

# **Basic Operations Manual**

for

## **MPROBE<sup>®</sup> 20**

### **Thin-Film measurement system**

Revision 4.5

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## **What is the MProbe® 20 used for?**

The MProbe® system is used to measure thickness and optical constants ( $n$  &  $k$ ) of translucent films. Some typical applications include semiconductor process films (oxides, nitrides, photoresist, polysilicon), hardness coating on plastics, adhesive layers, thickness of freestanding films/tapes (PET and other polymer materials), TCO (ITO, SnO, etc.), OLED films, PBO and other PCBA coatings, polyurethane, porous Si, Yttrium Oxide on ceramic and thousands of other applications.

The measurement principle is based on spectroscopic reflectance and wavelength range and spectral resolution of the system defines the thickness range and type of applications that can be measured.

Traditionally, spectroscopic reflectance based system could only measure optically smooth layers that give near perfect signal response. MProbe® system is able to measure many applications on rough, tilted surfaces, films that are non-uniform, include nano-particles or other imperfections.

## **I. Quick Start up Guide**

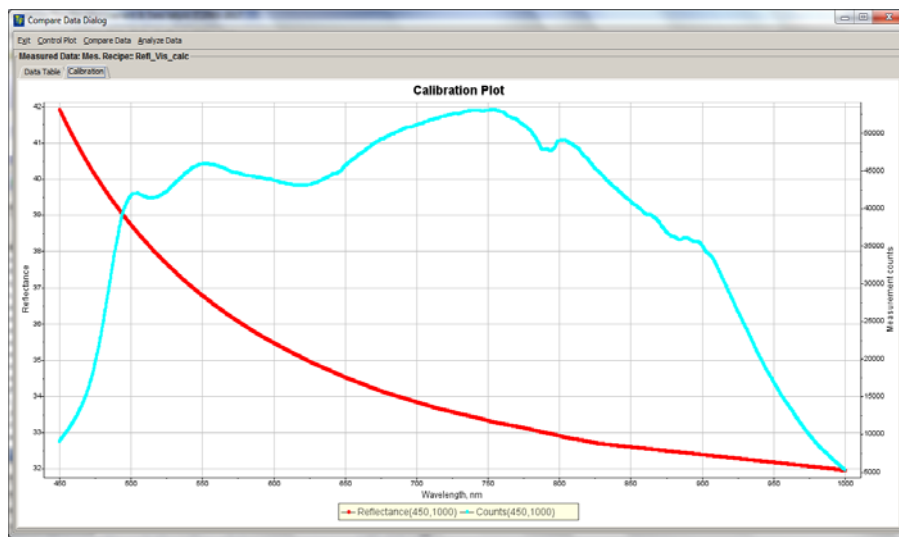
### **You just setup MProbe® - how to measure a sample?**

Measurement process includes several steps and conditions that are controlled by a Measurement recipe. Software automatically selects, optimizes and loads a standard Measurement recipe corresponding to connected MProbe system when it is executed the first time.

#### **a). Calibration**

**Place reference sample and adjust lens in the focused position (balanced maximum signal across the spectrum)**  
**Calibration is a two step process: measurement of the reference sample ( step 1), measurement of the black pad (step 2)**  
**Click Baseline button and follow a two step process as prompted**

Calibration (or Baseline) needs to be done before the measurement can be performed. The purpose of calibration is to map the light intensity measured by the system to a known reflectivity. The reference sample is supplied with the system and the type of the sample is set automatically in software based on configuration (it can be changed manually). It is important to remember that once calibration is done the configuration conditions should not be maintained. This means, in particular, that the distance between the reflectance/lens and the sample should be exactly the same as during calibration. If calibration/reference sample thickness is different from measurement sample – the position of the lens need to be adjusted to match the distance.

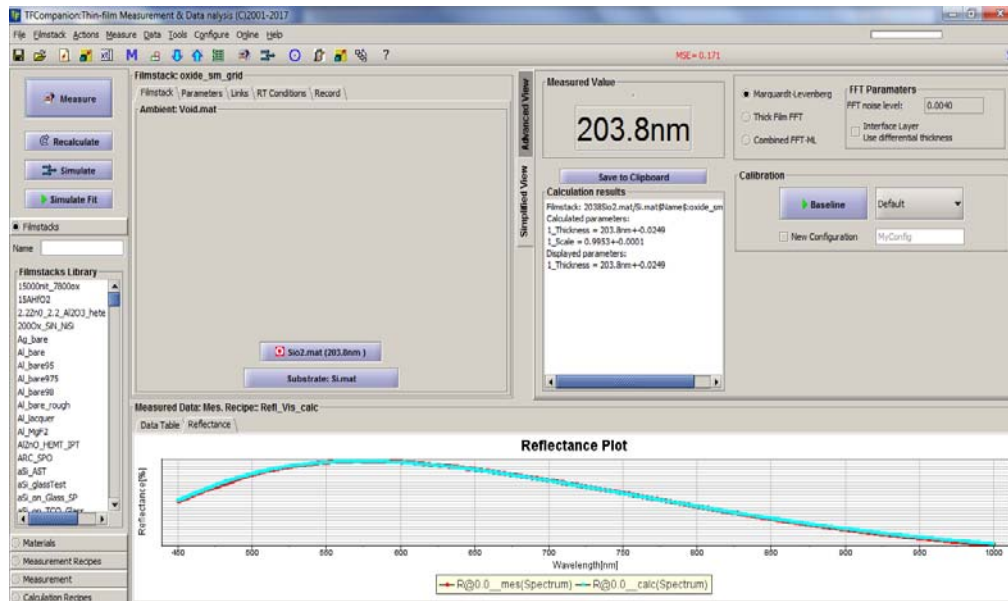


**Fig. 1.1 Results of the calibration/baseline for Visible system.**  
**Redline – reflectivity of the Si (reference sample), blue line –**  
**actual intensity measured by the system**

## b) Measurement

Optical measurement is indirect. Actual measured values are spectroscopic reflectance (or transmittance). A filmstack model that represents the measured sample structures is required to determine thickness and/or  $n$ & $k$  parameters of the layer(s). A suitable filmstack can be loaded from the database and adjusted to match the sample (it can also be build form the scratch using materials in the database)

