in the spectrum very near to the upper limit of the plot). If this happens a warning message will appear.
If you want to measure precisely (especially for extremely thin layers) repeat this reference from time to time (drift of lamps and so on).

If you use a double spectrometer, you have to adjust the "crossover wavelength". Below this wavelength the data are collected from spectrometer VIS-channel, above they are collected from spectrometer NIR-channel. Within the screen a small red line in the upper part shows the position of the crossover

You may use a **different** material for referencing than your substrate (but pay attention: do not run into saturation in either mode !). In the present version a reference material has to be a solid, nontransparent material like Si (where the optical constants n and k are well known).
If you choose a transparent material like glass (with a backside reflection !), NanoCalc will use a different formula to calculate the reference reflectivity. In this case you have to choose a "thick" glass (regarded as transparent), which means that the name of the glass material has to end with something like "_1.5_mm".
An example: you want to you use a thick BK7-plate with 2.3 mm thickness as a reference material. Then rename the material "BK7.dat" in the materials directory to: "BK7_2.3_mm.dat". Apart from that, please regard that the quality of the glass surfaces on both sides are important.

There is an option for arbitrary reference systems and for "thick" layers.

6.2 Measure

This routine measures the spectrum of your test device (after the reference!) and performs the following calculation:
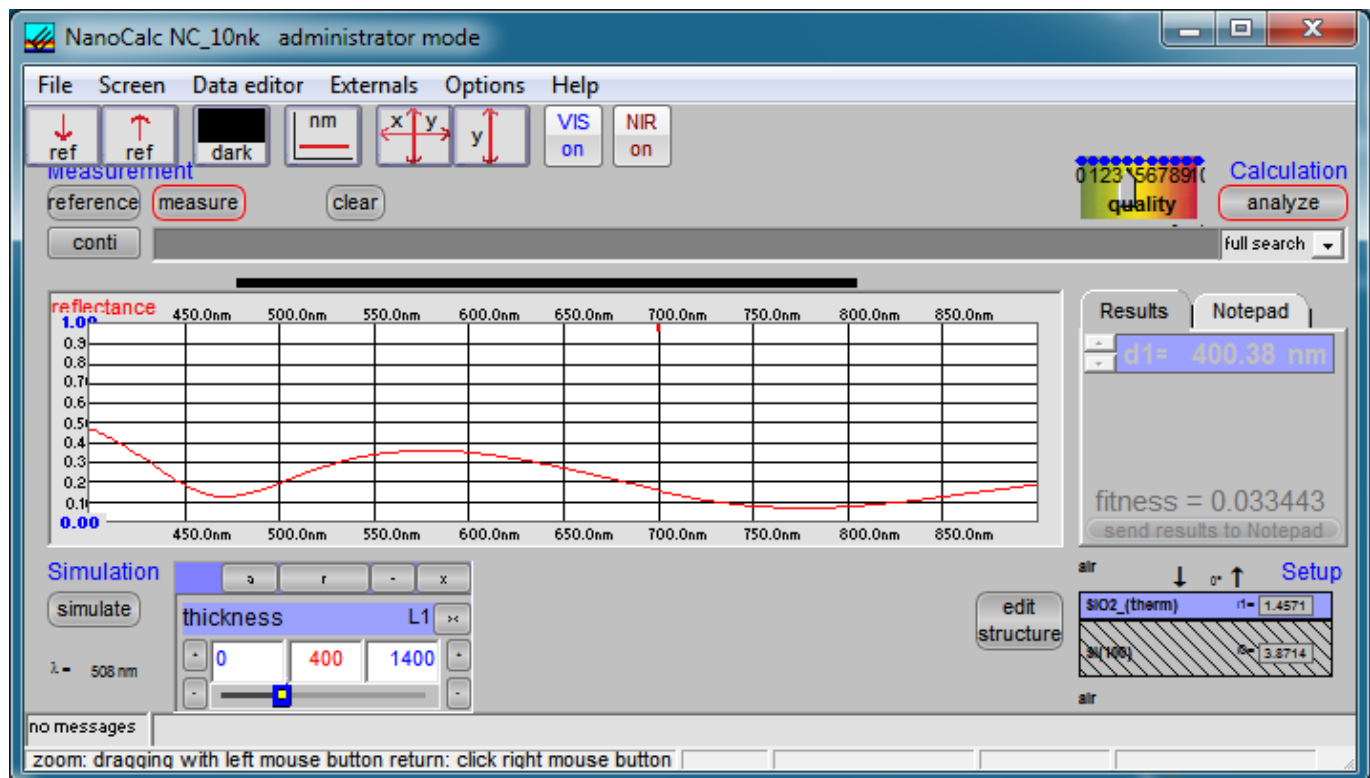
Reflectivity: $R = \dfrac{Meas - D}{Ref - D} \cdot R_{substrate}$

With:
Meas = measured spectrum
Ref = reference spectrum
D = dark spectrum
$R_{Substrate}$ = reflectivity of an uncoated substrate

As a result you get the reflectance (or transmittance) of your coated substrate.
If you are using a SCOUT-recipe the the measured data are transferred to SCOUT. This takes some time ….
The reflectivity R(substrate) is internally calculated from its dispersion values.

6.3   Simulate

This routine simulates a spectrum from the estimated thickness from „Edit Structure".
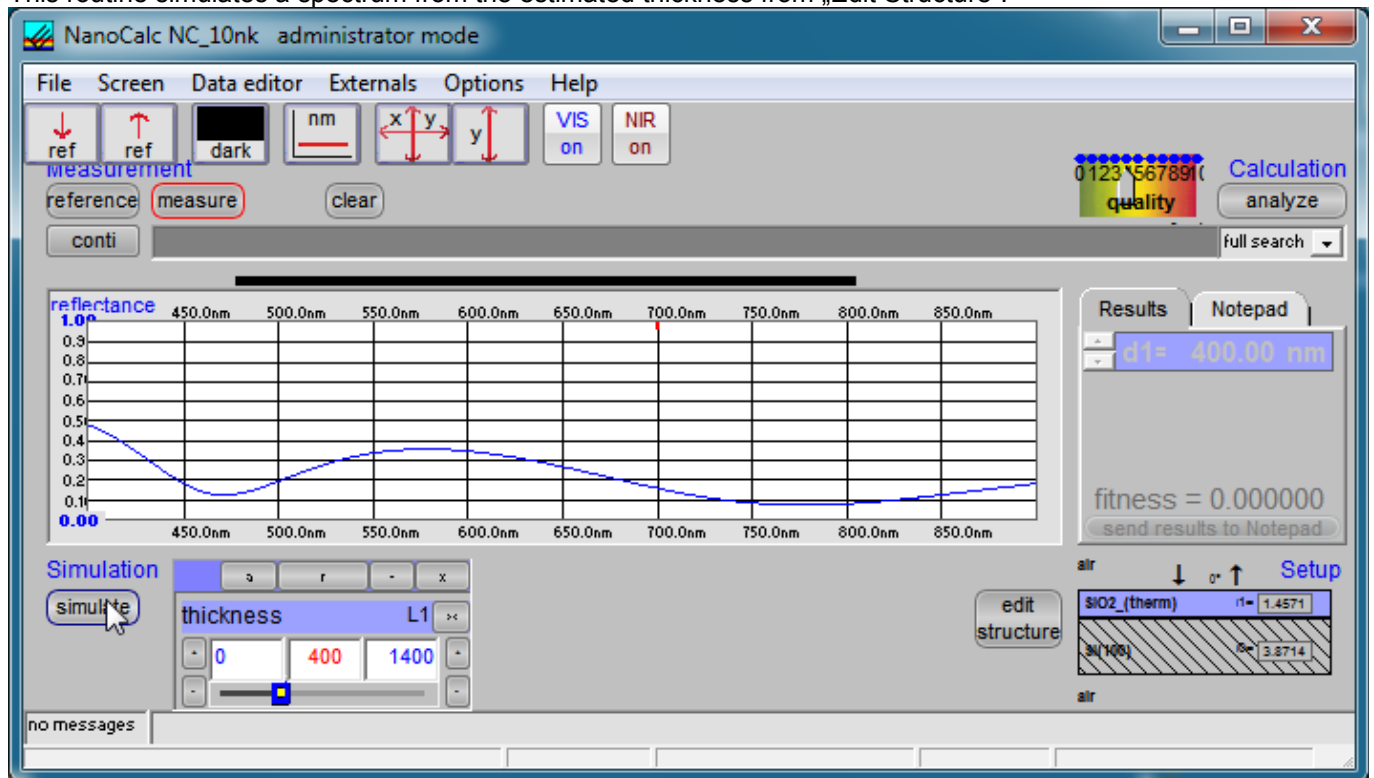
The structure that is simulated may be changed with button „Edit Structure", if you do not use SCOUT. Otherwise you need SCOUT experience.
Hint:
If you want to have a short check which structure is simulated at the moment, put the mouse cursor over the appropriate layer for some seconds and you see the layer thickness in a tooltip.
OR:
Leave your mouse cursor for some seconds over the button SIMULATE and look at the text in the status bar.

If you are using a SCOUT-recipe the calculation is done by SCOUT. This takes some time to transfer the data…..

6.4 Analyze

This routine analyzes a spectrum (either simulated or measured) within the data extraction limits.
The structure that is simulated may be changed with button „Edit Structure", if you do not use SCOUT.
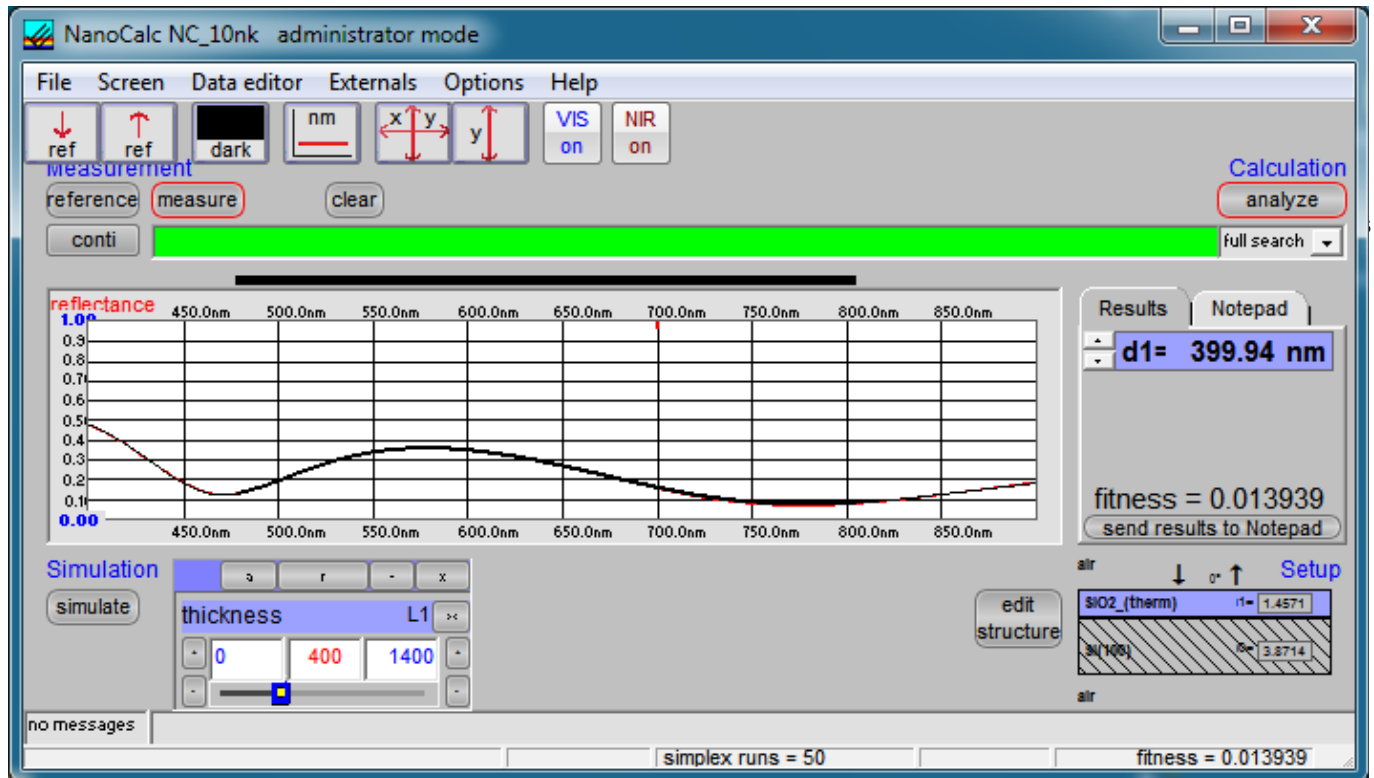
If you are using a SCOUT-recipe the calculation is done by SCOUT. This takes some time to transfer the data.....

6.5 Continuous mode

The continuous button switches between continuous: ON (=red button) and "continuous: OFF" (button =black). To use this option you have to switch either to "reference" or "measure" or "analyze". Then there will be a continuous measurement of the reference signal (very useful to adjust the intensity of your lamp) or there will be a continuous measurement or even analyzing of your signal (very useful if you want to move your sample to different positions).

All others buttons of NanoCalc are disabled until you finish the continuous mode.

You may adjust integration time by using the buttons -1/-10 / +1/+10 msec (separate for VIS-channel and NIR-channel spectrometer)
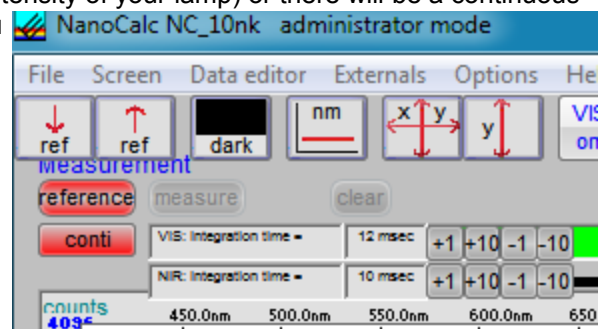
6.6 Measurement mode

There are different data extraction modes in NanoCalc (internal mode):

Full search

NanoCalc uses the lower and upper limit of your guess in EditStructure and tries to find the best fit to the measured values by testing <u>all</u> simulated curves in narrow intervals of 1 nanometer.
This is the preferable method in most cases, although it is not optimized concerning speed.

Fast search

NanoCalc extracts information from the (guessed) values in EditStructure to calculate thicknesses as precise as possible. The search region is still determined by your choice of narrow, wide or user limits.
This is the fastest method in most cases, nevertheless it may fail.

FFT

This method is very fast and applicable only for a single relatively thick layer, <u>but not extremely precise !!</u>
You will see the fouriertransformed spectrum on the screen. The width of the peak spectrum is inversely proportional to the width of your extraction region and does not give any information about precision. The main peak is marked with a colored green circle.

Be careful if you want to use FFT for layers thinner than about 1 micron. Try to use wide extraction regions, preferably more than 2 wiggles in the spectrum. Expect typical errors of 0-2%. If this is not good enough, use the FFT-value as a starting value for "fast search"
The scale in FFT mode is a scale of <u>optical thickness</u> (=product of geometrical thickness and refraction index), not of geometrical thickness. So the thickness value also depends on the quality of your dispersion data.
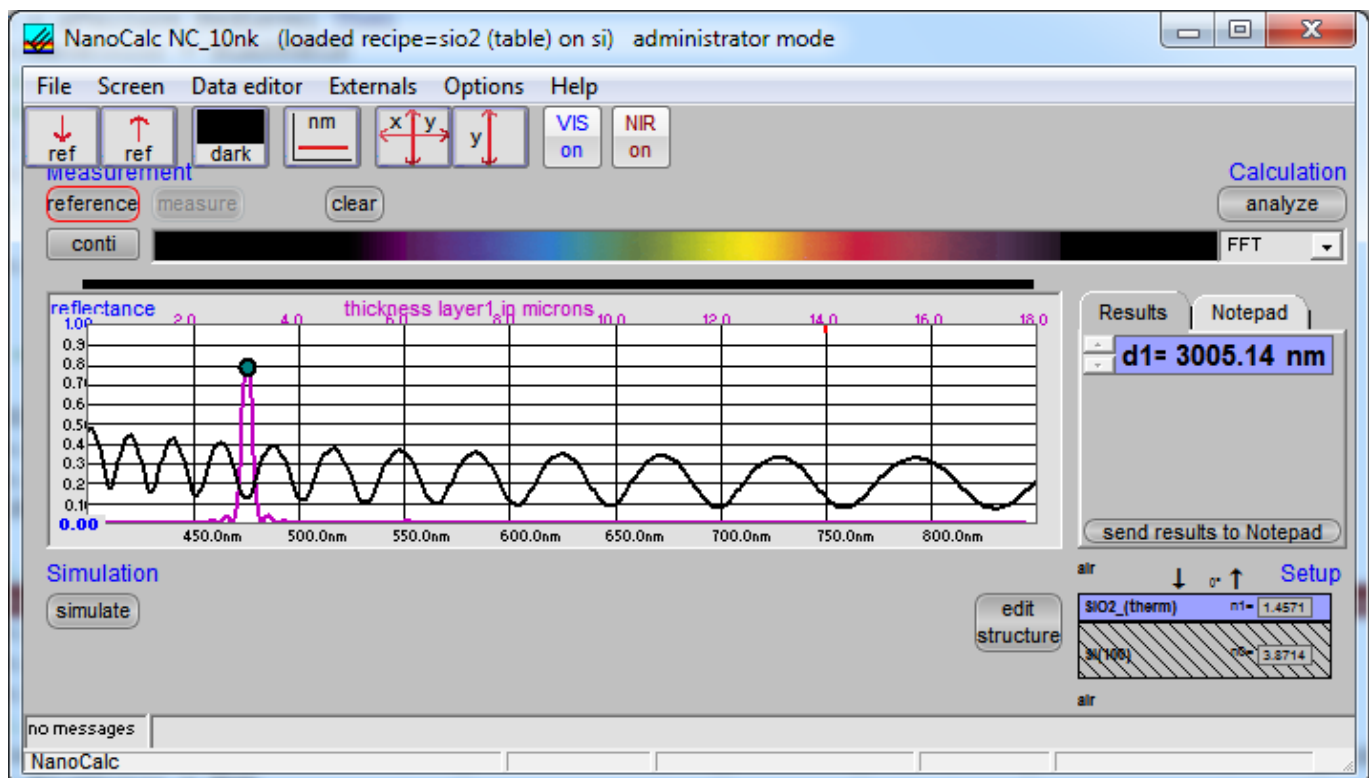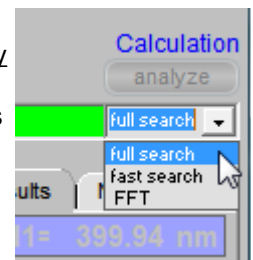
You have the choice between different options in menu EditStructure ("FixedLimits", "NarrowLimits", "WideLimits" and "UserLimits")

"FixedLimitsMode"
In this mode the values of low and high limits of your estimate are made <u>equal</u> to the thickness. This means that this layer is regarded as perfectly <u>well-known</u>.
Such a layer is excluded from data extraction algorithms.

"NarrowLimitsMode"
NanoCalc uses the value of your thickness estimation to calculate low and high limits which are quite narrow (about ± 100 nm). A search is done ONLY within these limits. If your limits were to narrow this search will fail and you have to try wider limits (like WideLimitsMode)

"WideLimitsMode"
The low limit and high limit is set according to the EditStructure setup menu:
1. relative wide limits: a symmetrical region is given, like ± 1000 nm
2. absolute wide limits: the values of lower and upper wide limits are given as absolute values
In any case: a search is done ONLY within these limits. This means that the user does not need any knowledge about the thickness. This option MAY be slow (but not necessarily !)

"UserLimitsMode"
NanoCalc fits the spectrum between low and high limits which were input by the user.

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.
<u>Any</u> deviation contributes to the value of fitness, also a shift of the measured curve relative the the simulated curve.
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.

<u>Fast and full search:</u>
The fitness is shown in the output table and in the statusbar.

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 "Options/Fitparameters"), the 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 YELLOW.
- If the fitness is above Failure_RedLevel=0.1 you will see RED.