**Place the sample on the stage. If the thickness of the substrate is different from the reference sample – adjust the position of the lens to focused position. Load or create a filmstack matching the sample structure and select the parameters to measure. Use MEASURE button to initiate the measurement. If you did not get good result – you can reuse the same measured data and fine-tune the filmstack and data analysis parameters. This can be done offline.**



**Fig.1. 2 Results of the measurement of SiO<sub>2</sub> coated Si wafer. The model fit the measured data and the thickness is determined from the measurement (203.8nm) is displayed**

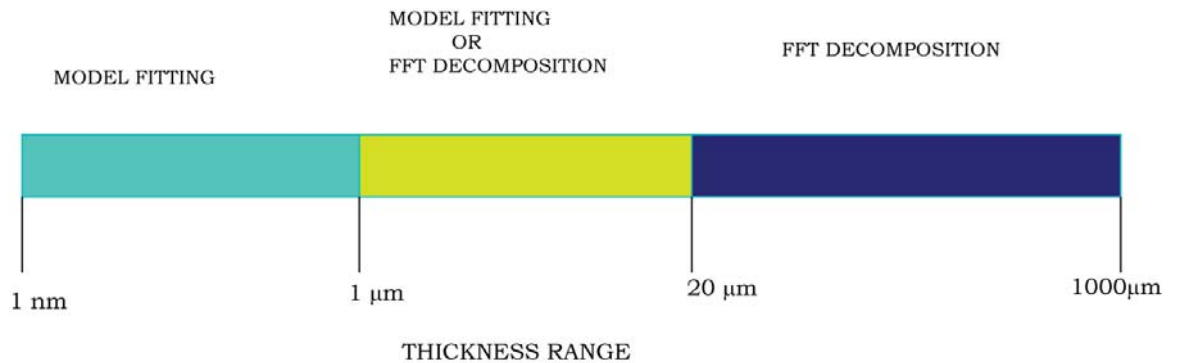
## Measurement recipe

The measurement process is controlled by a measurement recipe that should match the wavelength range and resolution of the spectrometer used. During first startup of the software standard recipe(s) are customized to match connected hardware. The most suitable recipe is automatically loaded during the startup. This can be changed manually. Calibration should match exactly to the recipe that is used for measurement (calibration recipe is generated automatically). If a different measurement recipe is used later, the mismatch error will appear – calibration need to be repeated.

## II. Software Overview

*MProbe® 20 uses TFCompanion -R advanced version. This software can be used standalone as well as with the hardware. Throughout this document –RE advanced version of the software is described. This version additionally support ellipsometry data analysis. Some features related to the ellipsometry measurement are not available in the –R version supplied with the system.*

The light spectrum reflected from the thin-film structure contains information about thicknesses, optical constants and interface roughness. By measuring the reflectance spectrum and analyzing this data MProbe® system is able to determine the parameters of the sample. There are two main methods of data analysis: curve fitting and FFT based thick film algorithm. In **curve fit** or **model fit** data analysis, parameters of the filmstack model are adjusted to achieve a good fit of the model to measured data. In **FFT/thick film algorithm** interference fringes structure is analyzed to determine the thickness of the layers-optical constants cannot be determined with this algorithm and it can be used only for thicker films (typically  $>1\ \mu\text{m}$ ).



**Fig. 2.1 Data analysis method based on the layer thickness**

The basic steps for any MProbe® measurement are selecting and/or editing filmstack structure (for measurement of known samples filmstack can be attached to a measurement recipe), taking calibration/baseline measurement and making measurement. The measurement itself includes

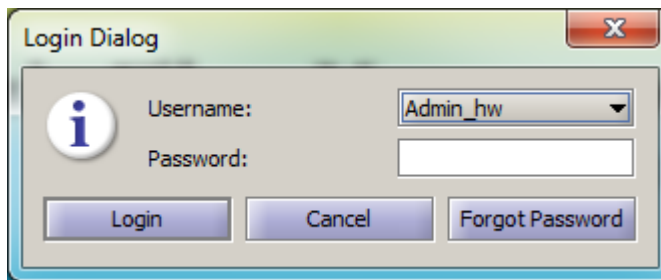


data acquisition and data analysis steps that can be performed seamlessly by the Measurement recipe.

The details of these steps and other functions of the software are detailed in the following pages.

Login dialog is appearing at software start up. Two default users: Admin\_hdw and Administrator are available. Default password: psw

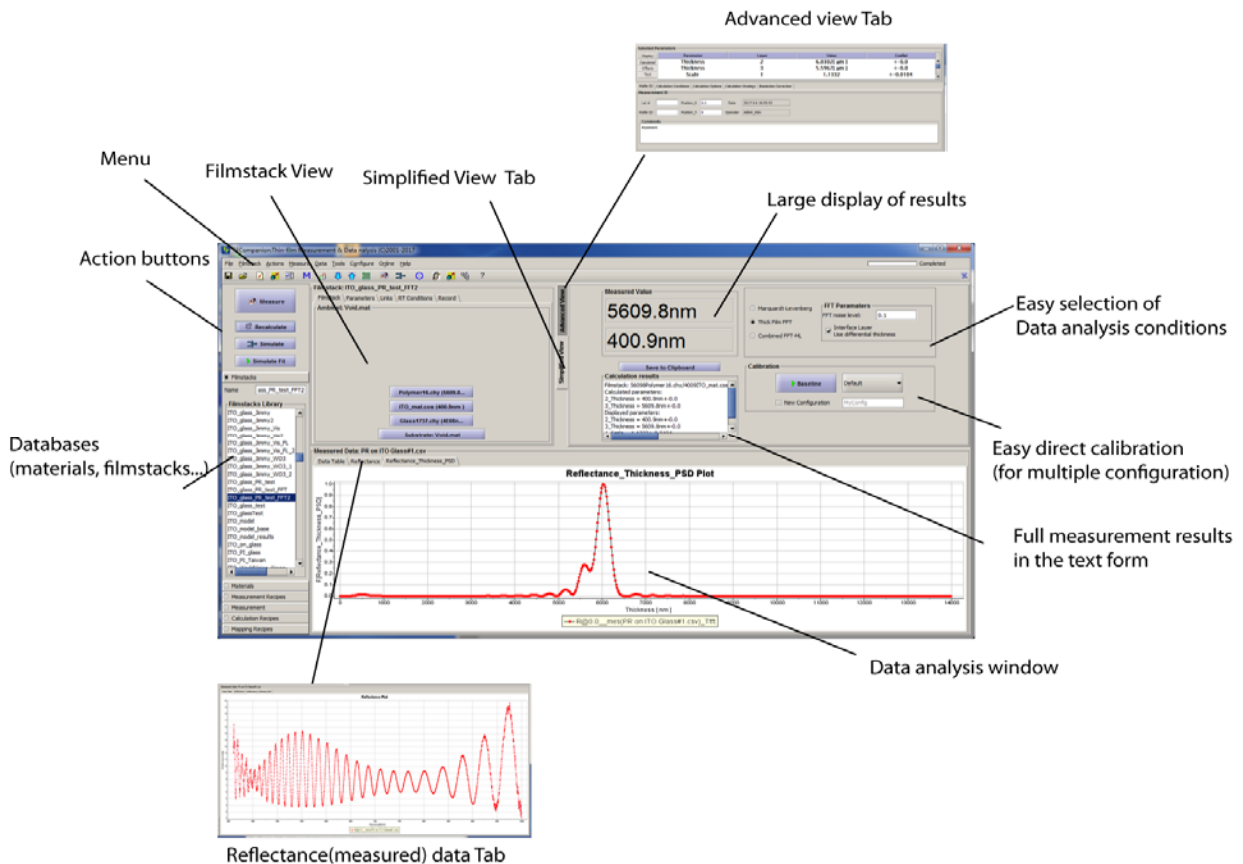
Using “Administrator” starts software in standalone mode (no hardware), “Admin\_hdw” starts in MProbe (hardware integrated) mode. Additional users can be created and assigned different access privileges.



**Fig. 2.2 Login dialog at start-up**

Standalone and MProbe software modes have the same user interface. MProbe mode interface has additional features related to measurement and hardware configuration.

Several optional software features are not included in the software build and can be installed as a separate plugins. Some of the plugins are Mapping, Dynamic measurement, Flash lamp control, optical switch control



**Fig. 2.3 Main window includes all the information needed during measurement and/or data analysis**

## **2.1 Main Window elements details**

### **2.1.1 Action Buttons**

- **Measure** - starts the measurement. Measurement is defined by the measurement recipe that is currently loaded.
- **Recalculate** – perform data analysis of the measured data
- **Simulate** – opens Simulation dialog that allows to generate/simulate data (like Reflectance/ Transmittance spectra) using current filmstack and different conditions
- **SimulateFit** – generate reflectance or transmittance spectrum (depending on the currently measured data) and overlay it over measured data, This feature is frequently used in filmstack development – to quickly see the effect of filmstack parameters change to the data.

### 2.1.2 Databases

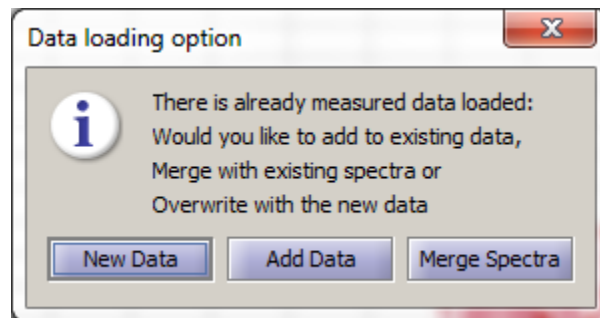
Several databases are available on the left side of the screen: Filmstacks, Materials, Measurement Recipes, Measurement, Calculation Recipes and additional databases depending on installed pluggins. All databases have context sensitive popup menu that is activated when item is selected and left-mouse button is pressed.

- Filmstacks database. Contains collection of filmstacks, new filmstack (created or imported) are also saved in this database. Popup menu has following items:
  - Review Filmstack – opens Filmstack Dialog with details of filmstack
  - Set Filmstack – loads selected filmstack. Double clicking the item is equivalent of this command
  - Delete Filmstack – permanently deletes filmstack from the database
  - Rename – allow to change filmstack name
  - Refresh – updates the list to show recently imported items
- Materials database. Contains collection of materials optical constants data. New materials (created or imported are saved to this database) Popup menu has following items:
  - Review/Edit - opens material dialog with details of material and ability to edit /modify the material
  - Add Layer - adds layer of selected material on top of current filmstack
  - Insert layer – insert the layer of selected material in user – specified location in the current filmstack  
**Note.** Double clicking on the item gives an option to select add or insert command
  - Delete Material – permanently deletes selected material from the database
  - Rename – allows changing the name of the material
  - Refresh – update the list of the materials from the database.
- Measurement recipes database contains currently available measurement recipes. New recipes can be created and saved in the database. Typically, one of the existing recipes is modified and saved under a different name. Popup menu has following items:
  - Review recipe - opens measurement recipe dialog with details of the recipe that allows to review/edit/ rename/save the recipe.
  - Load recipe – loads selected recipe and sets it as a current recipe. Double clicking on the item is equivalent of this command.

- Delete recipe – permanently delete selected recipe from the database
- Rename – allows changing the name of selected recipe
- Refresh - update the list of the recipes from the database
- Measurements database contains a list of measurements that were previously saved using File/Save Measured data from the main menu. Measurements are a reflectance and/or transmittance data.

Popup menu has the following items:

- Load measurement - loads selected measurement. Double clicking the item is an equivalent of this command. If there is measurement loaded of measured currently displayed – user is prompted to select on the option: New Data, Add data or Merge Spectra (this option is displayed only the cases when original and to be loaded data is defined in different wavelength ranges)



**Fig. 2.1.1 Loading data option**

- Delete measurement - permanently deletes selected data from the database
- Refresh - update the list of the items from the database
- Calculation Recipe database contains calculation recipes that were saved using File/Save calculation recipe. Calculation recipe normally includes filmstack and calculation conditions

Popup menu has the following items:

- Load recipe – load selected recipe. Double clicking on the item is equivalent of this action
- Rename – allows to change the name of the recipe
- Refresh - updates the list of the items from the database
- Mapping Recipes database contains mapping recipes that were created and saved in the mapping dialog. (This database is only available when the mapping plugin is installed)

Popup menu has the following items:

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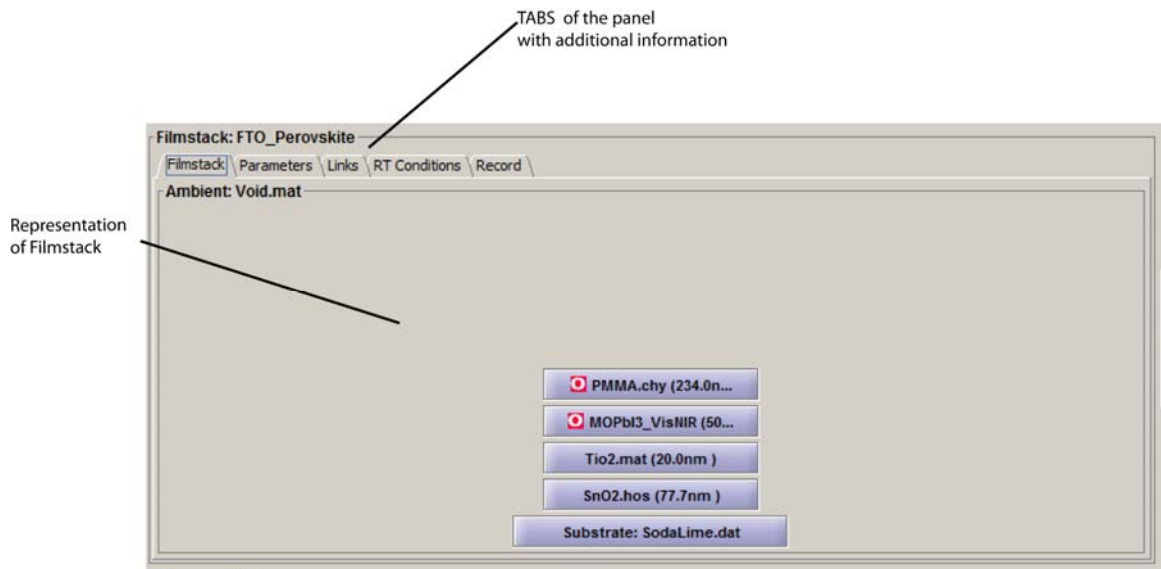
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- Review mapping recipe – opens Mapping Dialog to review/edit/save mapping recipe.
- Delete Mapping recipe – permanently deletes recipe from the database
- Rename – allows to rename selected recipe
- Refresh - updates the list of the items from the database

### 2.1.3 Filmstack Panel

For more details about filmstack please see [filmstack section](#)

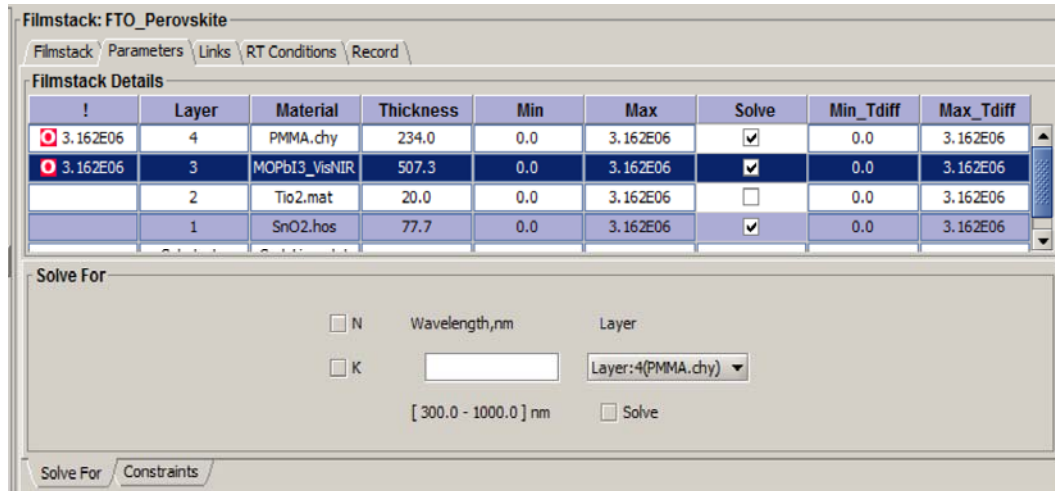


### 2.1.2 Filmstack main panel

Main filmstack panel has 5 tabs this all information related to filmstack.

- **Filmstack Tab** has graphic representation of the filmstack. Clicking on any layer of substrate – opens Layer/Material with relevant detailed information and ability to edit/replace the item.  
To change the ambient – right mouse-click new Ambient, Material dialog will open to enable change of the ambient material.

- **Parameters Tab**



### 2.1.3 Filmstack panel: Parameters Tab

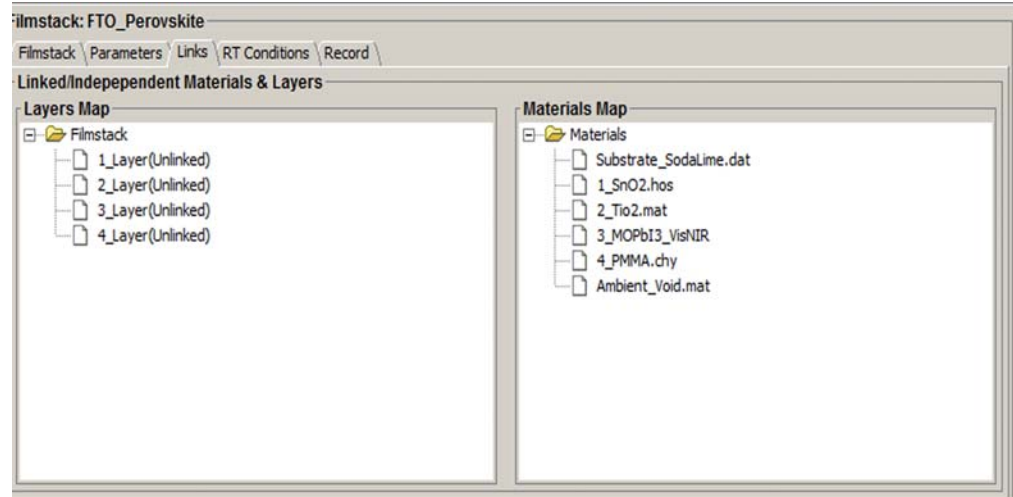
Parameters tab includes a table that lists all layer with their thicknesses and additional information.