<u>FFT search:</u>
There is no value of fitness for FFT because there is no comparison between measured and simulated curves. In menu Options/Fitparameters you may input a value for "FFT-Deviation" (in nm) to get an optical impression of the quality of the result. This feature is available only in NanoCalc version 10_nk. It is up to the user to choose a good value for this FFT_Deviation. It is helpful to make a larger quantity of simulations with the used layer structure and to compare the inputs with the FFT results.
Example:
If you believe (for statistical reasons!) that all FFT results have a maximum deviation of 1.5% compared to your inputs of the simulations and your thickness is about 2000 nm, then enter: "FFT_Deviation = 30" (30 nm=1.5% of 2000 nm).
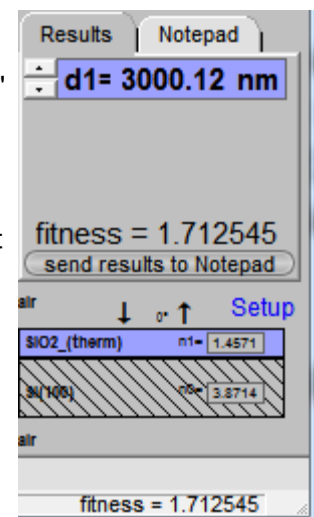
Then the lower and upper limit in menu EditStructure get a new meaning: the are regarded as limits to the accepted thickness interval. If your FFT-result together with the error margin of 30 nm lies completely outside of this interval you will be shown a RED color together with the text: "bad result" (the same with yellow=medium result and GREEN = good result). The limit interval is shaded in grey.
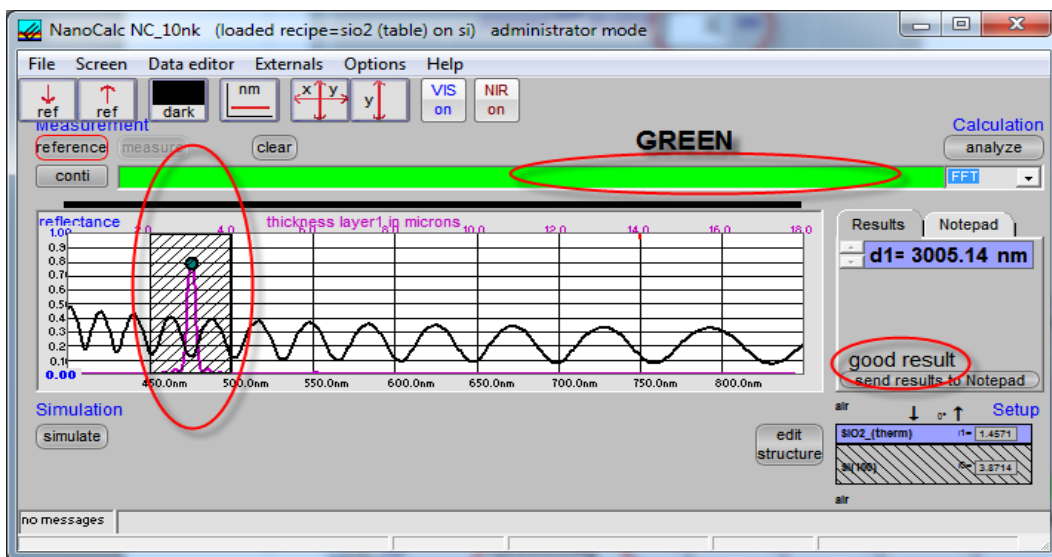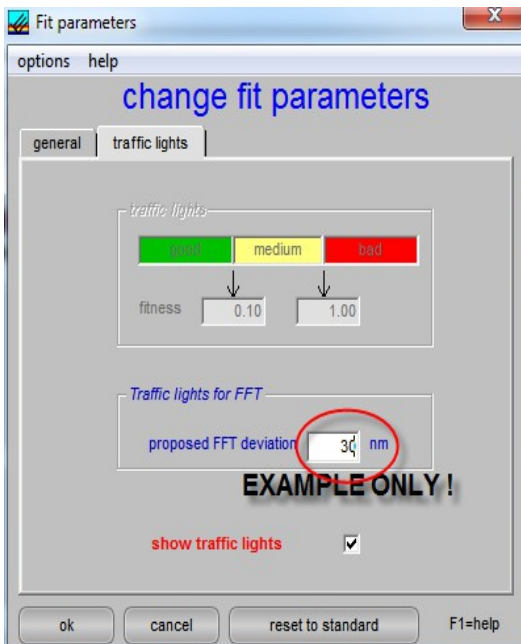

Important:
As there is an enormous number of parameters (among others: the width and position of the extraction bar) that influence the FFT result it seems impossible to make predictions from the factory side.

7 Description of NanoCalc menus

7.1 Fast buttons

Below the main menu commands you find some „fast buttons". Most of their features are also available via other menus.
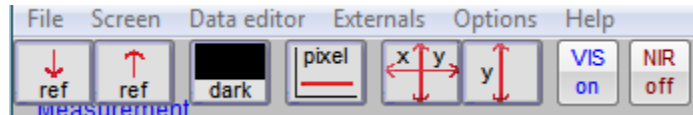
7.1.1 ref-buttons

If you measure a reference you may save this as a file (to directory Data/Internal_Files). If the dark button is active, also the dark spectrum is saved. Whenever you turn on the system again, you may load this reference (and dark) spectrum again via the fast buttons. If you measure relatively thick layers (like resist) this method may be uncritical and easy to use (you need not measure reference again with all its problems of changing wafers).

But if you measure <u>thin</u> layers a new and very recent measurement of the reference is strongly recommended ! The lamp intensity might have changed a little (or other reasons) and the result depends critically on a good reference. You could also use this function via menu Files/Load/Save reference and dark (pay attention to the directory! It is NOT recommended to use the Internal_Files directory)

7.1.2 Dark button

You can switch on and off the dark button also via menu Options/Change buttons

7.1.3 pixel

You can switch between pixel and nanometer mode also via menu Screen/pixel resolution
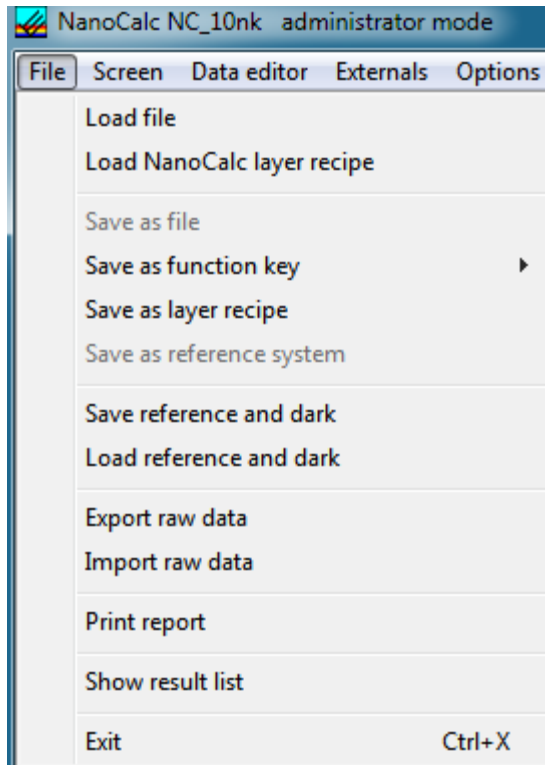
7.1.4 zoom options

This allows you to use the full plot range (either in xy or only in y direction).
You could also use this function via right mouse clicks in the curve area.

7.1.5 VI/NIR on/off

You can turn off either VIS or NIR channel (if you own a 2-channel-system).
You can switch between the 2 channels also via menu Screen/Spectrometer data (channel_activated)

7.2 Main menu "File"

7.2.1 Load file

(internal mode only)

This routine loads a measured or simulated spectrum that has been saved earlier (extension: .nan). Do not change the extension .nan.

It is assumed that all .nan-files are in the default directory "NanoCalc\data\nan_Files", but you can change the directory path to any other directory on your PC.

The *.nan-file is an ASCII file that contains most parameters of the software and the measured or simulated values of reflectance (or transmittance) as a function of wavelength (or pixel) within the plot limits.

If you load a recipe instead of a *.nan–file you will not see any curve on the screen, but a change in the setup or the limits. The only difference between a recipe and a *.nan-file is the additional list of data values.
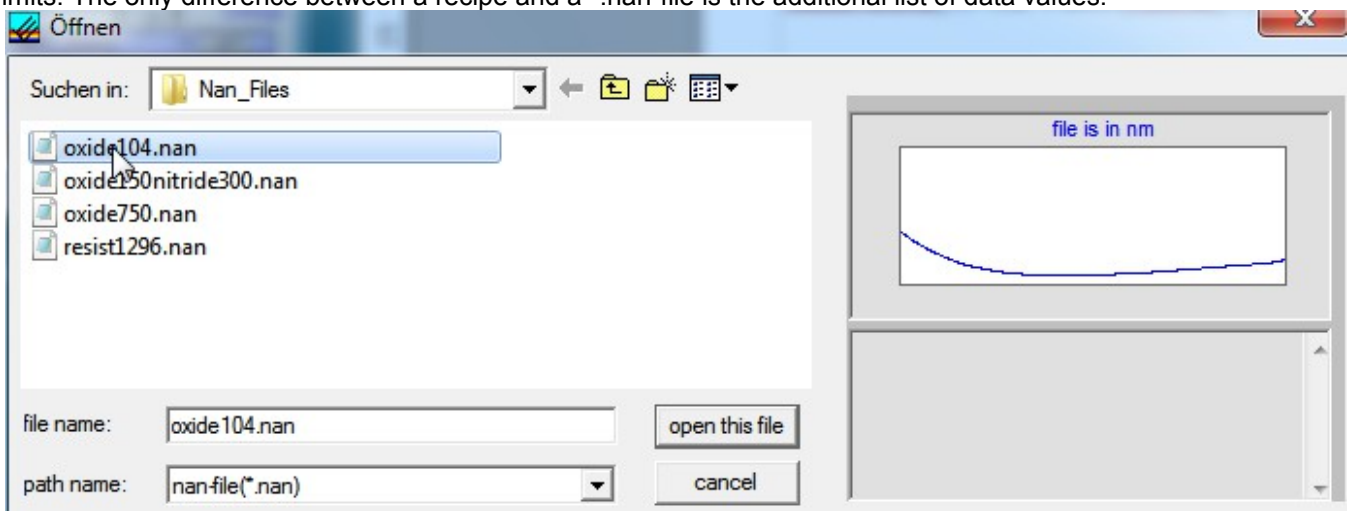
7.2.2   Load Scout/NanoCalc layer recipe
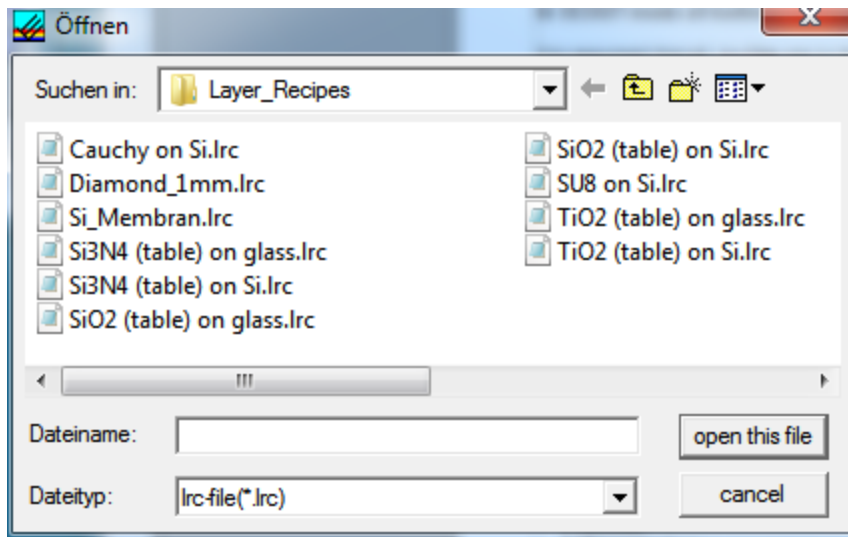
(internal mode and SCOUT mode)

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 NanoCalcs internal mode ("Load NanoCalc layer recipe").
In SCOUT mode all buttons captions are in *italic*, otherwise in normal.

It is assumed that <u>all</u> .lrc-files are in the default directory "NanoCalc\recipes\layer_recipes", but you can change the directory path to any other directory on your PC (provided that you did not use "UseLastFilenames_NC=False" in section [Filenames_NC] in Thinfilm.ini).

There is a section [Scout] in each layer recipe with an entry for "Scout_Recipename_NC". 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, NanoCalc will calculate without SCOUT = "internal mode" (at the moment only for thickness and Cauchy models!)

Example for SCOUT-mode (in ellipsometry):

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

Example for NanoCalc internal mode:

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

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.

7.2.3   Save as file

(internal mode only)

This routine saves the measured or simulated file as an ASCII file with the extension .nan. The name of the file may be chosen arbitrarily. Do not use any other extension than .nan.

The *.nan-file is an ASCII file which contains most parameters of the installation and reflectivity R(λ) as a function of wavelength (or pixel) within the plot limits.

7.2.4   Save as function key

(internal mode only)

You may save a recipe to a hardware function key F2, F3, F4, F5 and F6.

This is a very fast method of switching between different recipes.

7.2.5   Save as layer recipe

(internal mode only)

This routine saves all layer and screen settings as an ASCII file with the extension .lrc. The name of the file may be chosen arbitrarily. Do not use any other extension than .lrc.

The *.lrc-file is an ASCII file which does **NOT** contain and reflectivity R(λ) as a function of wavelength (or pixel) within the plot limits.

7.2.6   Save reference and dark

(internal mode and SCOUT mode)

This routine saves the current reference data to the file "NanoCalc\data\ref_files\name.ref" (nm-information) and to "NanoCalc\data\ref_files\name.rfp" (=pixel information).

This can also be done via the "fast buttons".

If the dark button was active also 2 dark files are saved (drf and .drp)

This function is easily accessible through function key **F8.**

7.2.7   Save as reference system

(internal mode only)

In Version NC_10nk there is an option to use "reference systems". e.g. a glass reference with a backside surface or even a stack of layers (e.g. native oxide). First you have to measure this reference system in the normal way = with silicon as reference. Then press the button file/save as reference system. Then choose this system as a new reference in EditStructure.

7.2.8   Load reference and dark

(internal mode and SCOUT mode)

This routine loads a reference from the directory "NanoCalc\data\ref_files". Eventually also dark files are loaded. Which of these files is displayed depends on the pixel or nanometers resolution.

This function is easily accessible through function key **F9.**

7.2.9   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.

7.2.10   Export raw data

(internal mode and SCOUT mode)

If a curve was produced by simulation or measurement it may be exported as ASCII-file ("raw data"). This file has a very simple structure: (lambda, value of reflectivity)

350,0.455
351,0.467
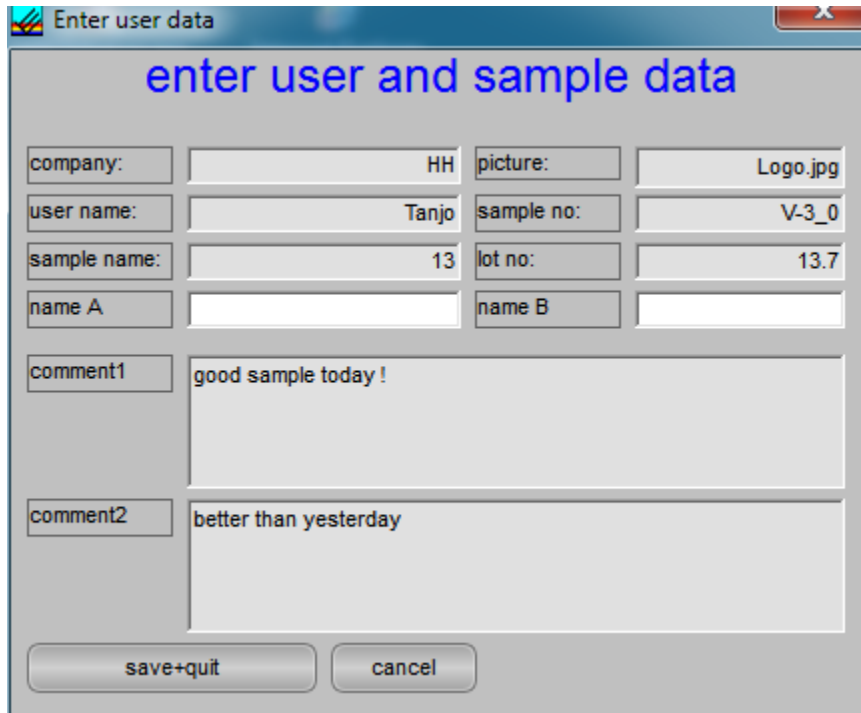352,0.479
353,0.490
354,0.501
355,0.512

356,0.522
You are asked for a directory to save this file. Please use the default directory \RawData_Files\Reflectometry

7.2.11   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.
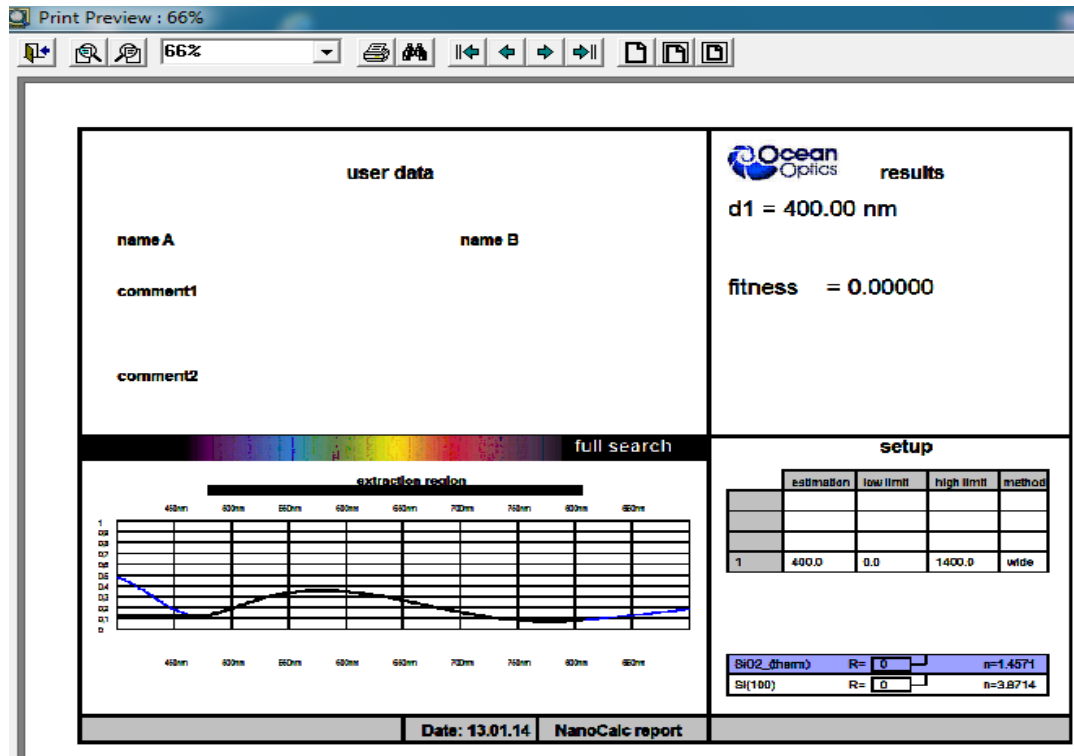Entering of user data: you may also change the names of the labels (empty labels: this line is not shown on the final print). In the preview window you may zoom in and out. After pressing the print button you have the chance to change some printer options.

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 NanoCalc-Online for printouts of multipoint measurement, result-windows with statistic data and Excel-connection.

7.2.12   Show Scout report

(SCOUT mode only)
Here all SCOUT results are displayed.
See chapter "Special features for SCOUT mode"

7.2.13 Exit

This routine exits NanoCalc 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 NanoCalc. The only way to restore this connection is to exit NanoCalc and restart the software !

7.2.14 Function keys

If you click on the buttons **F2 - F7** different spectra or recipes together with their layer data are loaded (for demonstration purposes or to get a faster access to recipes than by loading them via "files\load NanoCalc recipe"). You should be able to analyze these demonstration spectra by a simple click on the Analyze button.

How to add your own recipes to function keys:

Step 1: carefully adjust all parameters in EditStructure and all plot and extraction limits. Do not forget roughness parameters if necessary.

Step 2: save this setup with menu "files\save_as_recipe" as usual BUT save it to menu "data\internal_files" instead of saving it to menu "recipes\layer_recipes" AND save your setup with the name of the function key, e.g. save F4.nan or F6.nan (NOT F6.lrc !!). Recipes stored in function keys have the file extension .nan and not the extension .lrc (as usual layer recipes). Check for correct names with Windows Explorer !

7.3 Main menu "Screen"

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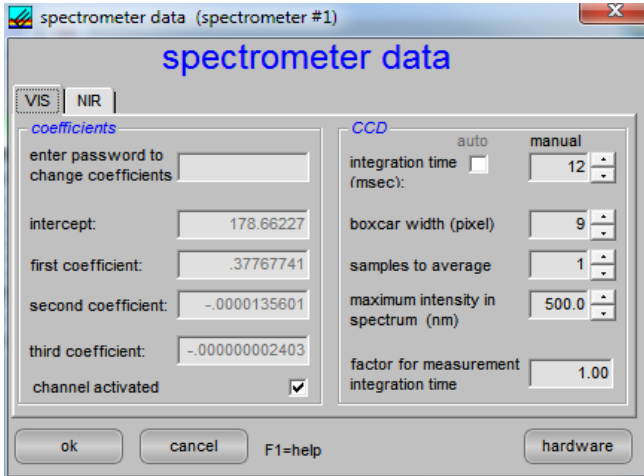
The 4 spectrometer coefficients are displayed for information purposes. They are automatically set by the Thinfilm.ini file which is specific for each single system.

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)

7.3.1.1 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:
To check integration time rapidly, use continuous mode button. You may change the value of integration time by +1 msec or +10 msec or -1 msec or -10 msec within a mouse click. Try to achieve a maximum signal of 20 - 90 % of total range. This value will depend very much on the reflectivity of your reference materials, your substrate material and your layer material.

An example:
If you use silicon as reference and substrate material and you want to measured silicon oxide thickness you should try to get reference signals of 80 - 90 %. An oxidized silicon wafer will NOT produce signal saturation and your signal-to-noise-ration will be as high as possible.
If you use a metalized surface as a reference (and you want to measure oxidized silicon wafers later on) you need to start with LOW reference intensities (like 20 %) to avoid saturation in your measured signal. Of course you get a lower signal-to-noise-ratio in this case.

After switching off continuous mode button, you do not have to press the reference button again as the last signal has been saved.

2. method:
use the menu "options/spectrometer data" and check by pressing the reference button once.

Tips:
Try to use short values of integration time while keeping the lamp intensity as high as possible (to get short measuring times). This is especially important in mapping mode.
If your integration times are too short, you will have problems with signal-to-noise. If your integration times are too long, you will get saturation of the signal and this may cause errors in data extraction.

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

7.3.1.2   Boxcar width

physical meaning:
The Ocean Optics spectrometer is able to average over some pixels to increase signal/noise-ratio.
A boxcar width of 1 pixel means no averaging at all. 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. Use a value of 1 for very thick layers.

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 tooltip will pop up to inform you about integration time, samples to average and boxcar width.
These values correspond to the **VIS-channel** spectrometer if you use a double spectrometer.

7.3.1.3   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. This ratio will increase with the root (!) of number of averages !
Example: to increase the S/N-ratio by a factor of 10 you need $10^2 = 100$ averages.

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 REFERENCE or MEASURE and wait for about 2 seconds: a small tooltip will pop up to inform you about integration time, samples to average and boxcar width.

Information: Internal correct for dark
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.

7.3.1.4   Dark button

If you choose this option, dark current is subtracted from the reference and measured signal. This is necessary if you can't protect your system against ambient light or stray light. Is is also necessary for real infrared spectrometers (e.g. NIRQUEST)

7.3.1.5 Maximum intensity

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

This value helps NanoCalc to achieve an automatic adjustment of the reference spectrum within the limits of the screen (=without saturation)

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

7.3.1.6 Crossover wavelength

If you use a double spectrometer with different sensitivity regions (e.g. 200-600 nm for the VIS CHANNEL spectrometer and 500-1100 nm for the NIR CHANNEL spectrometer), NanoCalc **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 in your overlap range of the two channels is possible, 550 nm would be a good choice in this case). It is marked by a little red line in the screen.
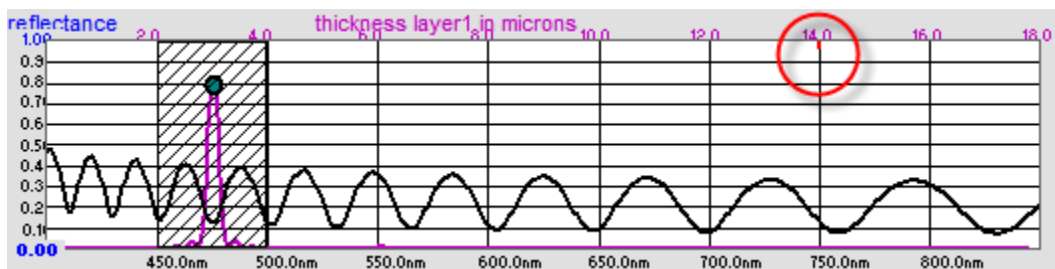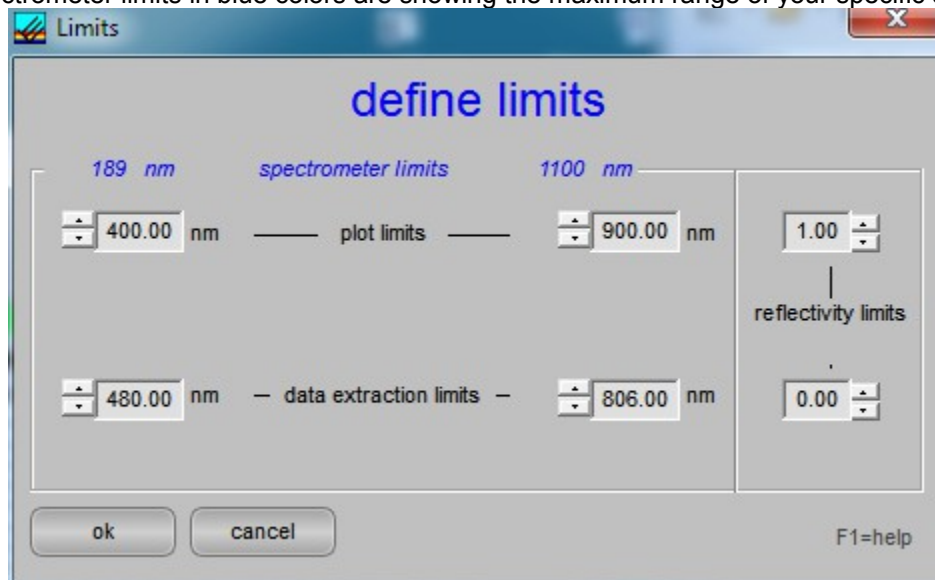

7.3.1.7 Hardware settings

Please find some information in Appendix A at the end of this handbook.

7.3.2 Limits

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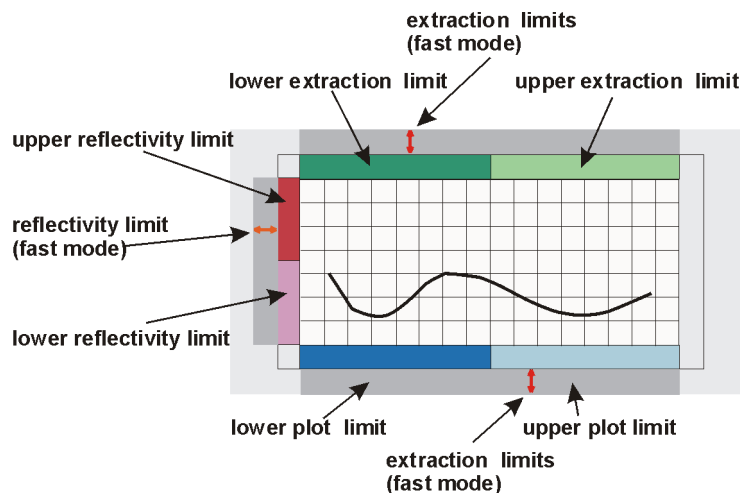

7.3.2.1 Plot limits

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 NanoCalc 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 gray 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.

   Please regard two of the "fast buttons", they allow a return to full screen (either in xy or y direction)

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.
   If you own a real infrared spectrometer these considerations apply to 800-2500 nm.
   If you own a double spectrometer VIS+IR, you will use 2 different directories "materials" (with limits 150 – 1100 nm) and "materials_IR" (with limits 800-2500 nm). For a full range data extraction the same material has to exist in BOTH directories (preferably with a perfect overlap of dispersion data)

7.3.2.2   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.
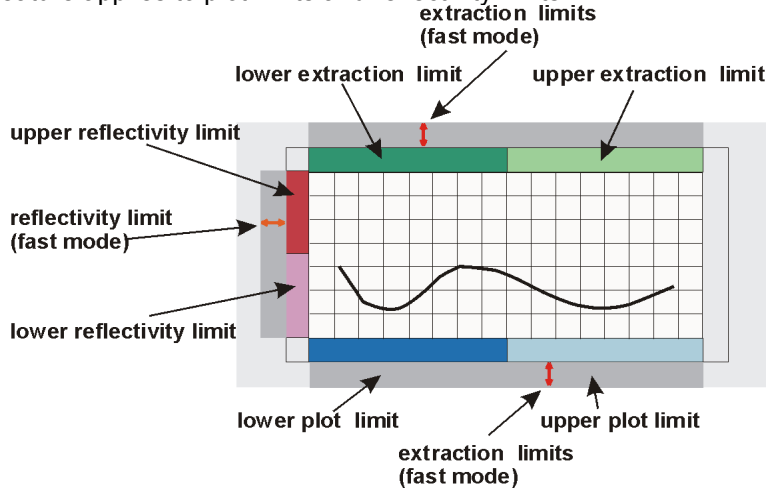
3. Fast and precise method to change the limits:
   If you move your mouse very near to the upper part of the plot window (but still in the grey part) you will see a little vertical arrow and the value of the wavelength is displayed. If you now click with the left mouse button, you are able to change 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.
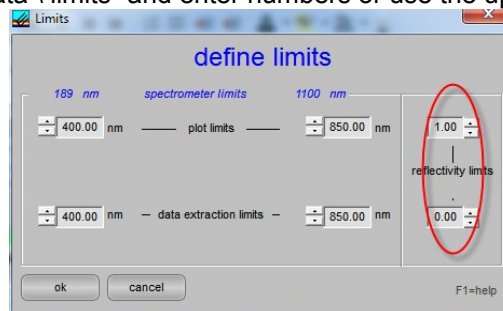
7.3.2.3   Reflectivity limits

Reflectance (and transmittance) are defined between 0 and 1.
To zoom in the plot and to see some more details you may change the reflectivity 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.

3. 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 gray 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)

7.3.3 Dispersion

This form shows the refraction index n(lambda) and the absorption index k(lambda) (within the plot limits) for different layers.
This form is just a tool to control your data, nothing can be changed in this form.
- You may use 2 cursors. 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 (= $k(\lambda)$) and red (=$n(\lambda)$)
- You may also zoom in and out and in an area
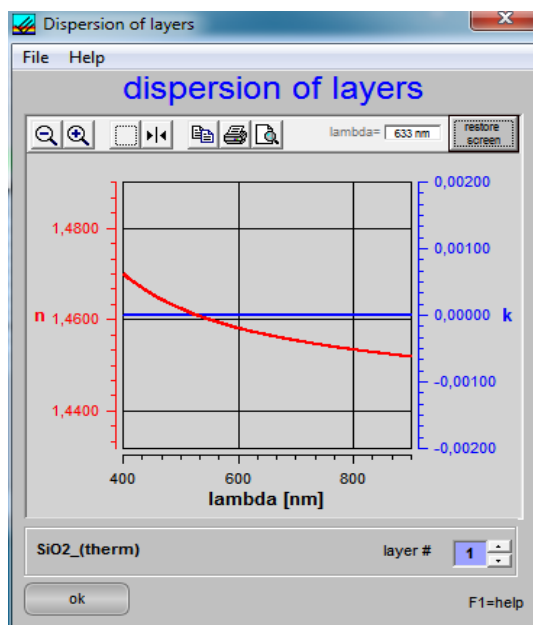
You may also save these dispersion values as a dat-file, but be very careful about the target directory !!
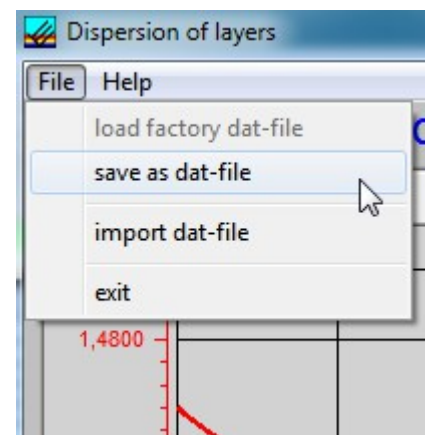
ATTENTION:
to be consistent with data handling, ALL materials files contain n and k data between 150 nm and 1100 nm. Usually only *parts* of these data are measured data (e.g. between 206 nm and 840 nm or between 300 nm and 1100 nm). If you simulate, the valid part of the curve is shown in *black* while the rest is shown in g*ray* (and you get a message).

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

7.3.4 Pixel resolution

This option is only useful for very <u>thick</u> films. If you use the option pixel resolution the software will acquire and display all data in spectrometer pixels and no more in nanometer resolution.

With pixel resolution data are displayed at exactly those wavelengths where there is a pixel in your spectrometer. If you own a high resolution spectrometer there is a spectral resolution down to 0.2 nanometer or less. For more precise information consult your hardware supplier.

7.3.5   Show intensity

If you use this option you will observe a value of "total intensity" in one of the panels in the status bar. This value is just the sum of all intensities between the extraction limit with a spacing of 5 nm.

Example:
    I(total)=234.45

So this figure gives a very rough information about the <u>area</u> under the measured or simulated curve. This might be used to maximize some intensity.

7.4 Main menu "Data Editor"

7.4.1 Modify old .dat-files

Modifying existing dat-files:
1. At first you will see two combo-boxes to choose a catalogue and a material.
2. Then click "open file". Some new features become visible: either a list with Cauchy coefficients or a table with dispersion data
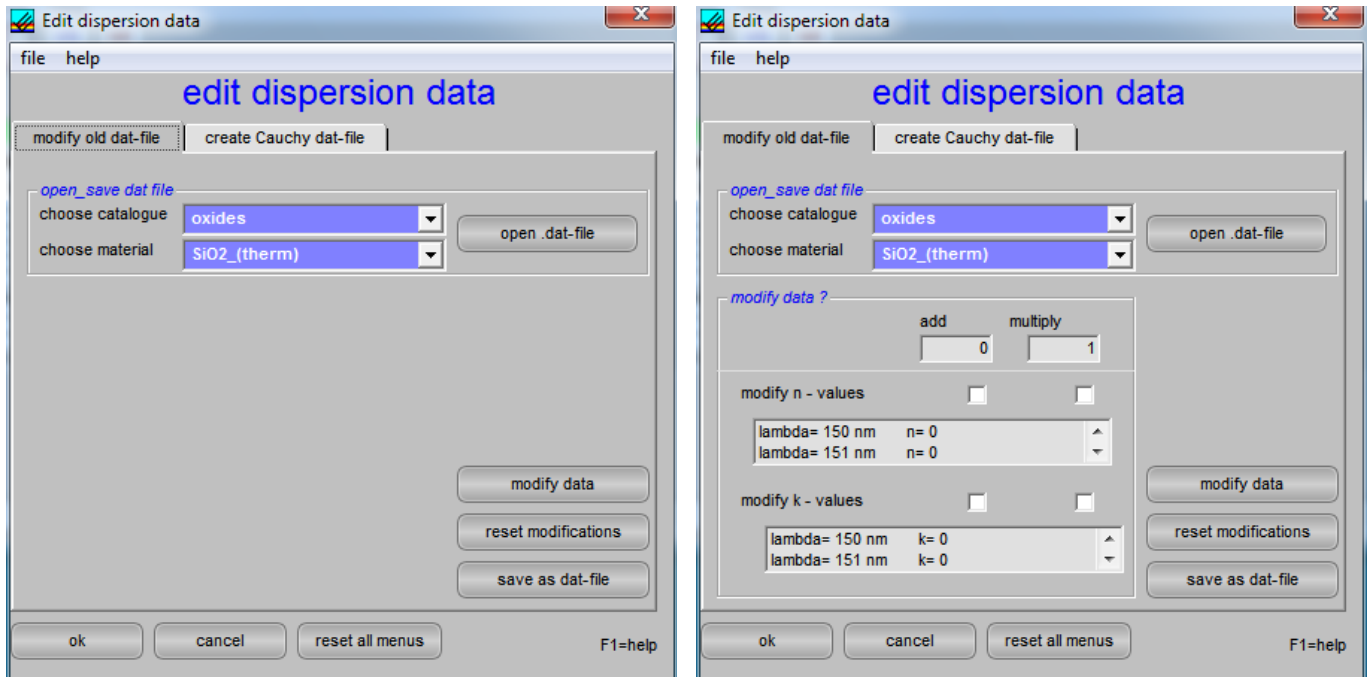

If you like to change these old data (=adding of constants or multiplying with a factor), just click on ADD or MULTIPLY in the appropriate row. It is possible to change each Cauchy coefficient separately, but not a single value in a table. If you want to change table values, you have to do this with an external text editor.

3. After adding or multiplying click on "save as dat-file" or click "reset modifications"
   Then the software will automatically switch to the page "save as dat-file".

7.4.2 Save as dat-file

Be careful where you save this "new" material !
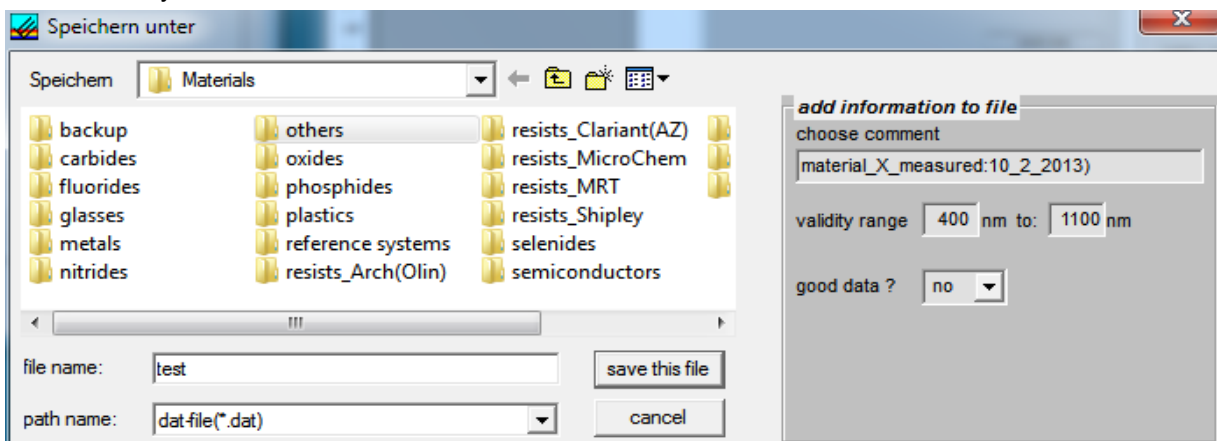
You should take the opportunity to add some comments to the file header, to give a validity range and to comment the quality of your data.
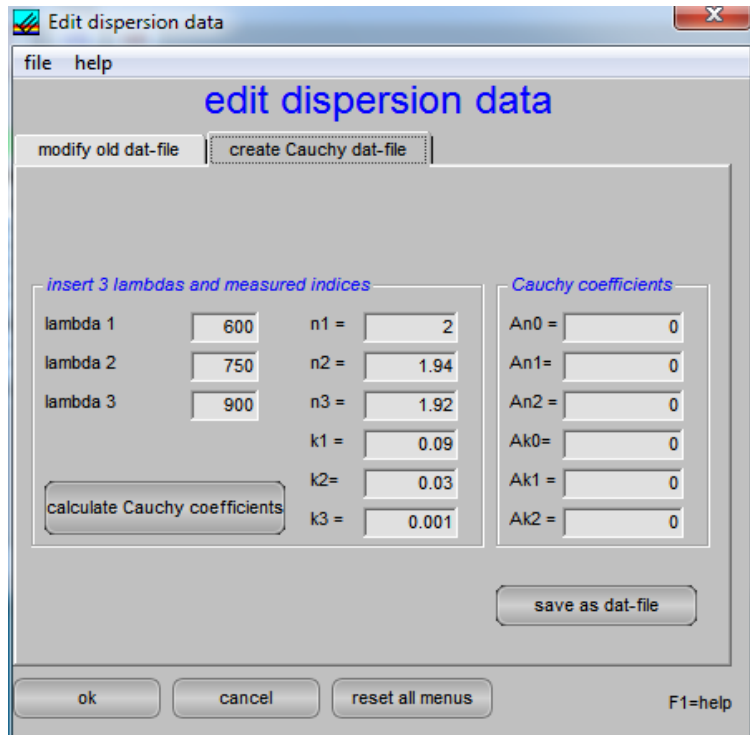
7.4.3 Create Cauchy .dat-file

Creating new Cauchy dat-files:
It is only possible to create new DAT-files with Cauchy coefficients, not as a table of index data. To create a table you have to use an external text editor.