Table includes following information:

- Column 1 : icon that shows special property of the layer is displayed. Special property can be Order Search or Incoherent layer. Otherwise – no icon is displayed
- Column 2: layer number
- Column 3: Material name
- Column 4 : current thickness of the layer (in currently selected units)
- Columns 5 and 6 are minimum and maximum constraints on the thickness of the layer
- Column 7 – Solve checkbox. If the checkbox is selected - thickness is set as a calculated/Displayed parameter
- Column 8,9 – minimum and maximum constraints on the thickness when Differential FFT method is used

The bottom **SolveFor** Tab/Panel is designed for quick access n&k parameters display. n and/or k value can be selected in the checkbox and wavelength entered in the text field. In case of MProbe (spectroscopic reflectance) and in most other case, n & k can be determined only through the use of parameterized materials. When layer with parameterized material is selected and “Solve” check box is checked – a list of material parameters that can be determined is displayed (use can select parameters to calculate). N & K a designed as a display parameters and they are calculated through parameterized

material. In ellipsometry measurement –  $n, k$ , values can be measured directly, in some cases however using parametrized materials is always preferred. The bottom **Constraints tab/panel** consolidate constraints of all the parameters in one place, except thickness.



#### 2.1.4 Filmstack Panel: Links

This panel allows to change the status of the layer or / and material from default unlinked to linked and display the current status.

Each layer in filmstack has at least two components: material and thickness. By default each parameter in each layer is determined independently. In some situations, filmstack has multiple layer with the same material. When materials in different layer are linked their optical constants are determined together (only exact same materials can be linked). When layer are linked – both material of the layer and thickness are linked.

Filmstack: FTO\_Perovskite

Filmstack Parameters Links RT Conditions Record

Reflectance/Transmittance correction coefficients

Use	Parameter	Value	Min	Max	Display	Fit
<input type="checkbox"/>	1_Rough	0.0	1.00	3.162E07	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/>	1_Scale	0.7669	0.0	3.162E07	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
<input type="checkbox"/>	2_Offset	1.00	0.0	3.162E07	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	2_Dull	0.0	0.0	1000.00	<input type="checkbox"/>	<input type="checkbox"/>

#### 2.1.5 Filmstack Panel: RT Condition

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There are four RT parameters: Roughness, Scale, Offset and Dullness. These parameters can be used to correct “imperfections” of the filmstack or measurement conditions.

To enable parameter setup one need to check the “use” check box (Column 1)

Starting value of the parameter is set in Column 3 “Value”. Columns 4 & 5 are used to set minimum and maximum constraints on the value of the parameters.

To activate the use of the parameter – check the box in the “Display” column. This will include parameter value in the model calculation. To make parameter adjustable during the calculation (fit parameter) – check the box in the fit column.

**Roughness** parameter corrects for light scattering that is causing wavelength dependant light attenuation (increased attenuation at shorter wavelengths)

**Scale** parameter corrects for small light intensity variations e.g. the difference in light intensity due to change in the distance during calibration and measurement

**Offset** parameter corrects for a large offset of reflectance due calibration or distance issues

**Dullness** parameter is somewhat similar to Roughness but it is not wavelength dependent. It can be used to correct the measurement of the samples that have extra light attenuation without scattering. For example, unpolished metal.

The screenshot shows a web interface for a 'Filmstack' record. At the top, the title is 'Filmstack: FTO\_Pervskite'. Below the title is a navigation bar with tabs: 'Filmstack', 'Parameters', 'Links', 'RT Conditions', and 'Record'. The 'Record' tab is currently selected. The main content area displays the record details for 'FTO\_Pervskite'. It includes fields for 'Name' (FTO\_Pervskite), 'Last Modified' (2016, 7:08:31 PM), 'Owner' (Administrator), and 'Access' (public access). Below these fields is a 'Comments' section with a 'Comment' label and a large text area for entering comments.

## 2.1.6 Filmstack record tab

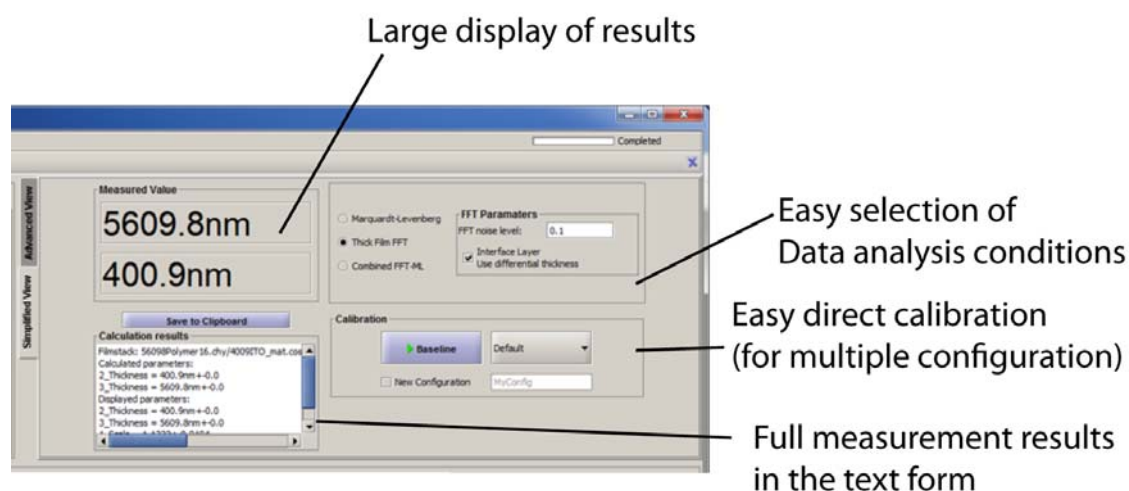


Includes information about the filmstack that is available in the database, such comments, last modified and owner.

## 2.1.4 View Panel

View panel includes measurement results and basic measurement conditions.

There are, actually, two view panels with overlapping functionality: **SimplifiedView** and **AdvancedView**.