1. At first you will see three wavelengths and 6 Cauchy coefficients n0, n1, n2, k0, k1 and k2

2. change these values according to your information. You have to add **ALL** three values.

3. click on create Cauchy coefficients

4. then click on "save as dat-file" or click "reset modifications"

    Then the software will automatically switch to the page "save as dat-file".

7.4.4 Create EMA dat-file

(possibly not active in current version !)
Creating new EMA dat-files:
An EMA-file is a mixture of 2 different dispersion values. There are different mixture algorithms in the literature. In NanoCalc only the simple Looyenga method (=a linear mixture) and the Bruggeman method are implemented.
The structure of an EMA dat-file is rather similar to 2 added normal dat-files. Here you see an example for Poly-silicon as a mixture of crystalline silicon and amorphous silicon (it is also possible to construct such a file manually with every text editor)

Si_cr.100(Aspnes_mod.)
633,3.8714,0.0158
150,1100

EMA_Mixture=Si_(100),a_Si,Bruggeman,50.0_Percent
Table
150,0.5100,2.1500
151,0.5000,2.1500
152,0.5000,2.1500

1098,3.5559,0.0014
1099,3.5557,0.0014
1100,3.5554,0.0014
a_Si(SOPRA_amorphousSilicon)
633,4.517,0.2312
240,840
EMA_Mixture=Si_(100),a_Si,Bruggeman,50.0_Percent
Table
150,1.6844,3.3312
151,1.6844,3.3312
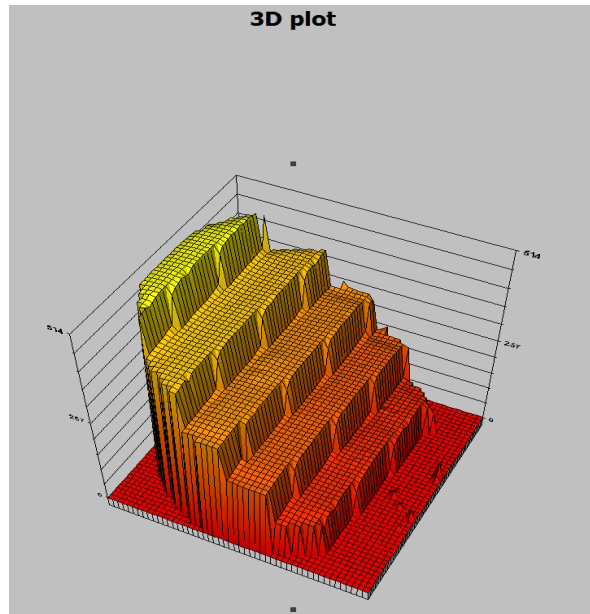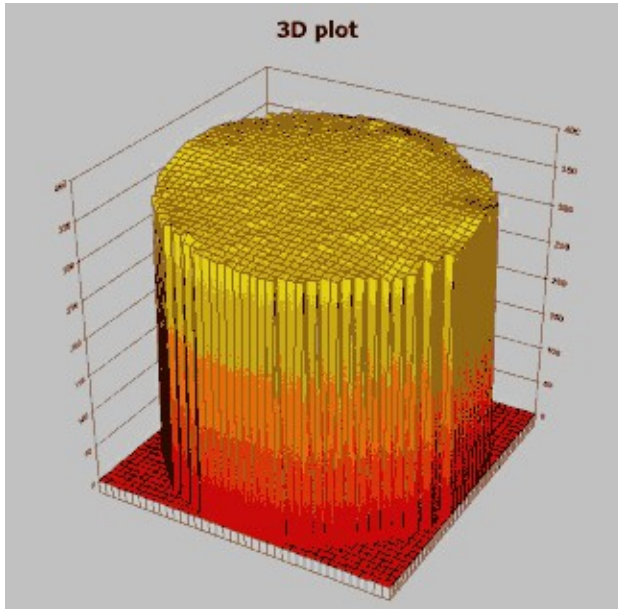152,1.6844,3.3312
153,1.6844,3.3312
154,1.6844,3.3312

Be careful where you save this "new" material !
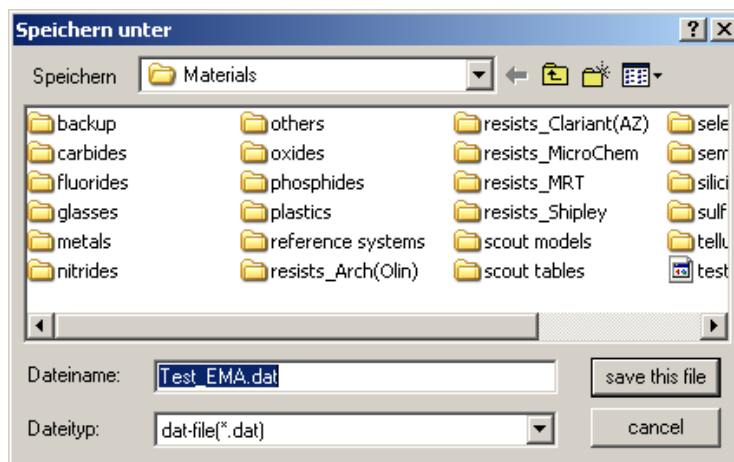
7.5 Main menu "Externals"

7.5.1 Mapping

You need a mapping-xy-stage and a special mapping add-on software for NanoCalc 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

These recipes are for mapping parameters only and are completely distinct from layer recipes !
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 a following section

3. menu "help"
This is the usual access to help functions

main buttons (lower right side)
reference
You can take a reference with a blank reference wafer (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
dark
Only if dark button is activated
clear
Clears the screen
analyze
You can analyze the layer thickness your sample. Thus you can control all settings before you start the mapping
init stage:
After starting mapping mode you have to initialize the mapping stage first.

Until the mapping stage is initialized the function start mapping is deactivated.

Conti

This has the same functionality as in main screen = continuous reference, measure or analyze

start mapping

this will start the mapping sequence

cancel

leave mapping mode
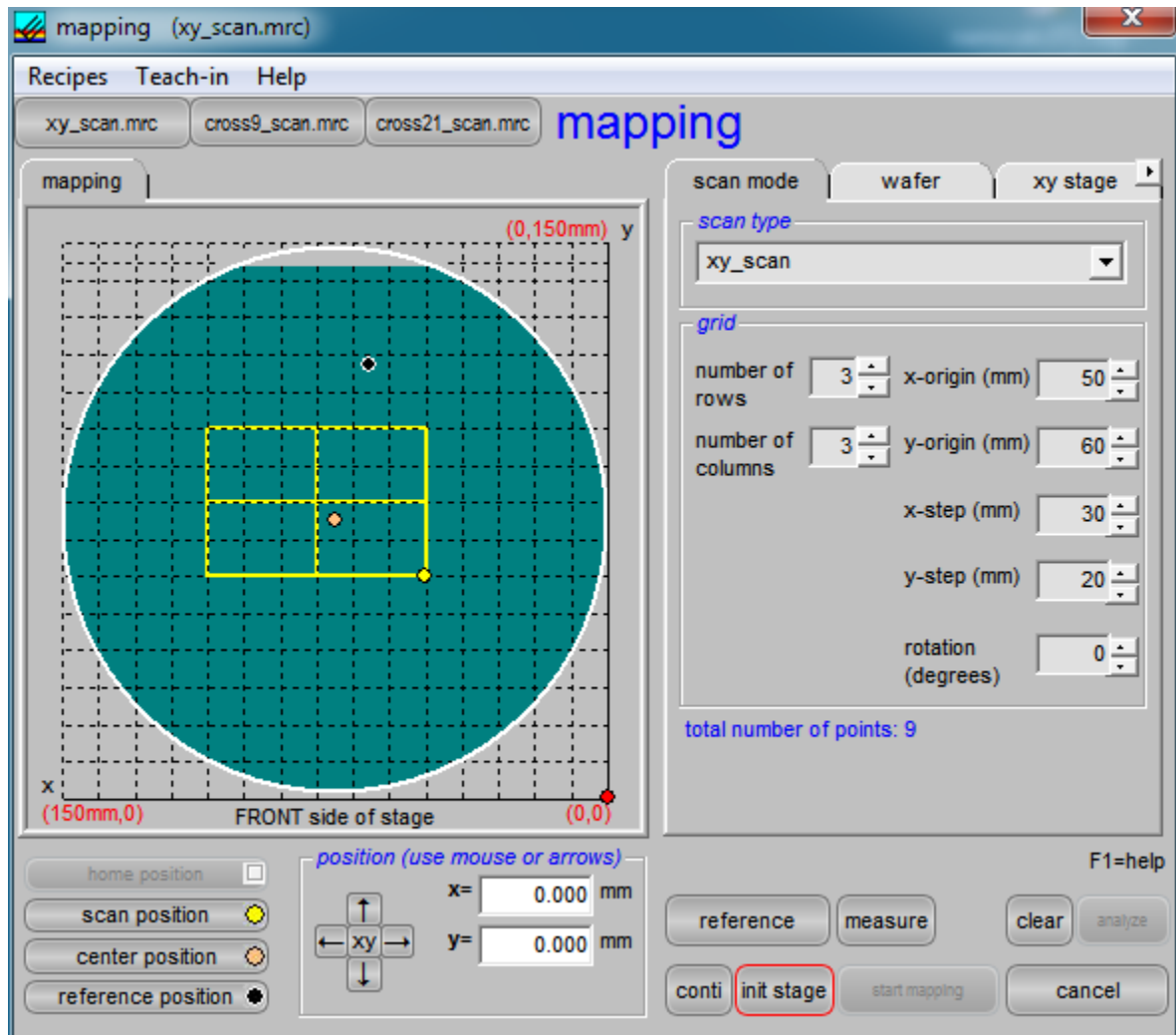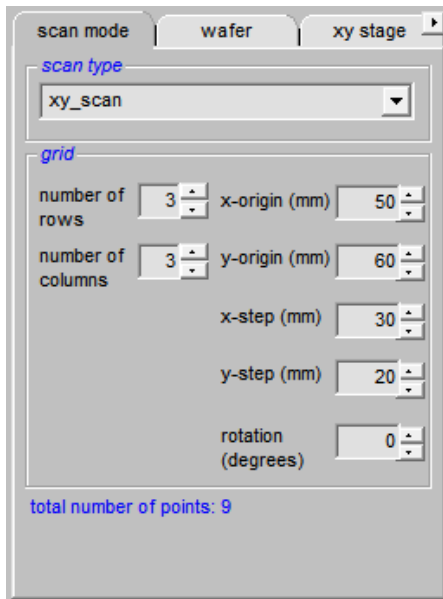
Here the origin of the wafer map is in the right lower corner and this is the view that you have if you stand in **front** of the stage. The hardware origin also is I this right, lower corner. The x-direction points to the left, the y-direction points upwards.

The yellow lines connect the scan points (here 9 points). The stage starts at the "scan position" (yellow circle) and the continues in x-direction (meandering).

In file "thinfilm.ini" you can change the position of the origi to the upper left corner (section [mapping], entry ZeroIsDown=True/False). This is consistent to earlier versions of NanoCalc.

The TabSheet on the right side has 6 tabs (scan mode / wafer / xy stage /....). If you want to see them all at the same time change the entry MultiRow=True/False in file "thinfilm.ini".

Tab 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 (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 (= 12"). 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)

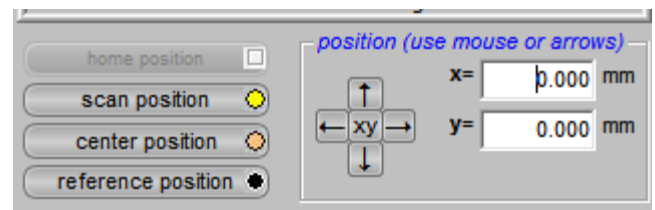The wafer plot shows what you are doing.

d. rotation

here you can rotate the scan region

e. mapping positions

measuring position:

If you press one of the position buttons (Home, Scan, Center, Reference), 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
   Usually 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
4. reference position
   this is the position where the reference measurement has to be done.
   this point (=the black circle) may be chosen by clicking with the RIGHT mouse button or by changing the numbers

The wafer plot shows what you are doing.
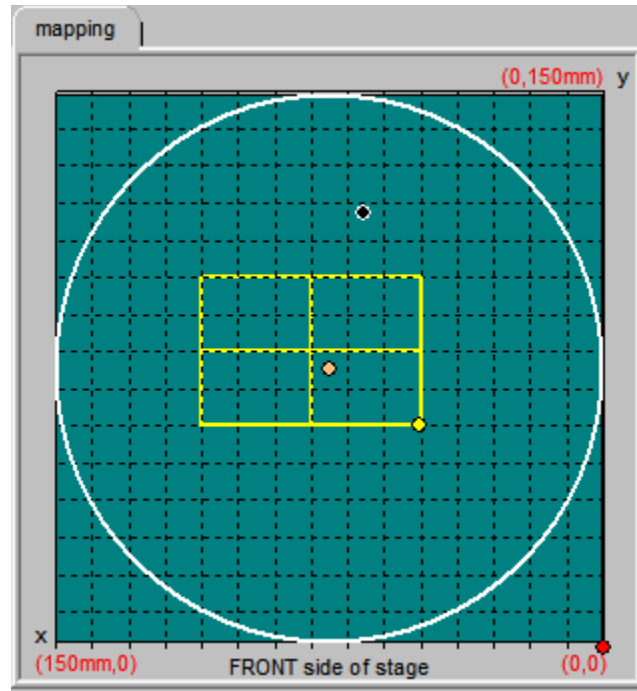
Tab wafer:

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 (= 12"").

Tab xy-stage:

Ocean Optics can deliver xy-stages up to 300mm (= 12")

a. xy reference position

with a <u>right</u> mouse button click you may change the position for measuring the reference. You may also enter numbers in this field. There is a possibility to build a wafer-chuck with a special area for a piece of reference-material even outside the defined wafer area. You may enter negative coordinates, but be VERY careful not to damage the stage. When the reference is taken, the stage drives to the set reference position and takes the reference measurement.

b. xy center position:

you may define a round (!) area which means the area of measurements. This area is not necessarily the same as the reserved area for the chuck

c. wait interval:

after each measurement the scanning may be interrupted for a certain interval of time

d. scanmode:

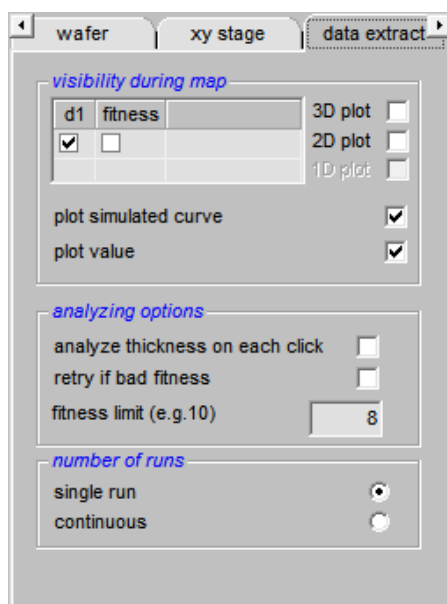If you activate this option each single measurement is waiting for a trigger signal (a keystroke with ENTER key or an external TTL trigger signal which is applied to the spectrometer. Ask your hardware supplier…)

e. single steps

mapping is down in single steps with ENTER (for test purposes?)

f. return to homeposition after scan

You decide whether the stage remains at the last measured point or returns to home

data extract:
a. visibility 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.)
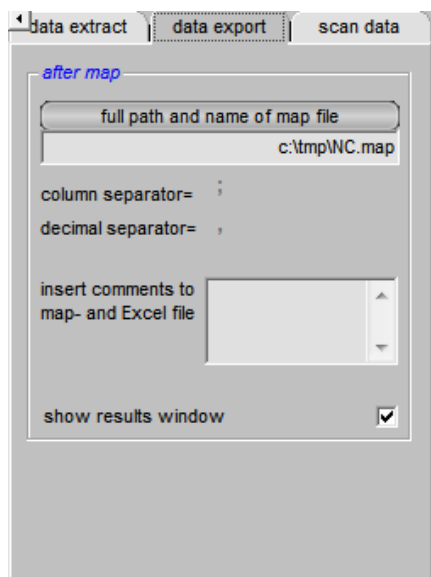   Only one variable is allowed to be seen during map.
b. analyzing options
   analyze thickness on each left mouse click. This is a very useful feature to make a quick check on thickness distributions on your wafer (do not forget to activate option "plot value ").
   fitness limit: if your results are 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.
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 thickness value

It is more informative to see the analyzed curve and the calculated value of thickness 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 thickness and fitness data together with some coordinate information are written to a ASCII-file in a (choosable) directory .
   Examples can be found in the directory "NanoCalc\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

7.5.2   Result List

As soon as the mapping is finished you will see a result list:
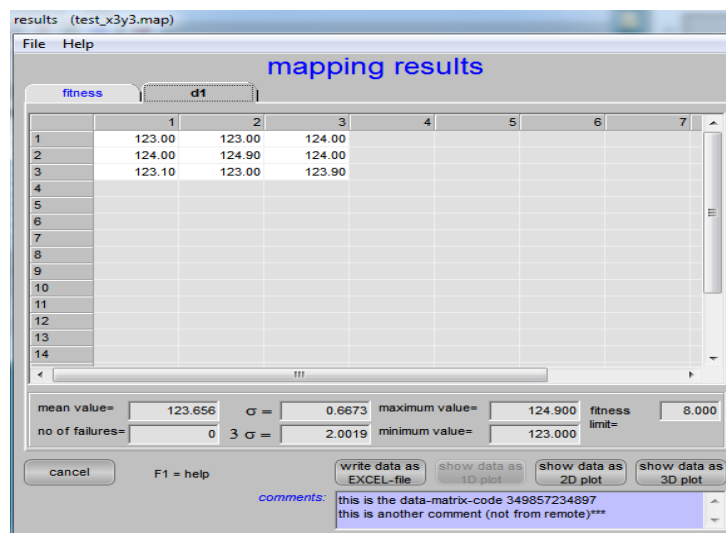
On the first page you see the measured thickness values for each layer. In the picture above there was just one layer and 3 x 3 = 9 measured data points. In the last page you can see the associated fitness values for each coordinate. In the text windows below the data window you see mean values, maximum 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).

7.5.3 Analyze mapped data

You may also analyze your mapped data at a later time, if you saved them to a .map file.