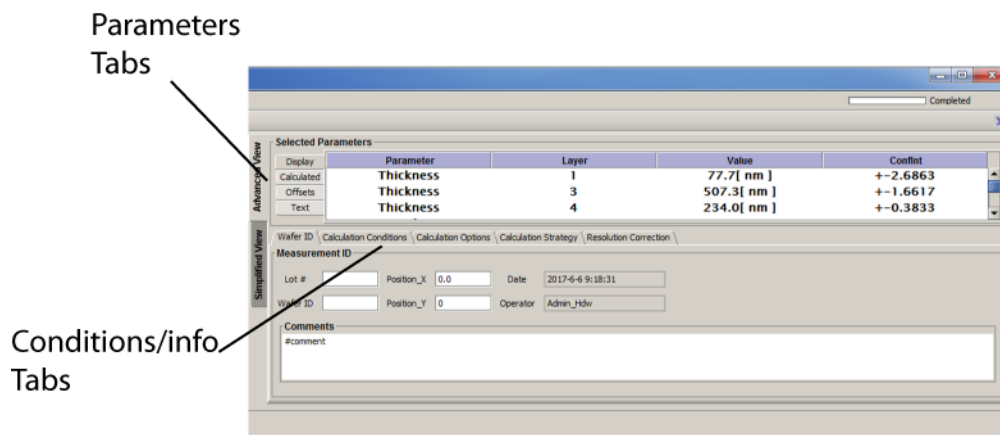
**Fig. 2.1.7 SimplifiedView Panel**

**SimplifiedView** panel includes results display of only up to 2 thicknesses – it does not show other parameters. Full measurement results are displayed in the text form and can be copied to the clipboard.

**Calibration Panel** can be used to create new calibration using Baseline button and follow two steps procedure as prompted. The active calibration defined in the drop-down box will be overwritten. It is possible to have several active calibration for different system configurations however, one calibration is used for MProbe 20 in most practical cases (different calibrations corresponding to different focusing lenses can be used in MProbe 40). To create a separate calibration (in addition to default calibration) select New Configuration check box, type in the name in the text box and click Baseline button.

**Calculation Options** panel allows to select one of the calculation options: Marquard-Levenberg minimization (curve fitting), FFT (thick film algorithm) or a combination of the FFT-ML.

**Advanced View** panel includes most of the information from the SimplifiedView panel (except calibration/Baseline) and additional options.



**Fig. 2.1.8 AdvancedView Panel**

**Advanced View** has two panels Parameters (4 tabs) and Conditions/Info (5 tabs).

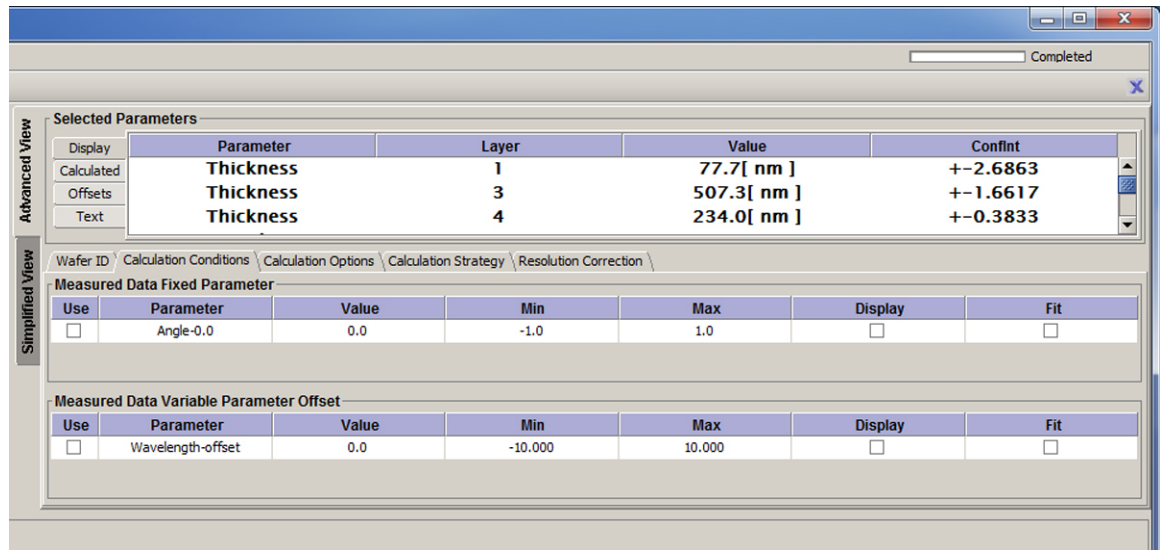
*Selected Parameter Tabs/Panels : Displayed, Calculated, Offsets, Text.*

Each parameter can have *Displayed* and/or *Calculated* property. The difference between these properties is easy to explain on an example of parameterized material: we directly calculate coefficients of the parameterized equation but, frequently, want to display corresponding n,k values (that are calculated indirectly). If parameter is both calculated and displayed, as thickness is, in most cases – it is listed in both Tabs. For each parameter - name, layer, value and confidence interval are displayed.

*Offset Tab/Panel* has a list of all displayed parameters with option to define an offset to the value. This offset can be used to correct displayed value i.e. defined offset is added to an actually measured value for display. *Text Tab/Panel* is the as the similar panel is SimplifiedView and displays all measured parameters.

*Conditions/Info Tab* panels: WaferID, Calculation Conditions, CalculationOptions, Calculation Strategy, Resolution Correction

*WaferID* panel includes information about Sample ID, Sample lot, measurement position (x,y) and comments. This information is stored with the measurement, Sample ID and lot are also displayed in the Measurement history.

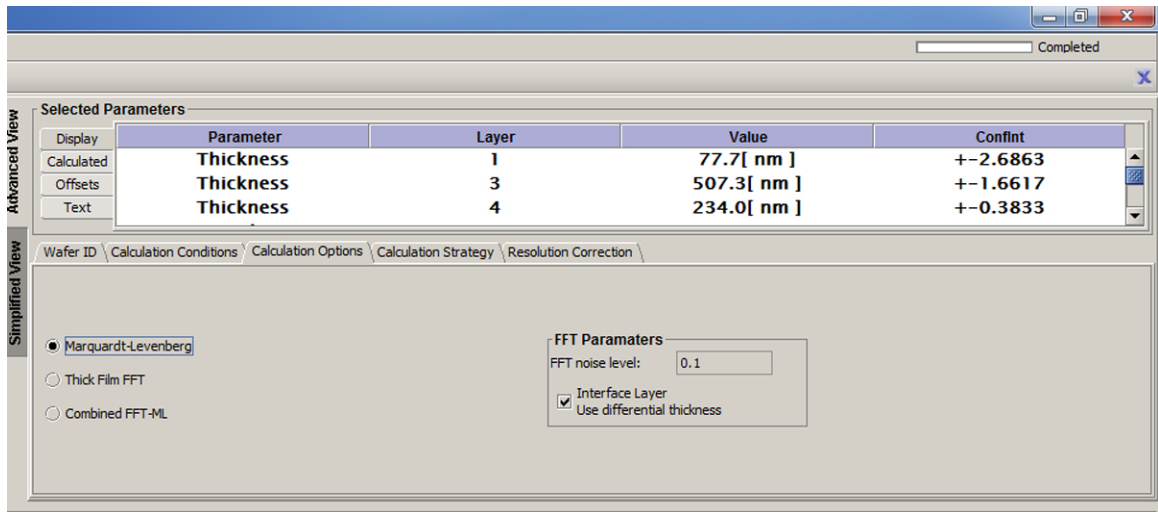


**Fig. 2.1.9 Calculation Conditions panel**

*Calculation Conditions* panel allows to add correction to fixed and variable spectrum parameters. In case of spectroscopic reflectance – fixed parameter is always the angle of incidence and variable parameter is wavelength. Fixed parameter – AOI or wavelength offset can be selected as a calculated/ measured value. This option is not used with MProbe 20 system.

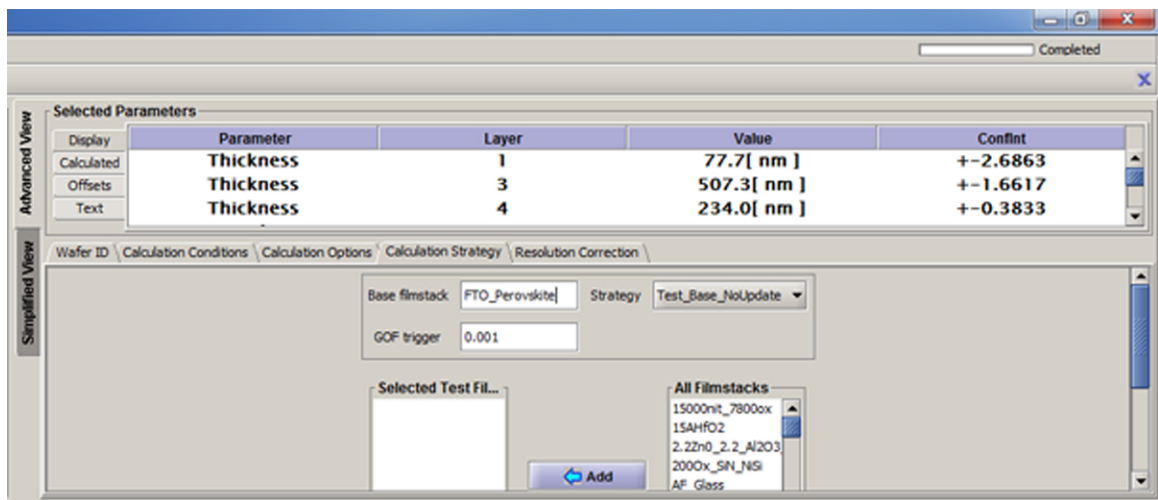
Like in all cases of correction parameters, use check box to enable parameter, minimum/maxium constraints limit the range parameter variation, display check box includes parameter value in the model calculation and fit checkbox enable it as a measured/fitted parameter. In case of in-situ measurement when oblique measurement is used, the AOI maybe no known very precisely. The common strategy is to use AOI as a measured/fitted parameter on the known sample like Si. After AOI is determined accurately, it can be fixed.

Wavelength offset is rarely used, mostly for debugging problem with high resolution spectrometers when measuring thick films.



**Fig. 2.1.10 Calculation options panel**

*Calculation options* panel is the same as in the **SimplifiedView**



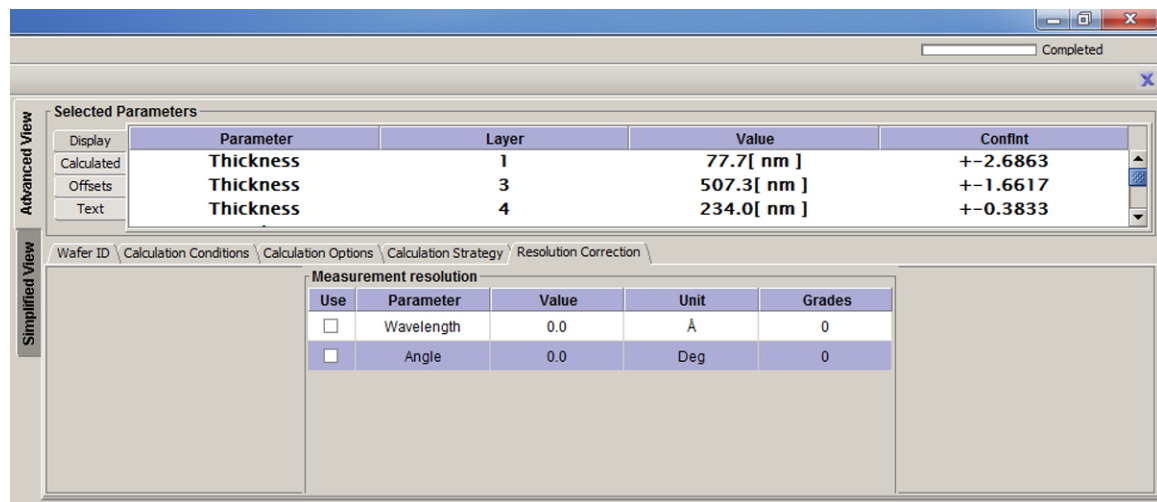
**Fig. 2.1.11 Calculation Strategy panel**

*Calculation Strategy* can be used in the cases when multiple samples or multiple points are measured (Production Batch, Dynamic Measurement, inline measurement) and filmstack can be different at different points.

*Calculation Strategy* panel allows to select a set of filmstacks that cover potential measurement points/samples and a strategy. Filmstacks are added from the database, strategy is selected from the drop down box and GOF trigger to determine if filmstack is suitable/measurement successful entered manually in the text box.

There are three strategy options:

- Base\_Test\_Update - if using base filmstack for data analysis is successful, update this filmstack parameters to the latest measured values
- Base\_Test\_NoUpdate - if using base filmstack for data analysis is successful, do not update it – use the original filmstack for next calculation.
- Test\_Update\_BaseUpdate - if using Base filmstack was not successful and another filmstack was selected, switch successful filmstack as a base.



## 2.1.12 Resolution Correction panel

*Resolution Correction panel* allows to add wavelength and angle resolution to the model calculation. Angle resolution is referred to a convergent cone angle of light striking the sample. Number of grades (typically 10) is referred to a number of slices the resolution value is divided into during the calculation.