7.5.4 Structure of .map-file

Map-files are used internally and are not intended to be a basis for data visualisation. All data are written in sequence of the measurement and this is normally a meander !
Please use Excel export via csv or xls-files, they are written in geometrical xy order

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
```

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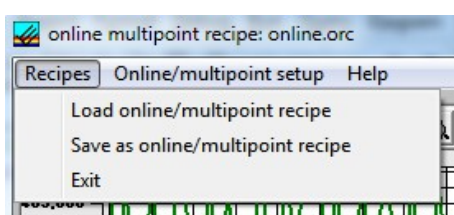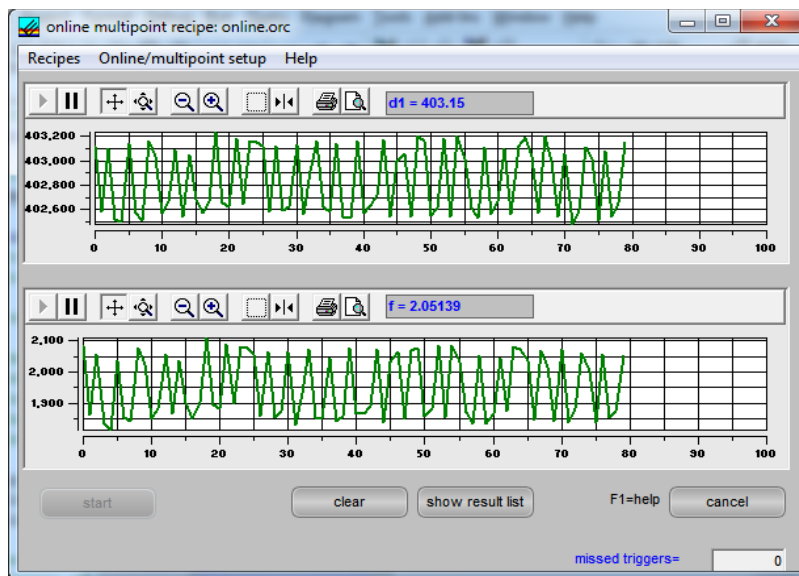
load online/multipoint recipe:
The online setup window contains lots of input data, so usually you will
want to use an online recipe to do that job for you.

You will be asked for a file name (usually in directory
"NanoCalc\recipe\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 "NanoCalc\recipe\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 recommen-
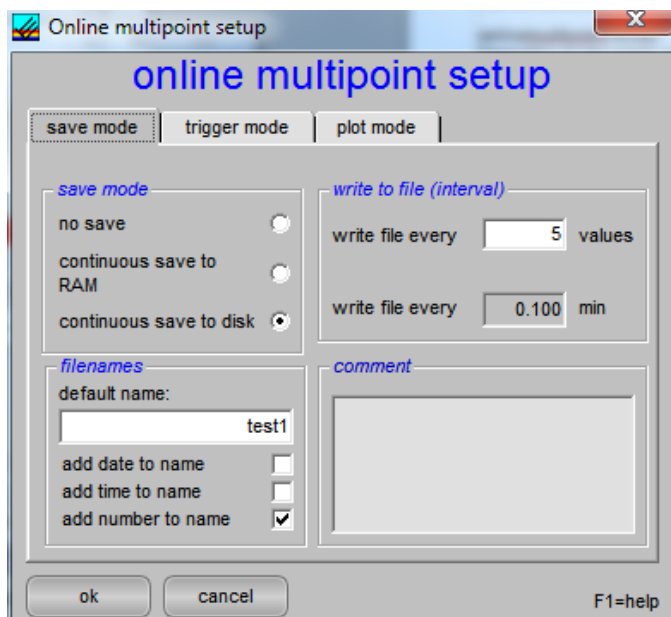ded to open the setup window first.

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. no save:
   all data are lost and only visible on screen
2. continuous save to RAM
   at the end of the run you may observe and analyze
   your data in the results window
3. continuous save to disk
   according to option "write_to_file_interval" all data are
   written to file in smaller portions with file names 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 file name 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.
e. comment
   you may add an ASCII-string, which will be added to
   every online file
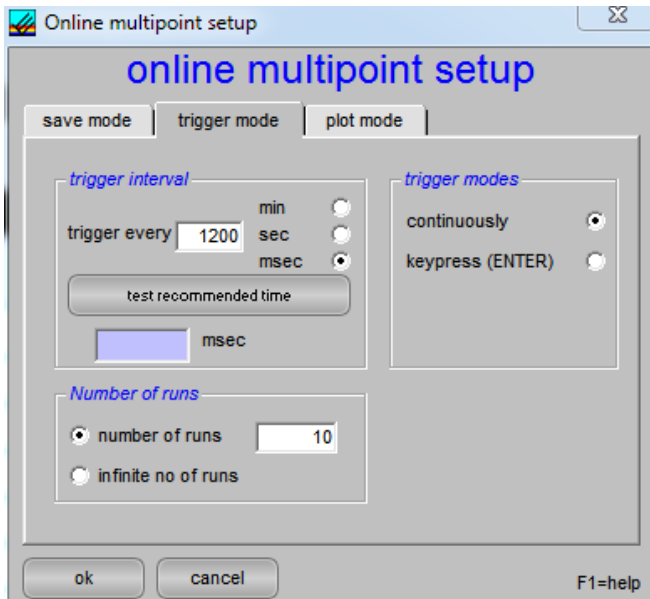
trigger mode:
In this second part of online setup you can choose:

a. option "trigger modes"
   you can trigger continuously by adjusting the appropriate software parameters like trigger interval. You can trigger manually with a keystroke.

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.
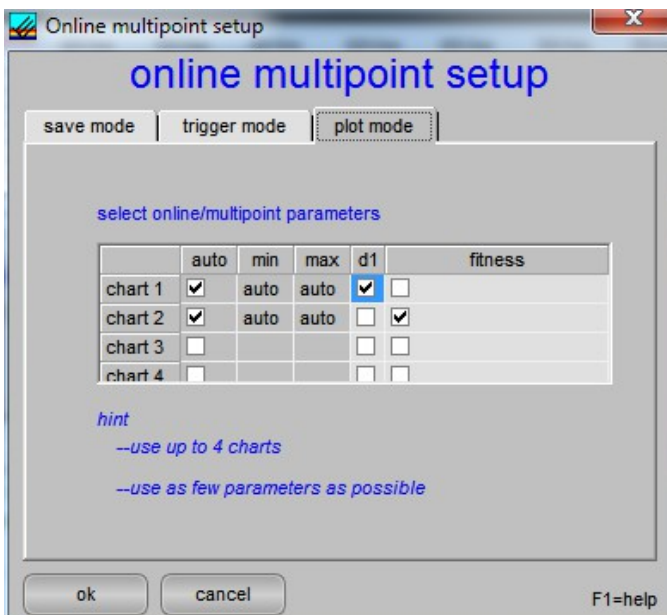
Plots:
In this third part of online setup you can choose plot parameters for up to 4 charts.
Each chart displays a single parameter

Result list for online/multipoint mode

On the first tab you see the fitness for each measurement, on the second tab you see the measured thickness values (for a one-layer system). In the picture above there 25 measured data points.
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.
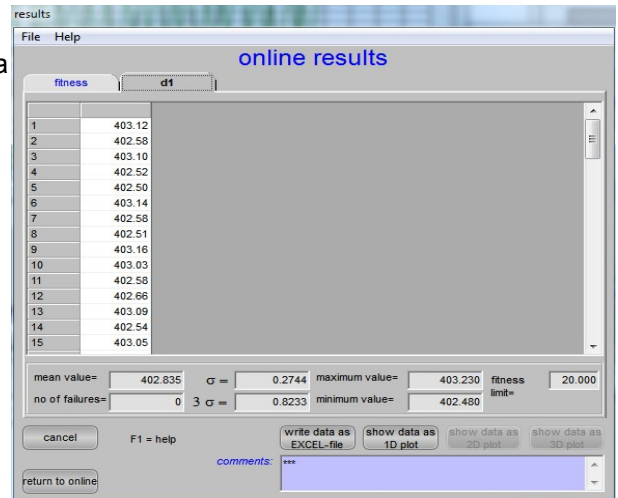
With "close all windows" you will return to NanoCalc main window and all online windows will be closed.

7.5.6 Analyze online/multipoint data

You may also analyze your online data at a later time, if you saved them to a .onl file.

7.5.7 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

7.5.8 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.
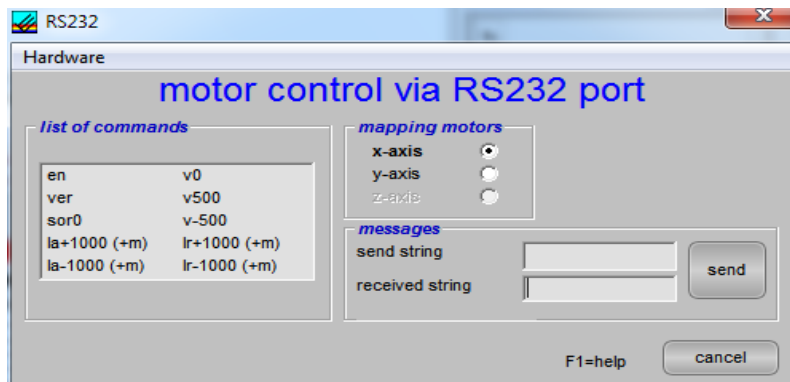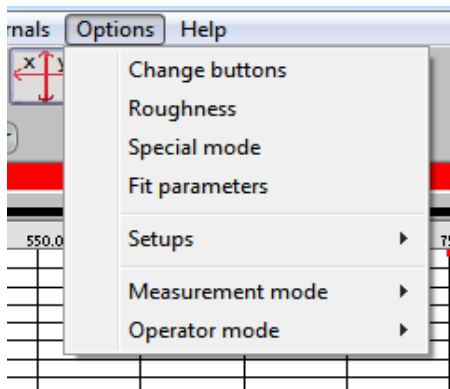
7.5.9   Vision system

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

7.6 Main menu "Options"

7.6.1 Change buttons

In this window you can make visible or invisible:

- a measure and analyze-button:
  to combine the functions to the measure and the
  analyze button
- factor for measuring integration time:
  Sometimes the signal intensities from the reference
  sample and the device under test are <u>extremely</u>
  different: e.g. the device might have an antireflective
  coating and does not show a good reflection signal.
  To avoid signal-to-noise problems, it possible to
  switch on the option "factor for measuring integration
  time" in menu "data extraction". If you now go to menu
  "spectrometer data" you will find a new item to change
  the integration time for the measurement task
  independently of the reference task.

  Example:
  Integration time for reference = 100 msec
  Integration time for measurement = 1000 msec
  Thus there is a factor of 10 between these two experiment. Internally the device signal will first be divided by 10
  (maintaining a good S/N-ratio) and then the calculation will be done as usual.
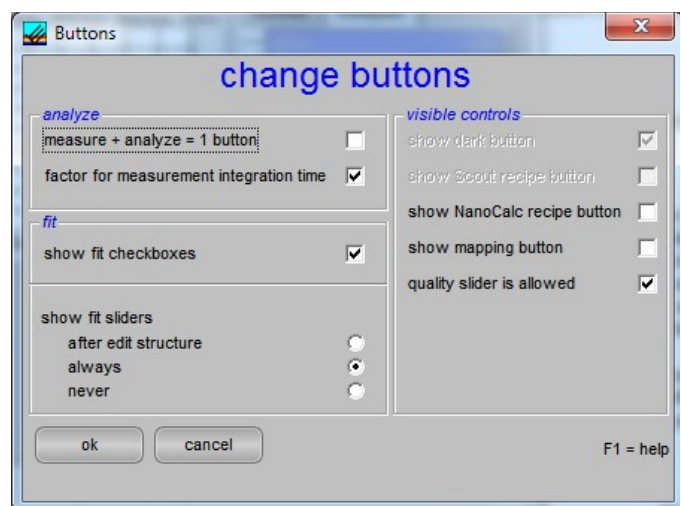
- show dark button:
  an extra dark button appears if it is necessary to measure any dark current (e.g. in a microscope setup)
- show SCOUT/NanoCalc recipe button:
  an extra "load recipe" button appears to make it easier to load recipes
- a mapping button:
  an extra "mapping" button appears to make it easier to use mapping
- a quality slider is allowed
  With this feature it is possible to set the speed (or the precision of the fit) for each individual measurement

7.6.2 Roughness

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

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 NanoCalc an empirical methods is implemented to deal with roughness:

1. **no roughness**
   No roughness is included in the calculation.
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.
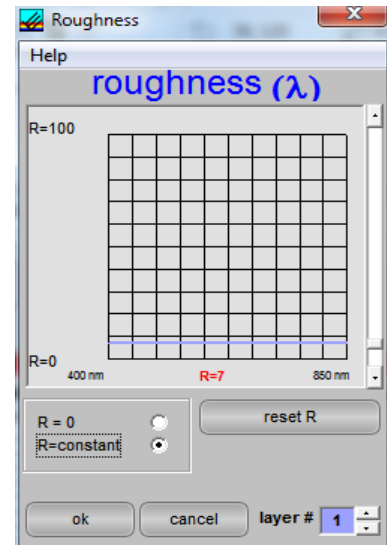
constant roughness
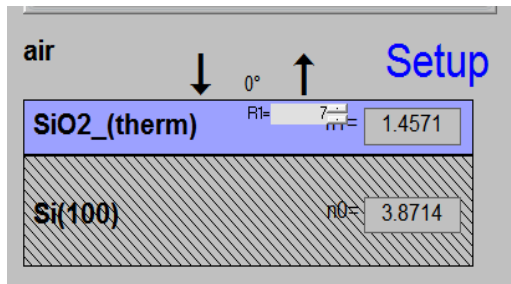
You may input roughness values in the roughness textboxes or use the slider in the roughness window.
Method:
At each interface a certain amount of light is regarded as lost. This percentage has to be input via roughness textboxes in the setup area. These R-factors are <u>not</u> dependent on wavelength.
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.
Try menu "Special modes" instead.

7.6.3 Special Modes

Please be aware of the fact that all actions within this menu are real manipulations of your measured data ! You change data to get better results, this maybe risky…
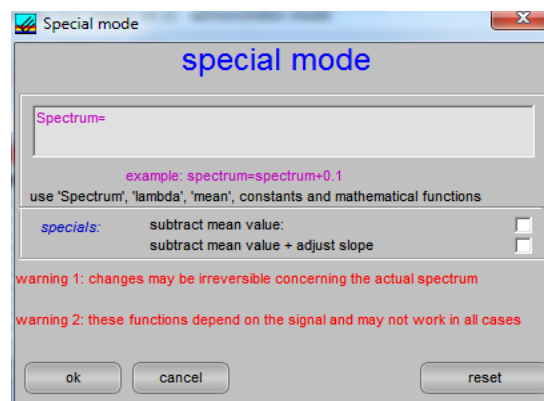
1. apply formula

It is possible to apply many reasonable formulae to the spectrum.
Example:
Spectrum=Spectrum*0.9
(all values are multiplied with a constant factor 0.9)
You may also try:
Spectrum=Spectrum*(1+lambda/800)
and many others …

2. subtract mean value

the mean level of the measured signal is adjusted to the level of the simulated signal, but NOT the frequency or the amplitude or the slope of the signal. This option is quite useful if for some reason there is a slight constant offset between signal and simulation.

4. subtract mean value and adjust slope

The **level** and the **amplitude** and the **slope** of the measured signal are adjusted to the level of the simulated signal, but NOT the frequency of signal modulation.
Only the frequency of the wiggles remain as information. Think about using the FFT method instead.

7.6.4   Fit parameters
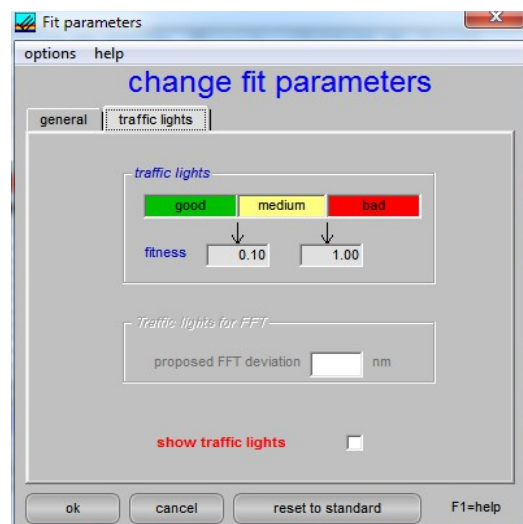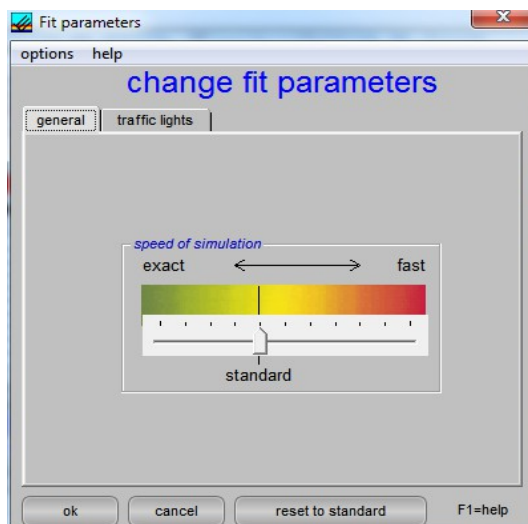
In the file "Thinfilm.ini" you will find 3 entries in section [fit]:
Failure_RedLevel=1
Failure_YellowLevel=0.1
RYG_LevelsAreDisplayed=False
If you change the variable RYG_LevelsAreDisplayed from "False" to "True" (in main menu "Fitparameters"), the usual rainbow pattern on the screen will disappear 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 resists (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.

7.6.5   Some setups

Change colors: Here you may change the colors of the layers. 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.
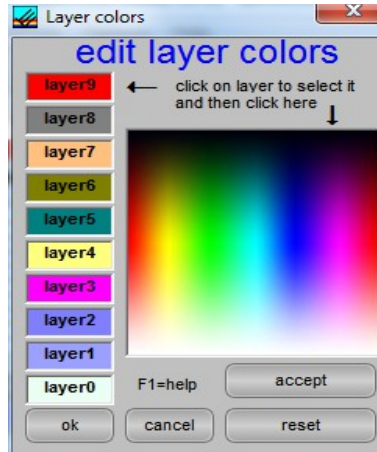
Change font sizes
Change size of sliders
Here a window (mainly a screenshot) opens and you may change most of the font sizes according to your screen an your needs. You may also change the size of the sliders.
Important: There are 2 <u>different</u> settings (saved in file thinfilm.ini). One setting for a maximized window and 1 setting for a normal (smaller) NanoCalc window.

Change all units

Here you may switch from nanometer to Angstrom resolution and background

7.6.6   Measurement mode

NanoCalc can be used in reflection or transmission setup.

7.6.7   Operator mode

NanoCalc can be used in administrator or operator mode.
The option expert mode excludes a lot of warning messages.
The language option is restricted to english and german (and a very crude french). If you need another language (and if you can help us with the translation): please contact your software supplier.
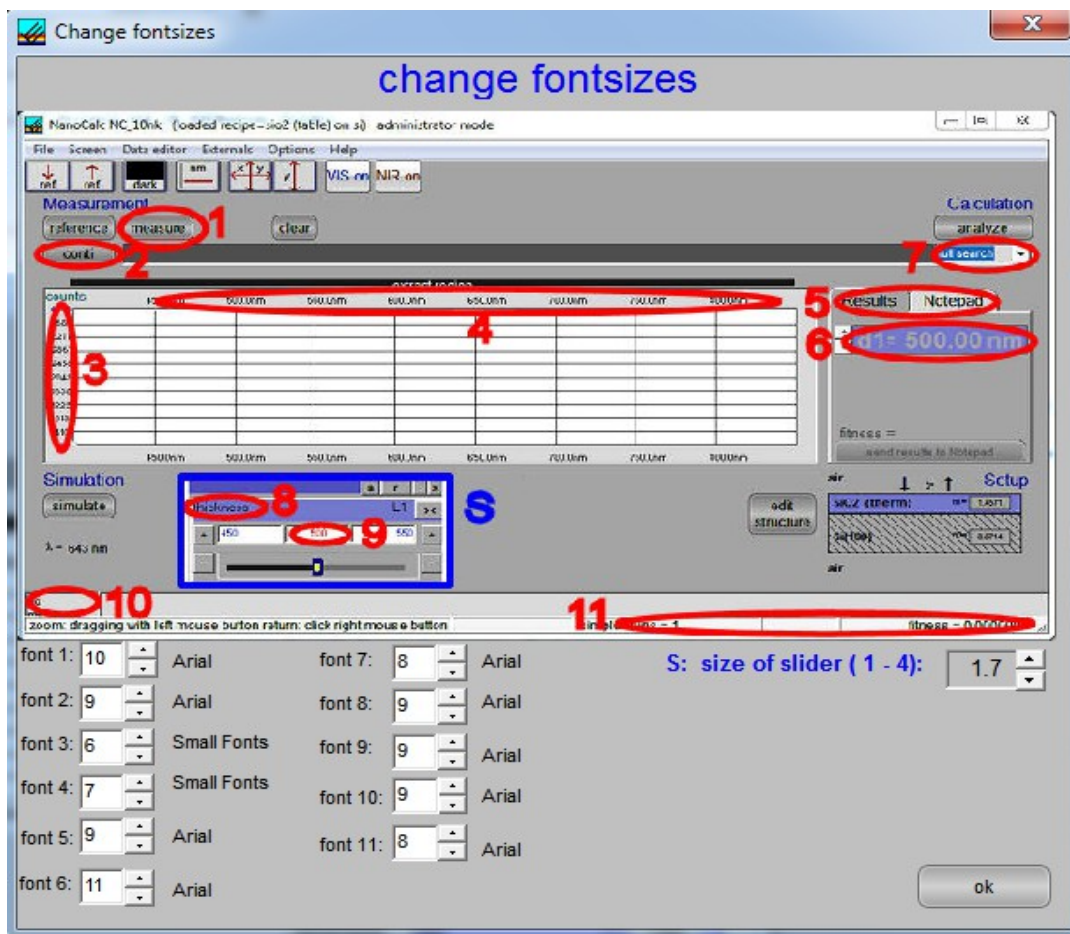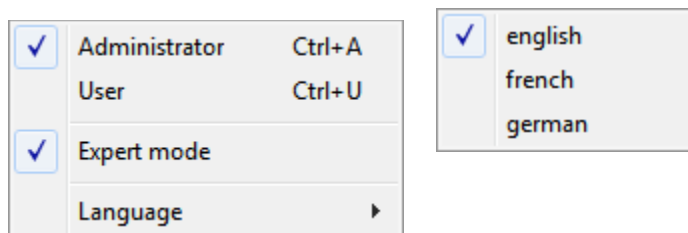

7.6.7.1   User mode

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.

7.6.7.2   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 on "administrator mode".

7.6.7.3   Rights of user

The administrator may set the rights for the user for nearly every single feature of the software.
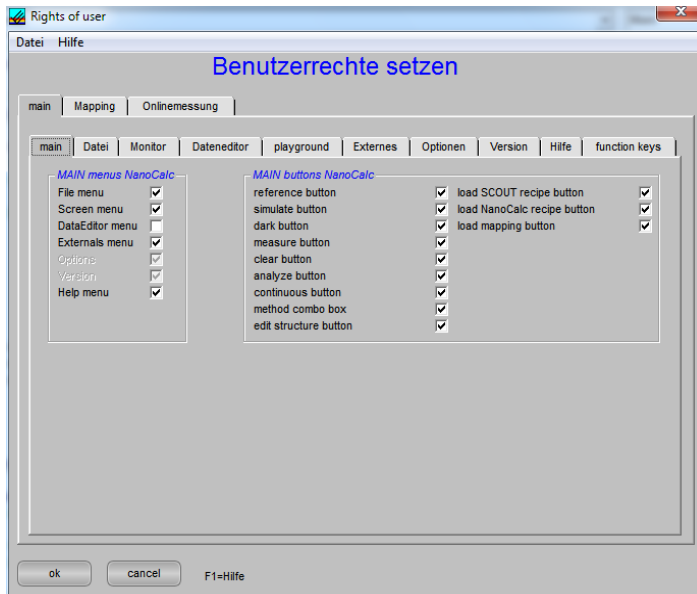
7.7 Main menu "Version"

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

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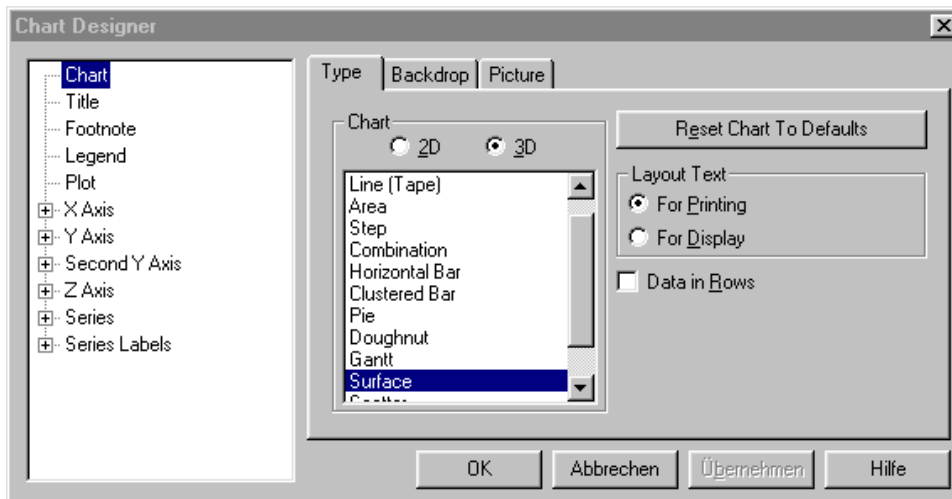
If you produced a 1D-plot or 2Dplot or 3Dplot you may change nearly ALL parameters of the plot by clicking with the RIGHT mouse button

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 NanoCalc installation.

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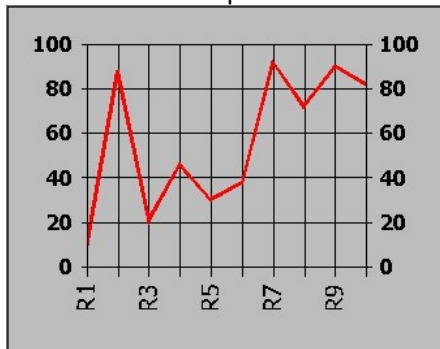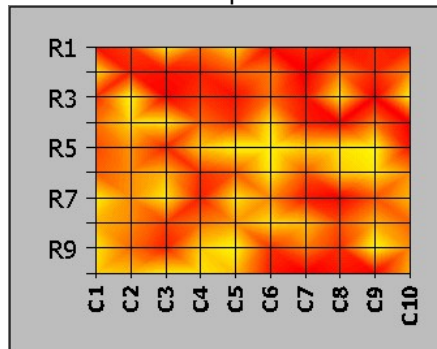
| 1D-plot | 2D-plot | 3D-plot |
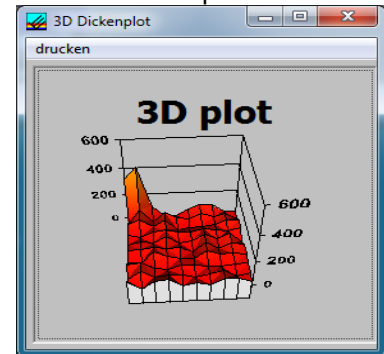
During mapping it is possible to produce 1D-plots, 2D-plots and 3D-plots.
These plot types can be changed interactively after the mapping was finished. Click with <u>right</u> mouse button on the plot to get access to the "chart designer".

8 Special features for "SCOUT mode"

8.1 General

If you activate the SCOUT window in menu Options/Change buttons you will see a separate SCOUT window.
Warning:
1. You should have some experience with this program if you plan to change anything inside this window !!
2. Do NOT close this SCOUT window directly !! It is closed by closing NanoCalc.
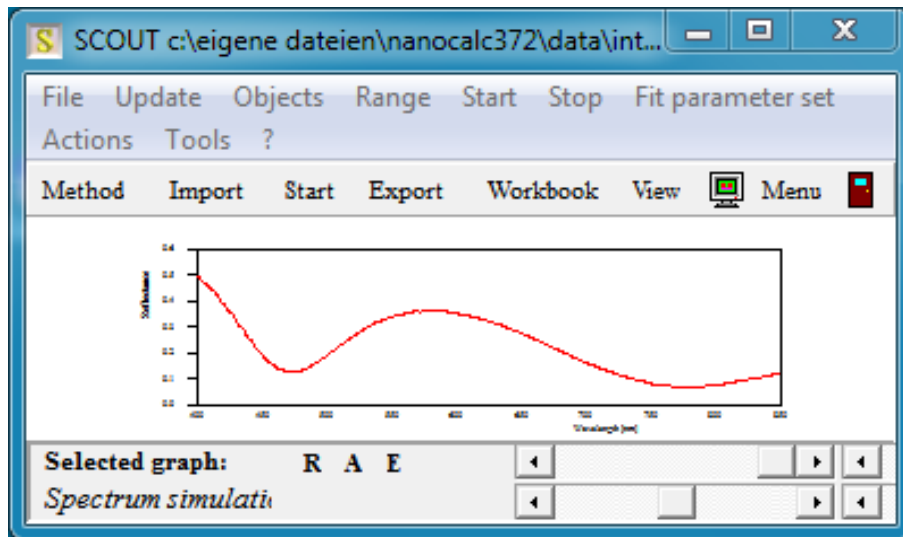
Normally NanoCalc uses SCOUT as an engine in the background. NanoCalc itself measures the spectrum, corrects for dark and so on. Then this spectrum is transferred to SCOUT and SCOUT does all data extraction. SCOUT has to know what to do, this is manifested in its .sc2-file. This .sc2-file is connected to the corresponding .lrc recipe.

If you load a recipe like „Cauchy on Si.lrc", you will find an entry in this recipe to a file „Cauchy on Si.sc2" in another directory. This SCOUT recipe was established by an experienced user (you or OceanOptics). In this SCOUT mode there is no EditStructure button, as all layer data are found within SCOUT.

8.2 Main menu "File"
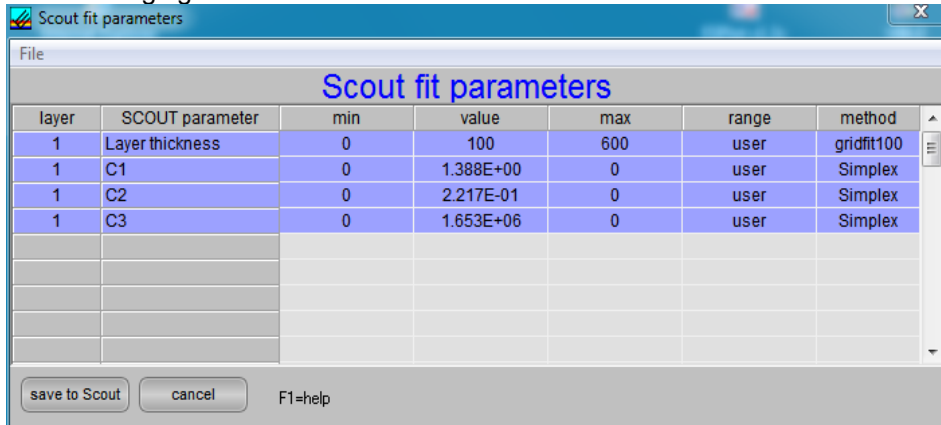
8.2.1 Change layer recipe

iI 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 NanoCalc.
The layer stack and all layer parameters are defined within SCOUT and are extracted by SCOUT. NanoCalc is only a user interface. There are lots of data in NanoCalc'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 <u>new</u> 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

layer	SCOUT parameter	min	value	max	range	method
1	Layer thickness	0	100	600	user	gridfit100
1	C1	0	1.388E+00	0	user	Simplex
1	C2	0	2.217E-01	0	user	Simplex
1	C3	0	1.653E+06	0	user	Simplex
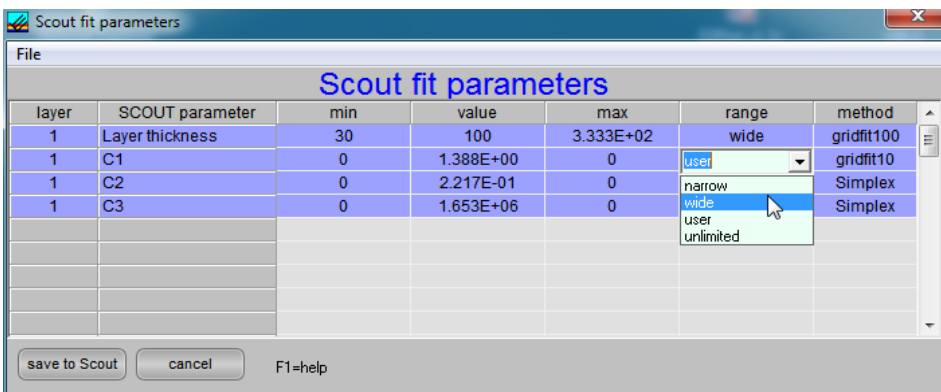
SCOUT fit parameters: Changing a range for parameters
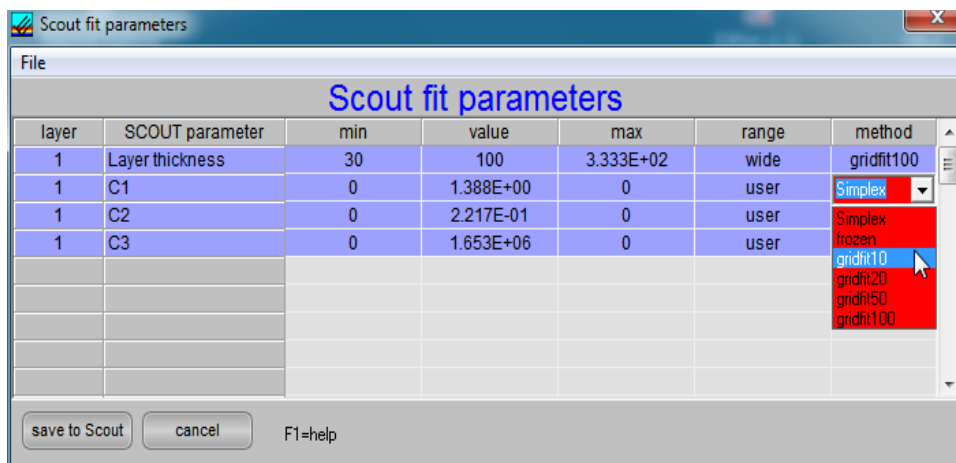
layer	SCOUT parameter	min	value	max	range	method
1	Layer thickness	30	100	3.333E+02	wide	gridfit100
1	C1	0	1.388E+00	0	user	gridfit10
1	C2	0	2.217E-01	0	narrow	Simplex
1	C3	0	1.653E+06	0	wide	Simplex
					user	
					unlimited	

SCOUT fit parameters: Changing an extraction method

layer	SCOUT parameter	min	value	max	range	method
1	Layer thickness	30	100	3.333E+02	wide	gridfit100
1	C1	0	1.388E+00	0	user	Simplex
1	C2	0	2.217E-01	0	user	Simplex
1	C3	0	1.653E+06	0	user	frozen
						gridfit10
						gridfit20
						gridfit50
						gridfit100

9 Special features for "internal mode"

This internal mode can only extract <u>thicknesses</u> 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_NC=name.sc2" in section [Scout].
  Be careful with this manual editing, make a safety copy! Finally the line should read:
  "Scout_FileName_NC="

After this change, you will see a new button "Edit Structure", which allows you to edit your own layer stack.

9.1 Edit structure button

You will see this button and this window only if you do not use a SCOUT recipe= if you use NanoCalc's internal mode (not yet fully supported). You could 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
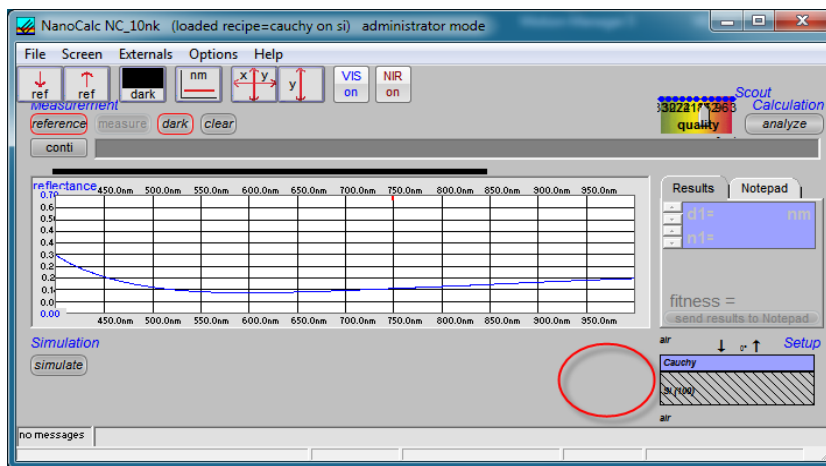
9.1.1 General

The full menu EditStructure is only available <u>if you do not use SCOUT</u>.
If you use SCOUT only the reference material may be changed.

In the menu Edit Structure you may enter:
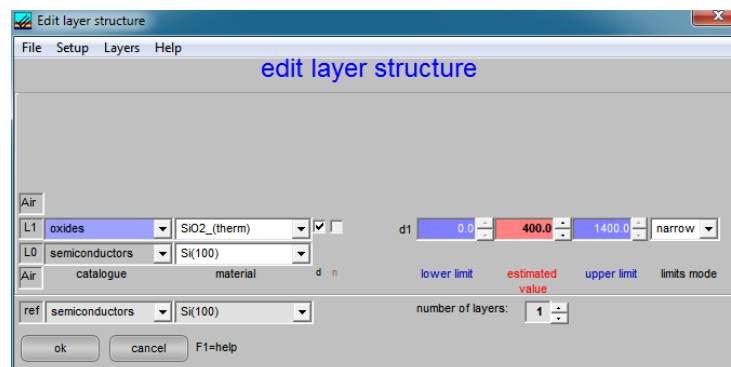
1. The type of catalogue like:
    oxides
    nitrides
    semiconductors
    .....
2. The type of material within one specified catalogue, like „oxides":
    SiO_2
    CuO
    TiO_2
    ......
3. The number of layers (in the present version: 1 to 10)

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".
   Restriction to NanoCalc_1: If you have two layers and one of them is fixed (= „well-known"), NanoCalc is able to determine the thickness of the second layer unambiguously. It is not important whether this layer is the upper or the lower one. The same applies to three layers: two of them have to be fixed, the third will be calculated.
    Of course it does not make sense to use three fixed layers, there is nothing left to analyze.

    This restriction will not apply to NanoCalc_10nk. This multilayer version is able to calculate several layers (Attention: in most cases you need moderate information, otherwise there are several nearly equivalent solutions to the problem)

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 Edit Structure 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 Clariant, Arch, 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 Edit Structure 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 Clariant, Arch, Shipley, MRT and others).

You may add a new material manually or use the menu Edit Refraction Index.

In Version NC_10nk there is an option to use "reference systems". e.g. a glass reference with a backside surface or even a stack of layers (e.g. native oxide). First you have to measure this reference system in the normal way = with silicon as reference. Then press the button file/save as reference system. Then choose this system as a new reference.

You may also change the top or bottom ambient material by clicking on the Label "Air"
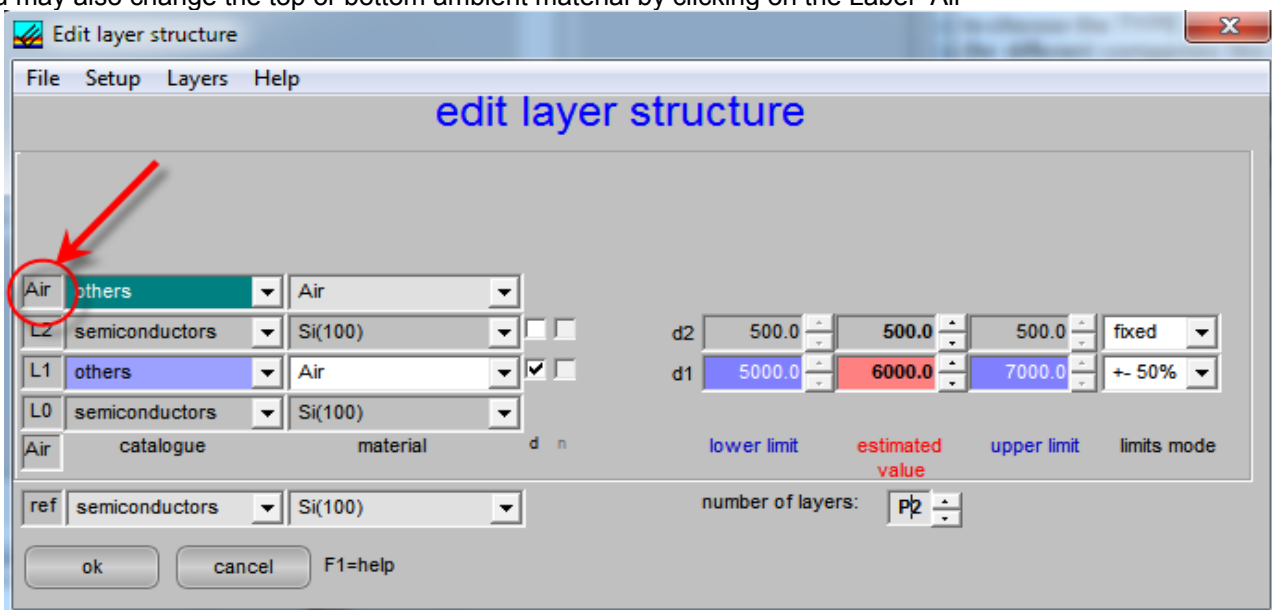
This feature is useful if you have a very thick glass or silicon plate above the system of thin layers. Such a glass plate cannot be simulated as a thin layer with coherent superposition of partial waves. It is advisable to change to top ambient material to glass as well (and perhaps to omit the glass layer).

9.1.4   Thickness

NanoCalc uses values for the thickness between 0 and 300000 nm (=300 micrometers). In the present version only thicknesses may be fitted (otherwise you need SCOUT)

9.1.5   Estimates

NanoCalc 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

NanoCalc_1 is able to analyze even 3 layers if **two** of them are "well-known" = fixed.
The same applies to 2 layers: **one** of them has to be fixed and the other may be analyzed. It is of no importance **which** layer is to be analyzed.
NanoCalc_10nk can extract 2 or 3 layers simultaneously. Of course this takes some time...
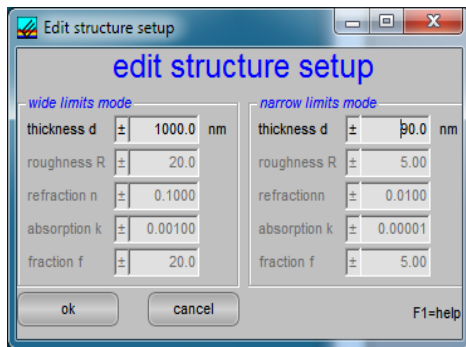
9.1.7 Narrow Limits

If you click "narrow limits", NanoCalc 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 "wide limits mode" (e.g. ±1000 nm and a thickness of 4000 nm), NanoCalc will search between 3000 nm and 5000 nm.
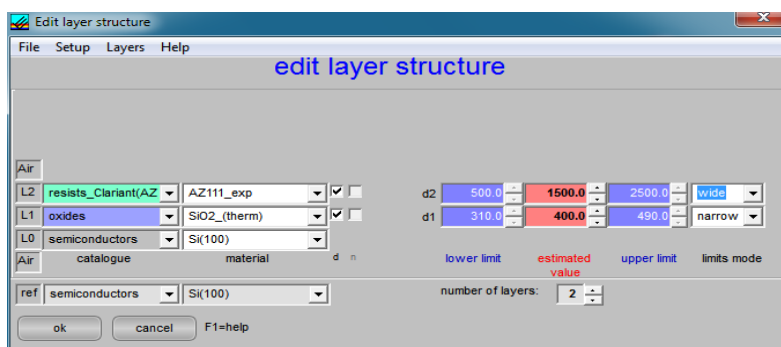
9.1.9 User limits

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

9.1.10 Number of layers

NanoCalc_1 is doing all simulations with a maximum of 4 layers (extraction: 1 layer)
NanoCalc_10nk can extract data from up to 10 layers simultaneously.
An example of two 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: "make a thick layer"
In most cases the substrate is the only "thick" layer and has layer number 0 (abbreviation: L0). As default this substrate is regarded as non-transparent: its backside is NOT included in the calculation, it is regarded as semi-infinite. In the software layer L0 owns a property "SUBSTRATE".
But if your substrate is transparent (like glass) you might want to include the backside. Then you have to change the property "SUBSTRATE" (= non-transparent) to another property "THICK" (=transparent).

example 1:
BK7-glass is the substrate and you want to include backside reflections (attention on rough backsides, oblique substrates and so on). Start with a configuration with glass as substrate, do not care about thickness values at the moment. Apply the command "make a thick layer". A little windows pops up, choose layer 0 (the glass layer) as "thick". Now you also have the chance to insert the thickness of the glass plate. Select "calculate backside=True". Now press "ok" in this little window (which will disappear). Now adjust all other thicknesses.
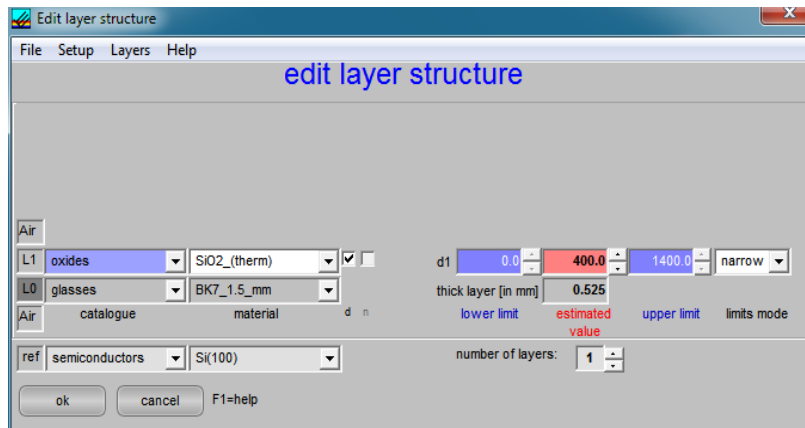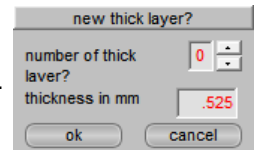
example 2:
you want to measure a thin film of Si3N4 on the backside of a thick glass plate
First establish the stack: Si3N4 as substrate with a glass layer on top. Do not care about thickness values at the moment. Then apply the command "make a thick layer". A little windows pops up, choose layer 1 (the glass layer) as "thick". Now you also have the chance to insert the thickness of the glass plate. You are not allowed to select "calculate backside" as this is always the case if the thick layer is not L0. Now press "ok" in this little window (which will disappear). Now adjust all other thicknesses.
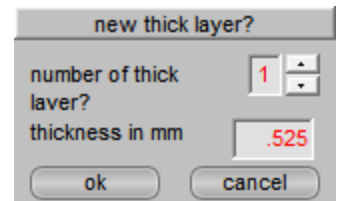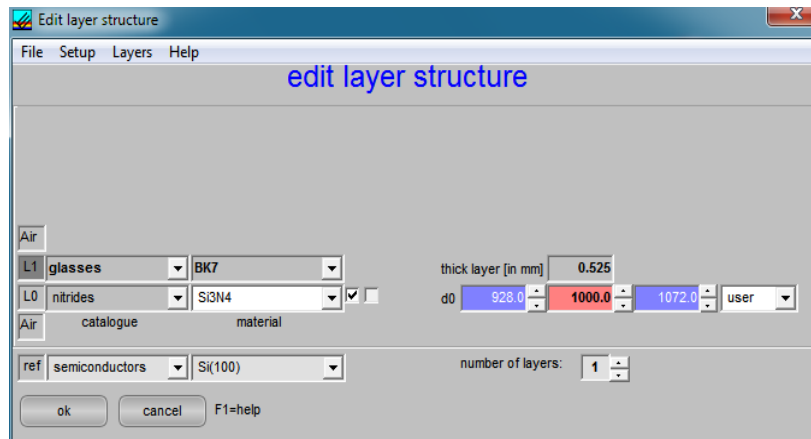
application 2: show layer commands

if this option is activated a small list of commands is shown (like PageDown, PageUp, …)
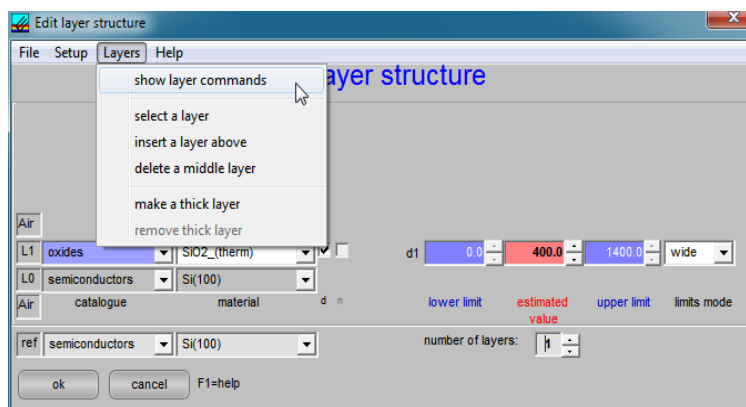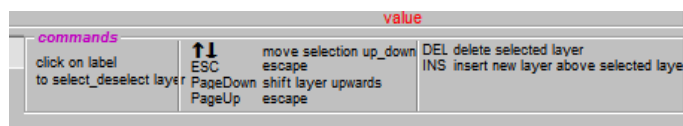
application 3: select a layer

To delete, insert or switch layers you first have to <u>select</u> 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"
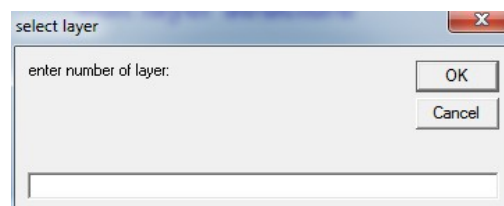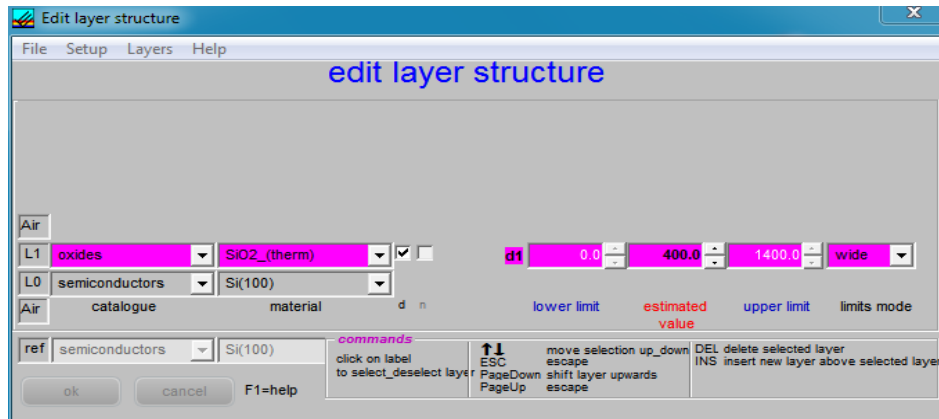
application 4: delete a layer
First select the layer that is to be deleted (see application 3). Then press the delete button on your keyboard
Or: select the layer and use the command "delete a layer" in submenu "layers"

application 5: insert a layer (above another)
First select a layer (see application 3). Then press the insert button on your keyboard
Or: select the layer and use the command "insert a layer above" in submenu "layers"

application 6: switch layers
First select a layer (see application 3). Then press the PageUp or PageDown button on your keyboard.
Thus you may also create backside layers.

10 Experimental setups and problems

10.1 General

10.1.1 Experimental setup

microscope setup:
- if you use a microscope you have the advantage of a high spatial resolution (depending on your lens system), but you should keep in mind:
- the angle of incidence is not well defined and you should repeat your measurement with different lenses to control your results (usually the results are slightly dependent on the magnification factor).
- you have a good chance to measure lots of stray light from your laboratory. Control your measured lamp spectra !
- If you use a fiber for illumination: turn off the usual microscope lamp.
- as your spot size is so small: pay attention on particles which may give wrong results
- if film thickness is high: such samples often are inhomogeneous. Try a different spot to measure.
- use reference wafers and device under test of the same height.

fiber setup:
if you use a simple fiber setup you should keep in mind:
- the spot size corresponds to the area of your fiber core (e.g. 200 micrometers or less)
- try to avoid stray light
- use a distance of at least 3-30 mm (otherwise the results are sensitive to different heights of your reference wafer and the device under test)

10.1.2 Reference spectrum

To measure the thickness of any thin film you have to measure a reference spectrum first. This is necessary to get information about the incoming amount of light as a function of wavelength.
Insert a blank (silicon?) wafer or your blank substrate in the measuring arrangement and press "reference".
You should get a typical spectrum of a halogen lamp (or a warning to increase or decrease the intensity of the lamp)
If you want to continue with measuring your thin films:
Do not forget to tell NanoCalc which substrate you used in this step (by pressing Edit Structure and adjusting the correct catalogue)

10.1.3 Maximum intensity

This value describes the maximum intensity in the spectrum of your amp (could be easily checked in Reference mode). This value helps NanoCalc to achieve an automatic adjustment of the reference spectrum within the limits of the screen (=without saturation)

If you use a double spectrometer there are TWO wavelengths corresponding to the sensitivities of the two spectrometers and your light source.

10.1.4 Polarization

In case of oblique incidence polarization plays an important role. In a vertical arrangement (like NanoCalc) the polarization does not play any role.

Attention: in microscope arrangements this condition of vertical incidence may no longer be fulfilled. You should test your results with different magnifications.

10.1.5 Angle of incidence

"angle of incidence" is defined as the angle between the direction of incoming light and an axis vertical to the surface.

In the current version of NanoCalc only vertical incidence is allowed.

10.1.6 Signal to noise ratio

The intensity of your acquired signal depends on:

 the adjustment of the lamp (see light source or NanoCalc-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

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

10.1.7 Stray light

Especially in a microscope setup there is a risk to catch stray light from your laboratory lamps. Try to avoid this as much as possible or use the simple fiber setup. External light sources usually changes and will produce errors.

10.1.8 Fiber

You may use different fibers with core diameters between 8 and 800 micrometers.
There are special fibers (Y-fibers, fibers with 6 outer fibers to illuminate and 1 inner fiber to detect the reflected light, fiber cables for double spectrometers). In most cases it is easily possible to detect more or less light through a different fiber constellation.

Consult your hardware supplier.

10.1.9 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 values of $n(\lambda)$ and $k(\lambda)$.

10.1.10 Passwords

There are several passwords within NanoCalc:

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 spectro-meter) 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…

10.1.11 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. You should be able to analyze these demonstration spectra by a simple click on the Analyze button.

F8 is used to save the reference and dark spectrum to disk.
If you click on the button **F8** a file "reference.nan" is saved (in an internal directory) and may later be used as a reference spectrum (to avoid a real measurement with a blank substrate). Of course this is only a very inaccurate method.

F9 is used to load the reference and dark spectrum from disk.
If you click on the button **F9** the file "reference.nan" is loaded and may be used as a reference spectrum (to avoid a real measurement with a blank substrate). Of course this is only a very inaccurate method for fast.

If you click on the button **F11** the last measured file is loaded again (if it was cleared). This file was saved on disk as "LastMeasured_File.nan" in directory \data\Internal_Data.

11   How to measure very thin films

It depends very much of the type of layers whether it is difficult to measure <u>very</u> thin films or not. As we have seen in the first section it is necessary to expand the spectral measurement range as wide as it is possible with this system. See chapter Frequency Limits.

1st example: 20 nm SiO_2 (=transparent) on Si
This is difficult to measure because the intensities and the spectral information of the signals with and without the
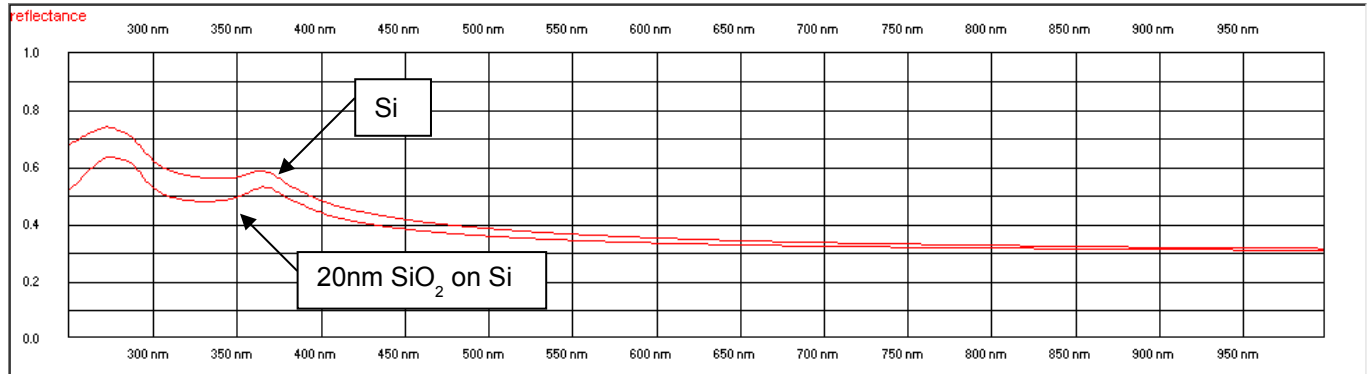
SiO_2-layer do not differ very much. The problem reduces more or less to an **intensity measurement**.
This means that you should use a light source with a extremely high stability and measure the reference signal immediately before measuring the SiO_2 sample to avoid any drifts. (You should use a UV/VIS/NIR System with a large spectral range (and a suitable lamp as well).
Try to measure in the UV-Range, as the changes of the signal are more pronounced.

2nd example: 5 nm Si on BK7-glass
You can see that it is rather easy to measure such an absorbing thin film.
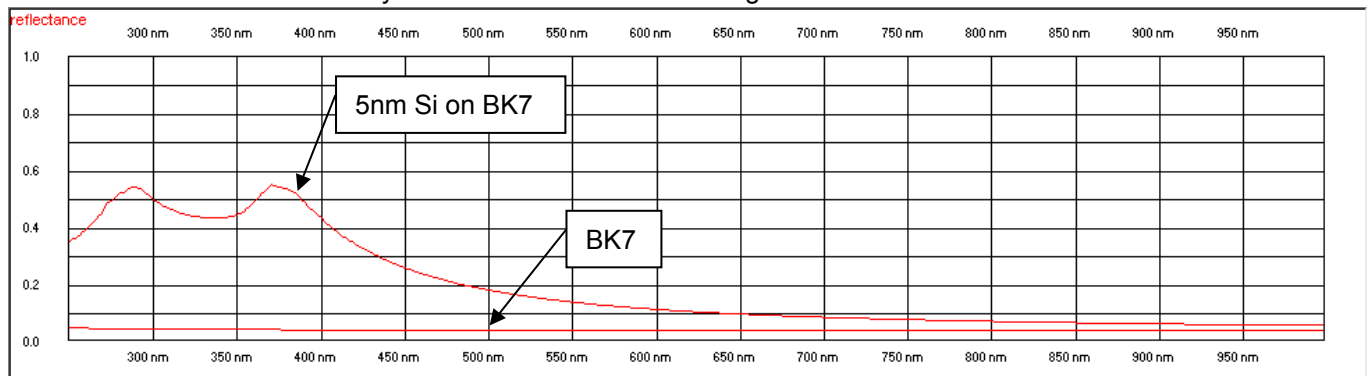
12   How to measure very thick films

Here you see a (simulated) example of 11µm resist on silicon
If the film thickness increases above 5 - 10 micrometers it gets more and more difficult to get good results because the numbers of extrema in your spectrum increases. This is in conflict with the spectral resolution of your spectrometer and the thickness of the fiber.

- choose pixel mode
- reduce the Boxcarwidth down to 1
- measure in the NIR region as the wiggles are further apart
- use FFT or "special modes" to get less influence from offsets or roughness effects
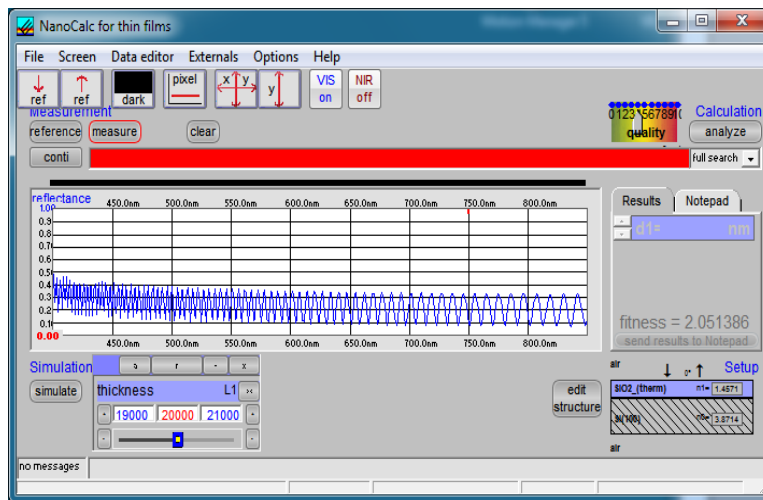
You get the best results (concerning spectral resolution) if you are using a system with a narrow slit. This means that you probably do not get enough intensity. To avoid problems with signal-to-noise-ratio try the following:

- adjust your lamp intensity to maximum
- minimize distance fiber – wafer
- adjust integration time (menu options)
- be careful in your choice of extraction and plot limits
- try manual measurement mode instead of automatic mode

Quite often thick resists are inhomogeneous or have a rough surface. This may destroy the signal completely or reduce the amplitude compared to theory.

13   How to measure rough, thick films

If the films or the substrate surfaces are rough it gets more and more difficult to get good results because of scattering effects. Sometimes it is still possible to measure a signal, but usually the amplitude and offsets are drastically different from theory. Nevertheless: if the film thickness is big enough, the spectrum has enough wiggles so that analyzing becomes possible. Use FFT or "special modes" to get less influence from offsets or roughness effects

In menu "data extraction" you find some options to adjust to roughness problems.

14 Physical explanations

14.1 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 dielectric function $\varepsilon(\lambda)$.
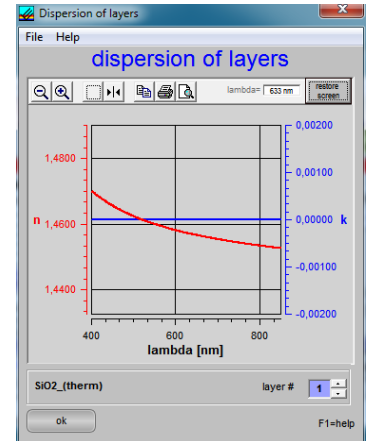
14.2 Cauchy coefficients

These coefficients empirically describe the dispersion functions of n(λ) and k(λ).

In many cases the 6 Cauchy coefficients are sufficient to describe the spectral behavior of resists, glasses etc. Normally NanoCalc 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	arbitrary 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 <u>measured</u> (=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 !!

14.3 Interference

The arrangement in the picture below shows the case of an oblique incidence (just to explain „angle of incidence") in contrast to usual experimental setup of a vertical incidence.

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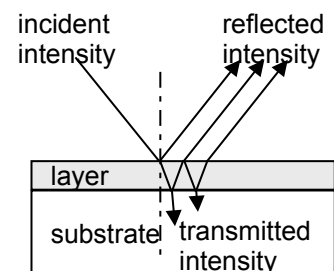
1. angle of incidence (if this angle is >0, then polarization plays an important role)
2. refraction index and absorption index of all layers

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.

15 Thinfilm.ini

This *.ini-file has to be located in the working directory of NanoCalc 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).

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 NanoCalc because only special users need these features.

```
[UserEdits]
WriteTmpFile=False
WriteRefFile=False
MinimumSearch=False
AllowPixels=True
Plot_During_Online=True
Save_During_Mapping_or_Online=False
ShowHistory=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=True
SpecialLambda=-1
UseClipBoard=True
HideNanocalc=False
StopMappingStage=False
SpectrometerSleepTime=30
NonLinearityCorrection=True
Lower_DeuteriumPeak=662
Upper_DeuteriumPeak=662
FastMode=False
ExpertMode=True
AxisTextStep=1
```

WriteTmpFile:
if this flag is set to TRUE, NanoCalc 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, NanoCalc 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

not active at the moment

Plot_After_FFT

If this variable is set to FALSE only the FFT peak will be plotted and not the extracted (=simulated) curve

YScale_FFTLayer

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=;)
You should choose a different string than csvExcelNumberFormatter to avoid confusion

csvExcelNumberFormatter

here you may enter the number formatter for the Excel-format, like "," oder"."
example: csvExcelNumberFormatter =.
If you own an american Excel, then a point will be correct, for german versions of Excel a comma will be correct.

ExcelMargins_LRTB

If you print Excel data LRTB means Left, Top, Right, Bottom as margins for the printout

UseShutter

In case an optical shutter exists this is a flag to use it or not. At the moment this feature is deactivated

SpecialLambda

this is reserved for a special customer

UseClipBoard

Setting this value to False: the last measured value is NOT saved to clipboard

HideNanoCalc

Setting this value to True hides NanoCalc in the taskline (for remote)

StopMappingStage

Setting this value to True: after each new position the motors are disabled (to get rid of spurious noisy movements)

SpectrometerSleepTime

If the spectrometer si not used for some time (SpectrometerSleepTime) the first results are not correct. This can be avoided by reading the spectrometer data several times. Within this SpectrometerSleepTime there are no repeated measurements.

AxisTextStep

On small monitors the x-axis texts might overlap. Then choose AxisTextStep=2 and only every second entry will be displayed.
In some cases this is done automatically .

16   Appendix A

16.1 NanoCalc-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 NanoCalc software

Start the computer and light source

Plug-In the USB-Cable, then install fiber cable between the spectrometer and light source.

Start the NanoCalc software

Put the reference (Si-Wafer) on the table (Bare Silicon)

Click the "Continuous mode" and "Reference" button

Set the integration time to 50 ms

Now adjust the fiber distance between wafer and fiber in that way that you get the highest possible signal. A typical distance is 1 - 5 mm
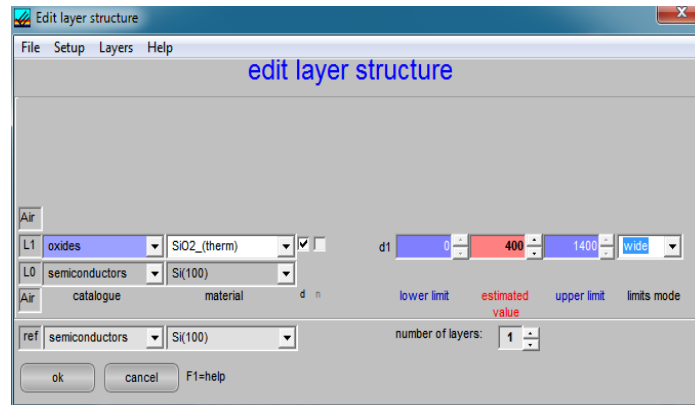
Now adjust the integration time in that way that the Max-Level is around 0.8 on your screen

Click again the "Continuous mode" button to stop the measurement

Click the "Reference" button

Now you are ready to work with the NanoCalc system!

Example I: Measure SiO$_2$ on a Si-Wafer
Go to menu Edit layer structure.

Settings:
L1 (layer1)   oxides   SiO$_2$_(therm)
bulk (substrate) semiconductors   Si
ref (reference)   semiconductors   Si
wide limits   => automatically: 0 nm – 1400 nm
estimated thickness   400 nm

Go to menu Screen > Frequency limits
        adjust the plot limits and the extraction range to:

System	*max. plot limits [nm]*	*max. extraction range [nm]*
VIS	400 – 850	450 – 800
XR	250 – 1050	300 – 1000
DUV	190 – 1100	200 – 1050
NIR	900 – 1700	950 – 1650

For thin materials choose a bigger range, for thicker materials (NIR) choose a smaller range and set the smoothing factor 1.

Measure the reference again

Then put the first step of the wafer under the fiber and push the button "Measure", then "Analyze".
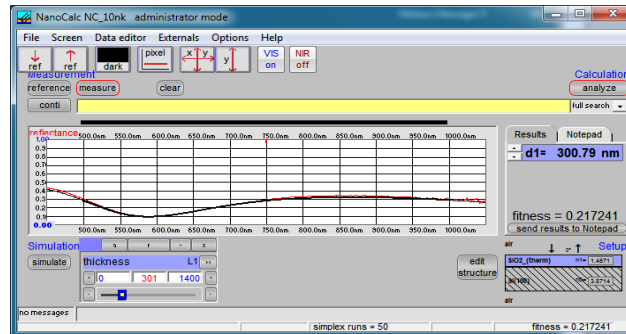
The two curves from measure and analyze should be nearly the same. How good they fit can you see in the right lower corner as Quality of Fit.
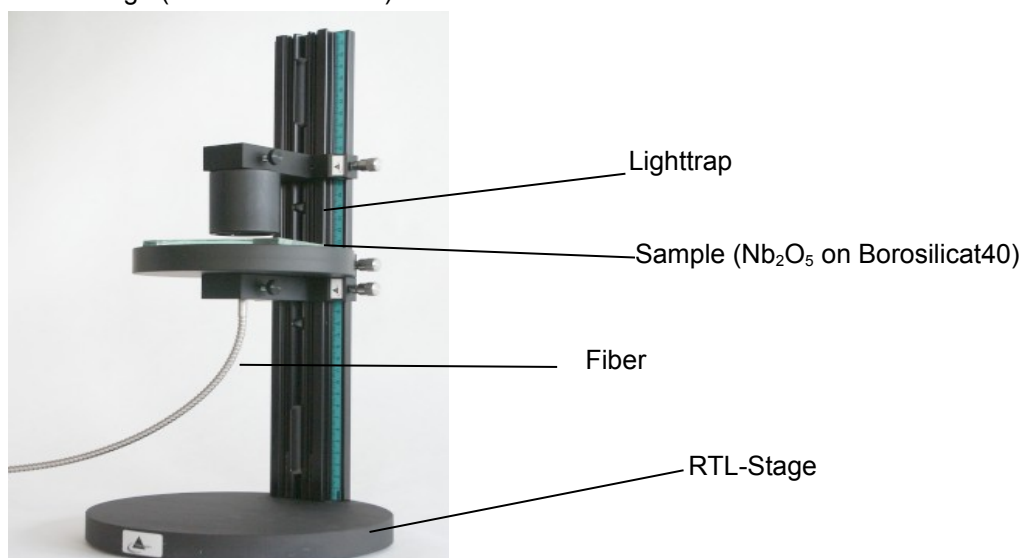
Please try the other steps on the wafer.

Save these settings as a recipe in menu "File" and "Save as recipe" under the name "Si_SiO2.lrc".
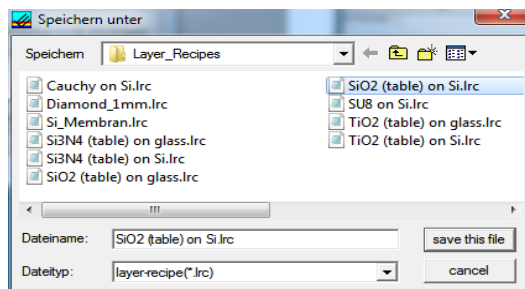
Example II: **Transparent Samples**
Nb₂O₅ on Glass (Borosilicat 40)

a.)   RTL-Stage (Reflectance mode)

Lighttrap

Sample (Nb_2O_5 on Borosilicat40)

Fiber

RTL-Stage

Please accept that Nb$_2$O$_5$ has a higher reflectivity than glass without coating, therefore we have to adjust the integration time with the substrate plus layer first and take the reference from the substrate without any changes.

Put the Nb$_2$O$_5$ glass onto the RTL-Stage. We need a light trap (black absorber material) behind the glass material, to prevent reflections or ambient light.

Click on the "conti" button and the on the "reference" button.

Adjust the fiber distance between sample and fiber in that way that you get the highest possible signal. A typical distance is 1 - 5 mm

Now adjust the integration time in that way that the Max-Level is around 0.8

Now put the reference glass (BK7) on the table.

Click the button "reference".

Now you are ready to measure, but as every time we have to go to the menu Edit layer structure first.
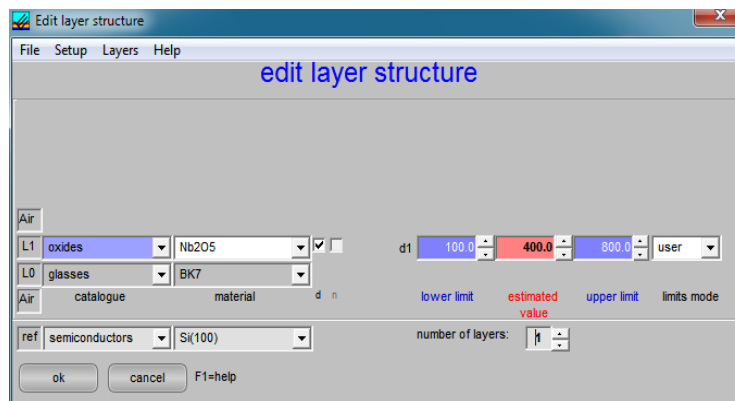
Settings:
L1 (layer1)   oxides   Nb$_2$O$_5$
bulk (substrate) glasses Borofloat40
ref (reference)   glasses BK7
user limits   100 nm – 800 nm
estimated thickness   400 nm

Go to menu Screen > frequency limits
adjust the plot limits and the extraction range to:

max. plot limits [nm]	max. extraction range [nm]
350 - 1050	400 - 1000

Please make again a reference measurement.

Now put the test-glass under the fiber and push the button "measure" than "analyze".

The two curves from measure and analyze should be nearly the same. How well they fit you can see in the right lower corner as "fitness" (?quality of fit). The difference in amplitude comes from the "wrong" reference BK7 instead of Borosilicat 40 and the inexact values for the n(lambda) and k(lambda) from glass and layer. This does not effect the thickness value in this case.
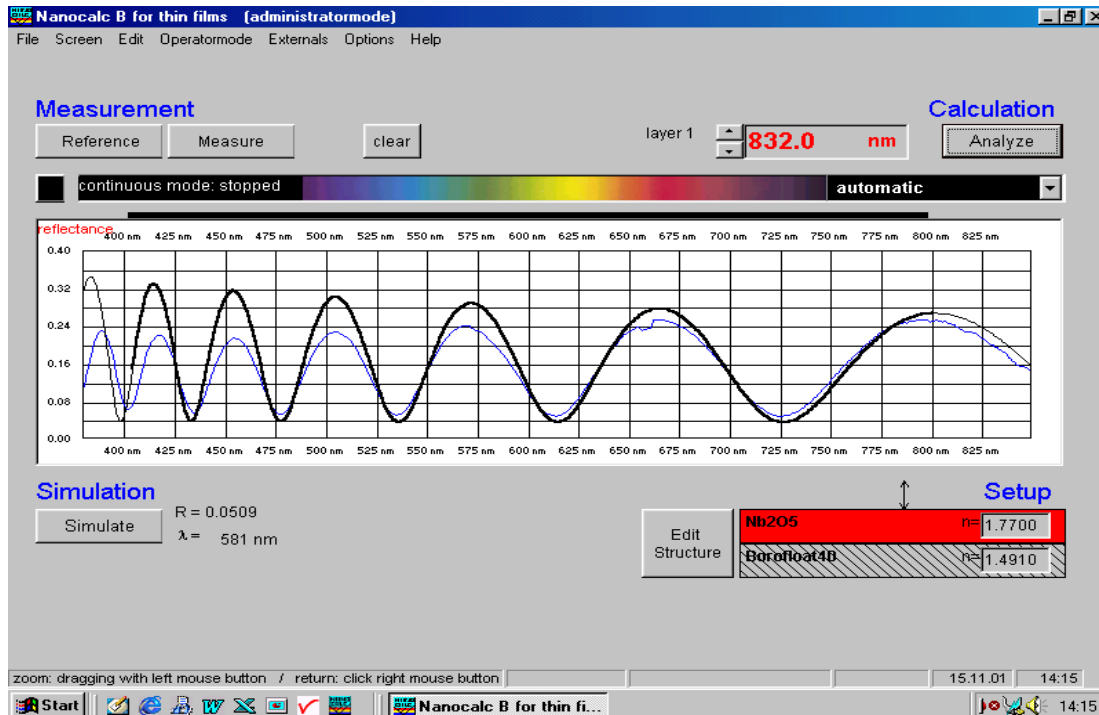
Please try different points on the wafer. Activate the continuous mode and analyze, and move the wafer by tweezers.

Save these settings as a recipe in menu "File" and "Save as recipe" under the name Nb2O5_Boro40.lrc".

RTL-Stage with 2 COL-UV lenses (Transmission mode)
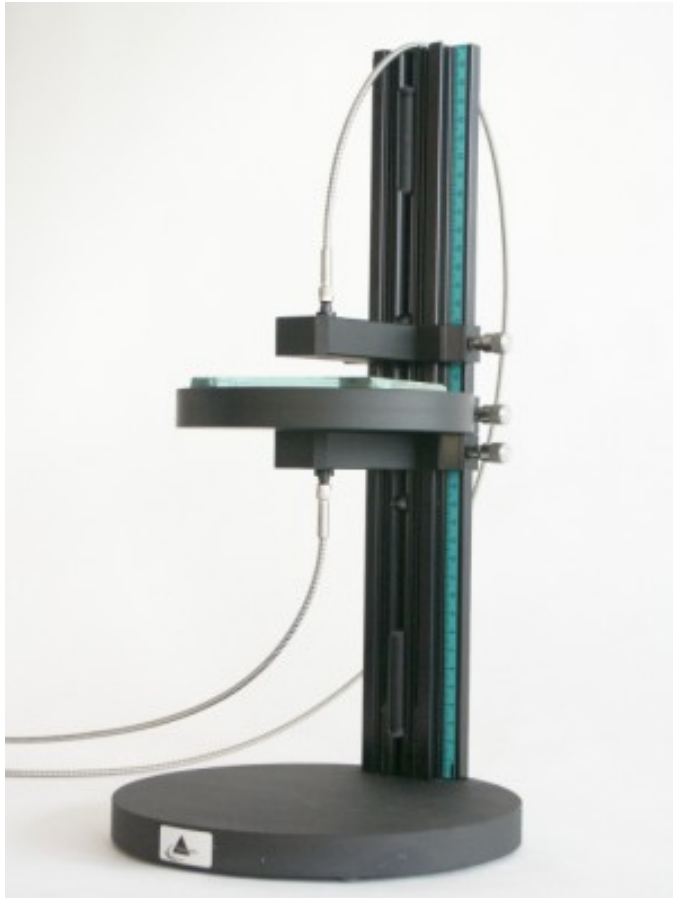
Fiber to the spectrometer

COL-UV lenses

Sample (Nb_2O_5 on Borosilicat40)

Fiber from the lightsource

RTL-Stage

Change to Transmission mode: go to menu Options > Measurement mode > Transmission

Please accept that Nb_2O_5 has a higher reflectivity than glass without coating, therefore we have to adjust the integration time with the substrate plus layer first and take the reference from the substrate without any changes.

Put the Nb_2O_5 glass on the RTL-Stage.

Click on the "conti" button.

Adjust the fiber distance between wafer and fiber in that way that you get the highest signal. A typical distance is 1 - 5 mm.

Now adjust the integration time in that way that the Max-Level is around 0.8.

Now put the reference glass (BK7) on the table.

Click the "reference" button.

Now you are ready to measure.