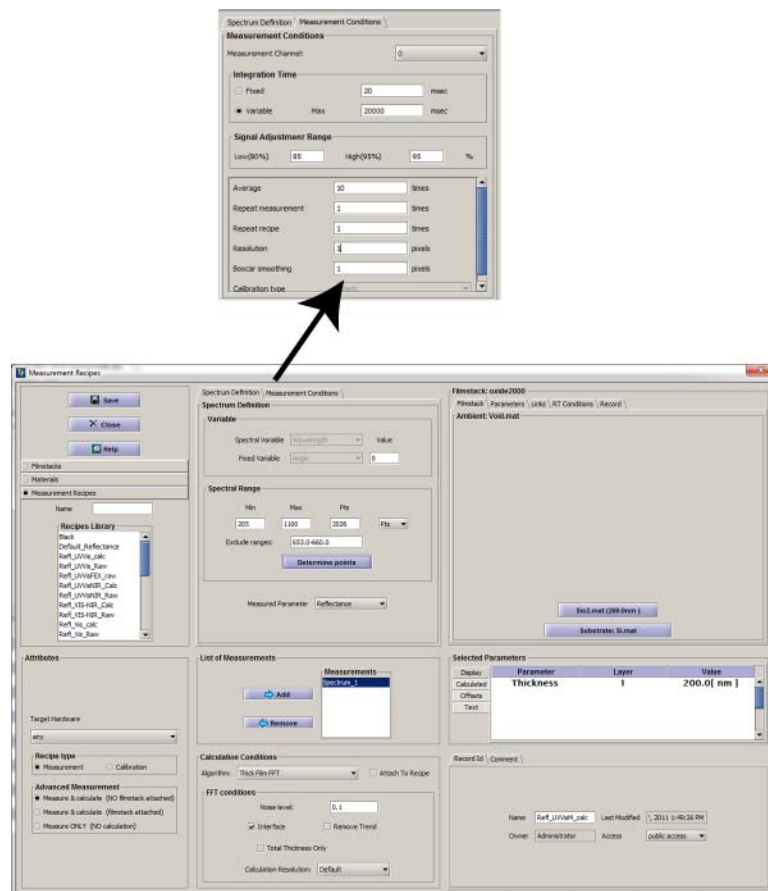
*This option is not , typically, used for MProbe 20 system.*

## 2.2 Measurement Recipe Dialog

### What is measurement recipe?

The measurement process is controlled by a measurement recipe that should match the wavelength range and resolution of the spectrometer used. During first startup of the software standard recipe(s) are customized to match connected hardware. The most suitable recipe is automatically loaded during the startup. This can be changed manually. Calibration should match exactly to the recipe that is used for measurement (calibration recipe is generated automatically). If a different measurement recipe is used later, the mismatch error will appear – calibration need to be repeated.

To start dialog, select Measurement recipe record in the database, right-mouse click and use “Edit”.



**Fgi. 2.2.1 Measurement recipe dialog.**

Measurement recipe includes five elements: Spectrum Definition, Measurement Conditions, Attributes, Calculation Conditions and Filmstack. Spectrum Definition defines measured spectrum. One measurement recipe can include several spectra corresponding to different spectrometer channels.

**2.2.1 Spectrum definition:** wavelength range, number of points and measured parameter.

Wavelength range can be entered manually. If the target MProbe system or spectrometer is currently connected – number of available pixels (points) can be automatically calculated using *Determine Points* button. Some parts of the wavelength can be excluded to remove large peaks (e.g. in the case of De lamp  $\alpha$ -line) by entering data in exclude range in nm in text box. For example, 653-660 will excluded 653-660nm wavelength range from the measured spectrum. Several excludes range can be added, separated by comma.

**2.2.2 Measurement Conditions**

Include following parameters, the values are pre-populated and can be edited/

- Channel: the spectrometer channel as defined by spectrometer driver is selected in drop-down box. MProbe system has always channel =0. (Some spectrometers like StellarNet has always channel=1)
- Integration time: fixed or variable can be selected. Variable integration time (default) allows software to adjust time to achieve the maximum signal (ADC range). In this case, measurement of different samples or different point on the sample can be done using best signal/noise. The acceptable ADC % range can be set in the recipe.
- Signal Adjustment range is used in case when Variable integration time is selected. Typical range is 80%-92% of the ADC.
- Average – defines the number of signal averages performed in spectrometer driver. Typically, 10 averages are used in desktop measurements
- Repeat measurement – has the same averaging effect (as Average above ) but it also calculates actual standard deviation and add it to the measured data. *Typically, not used with MProbe system*

- Repeat recipe – similar to Repeat measurement but, in case of variable integration time, time is adjusted for each measurement. *Typically, not used with MProbe system*
- Resolution – number of pixels read independently, e.g. 2 mean that each 2 pixels will be averaged
- Boxcar smoothing – signal smoothing performed by spectrometer driver. For example, during measurement of thin films (< 1µm) high-wavelength resolution is frequently not required. In this case, smoothing of 5 pixels helps reduce the noise without effecting accuracy.

Once Spectrum definition and Measurement conditions and defined – new spectrum can be added to the list using *Add* button. Variable Integration time and 10 averaging is, typically, used for standard desktop measurement. Fixed time and no averaging is used for inline and, frequently, mapping to reduce the data acquisition time.

### **2.2.3 Attibutes** define the type of the measurement recipe

Recipe can be:

- Measure and calculate (No filmstack). This means that filmstack is not defined in the recipe but loaded independed. Data acquisition and data analysis are performed.
- Measure and calculate (Filmstack attached). Name of the Filmstack is attached to the recipe and it is loaded from the database when recipe is loaded. Data acquisition and data analysis (using attached filmstack)are performed.
- Measure only (no calculation). Only measurement is performed. Data analysis can be done at a later time.

Names of recipes that perfume only data acquisition, typically, end with `_raw`, other recipes names ends with `_calc`

The recipe can also be either for “Measurement” or “Calibration”. Calibration recipes are, typically, created automatically when Baseline is selected.

Only special calibration recipe are created manually. The main case for special recipes is using two separate recipes for reference sample and black pad. This is needed when system is remotely controlled by third party software (e.g. via Modbus or PLC). In this situation, time need to be given place reference wafer and black pad and this is easily accomplished using two separate recipes.

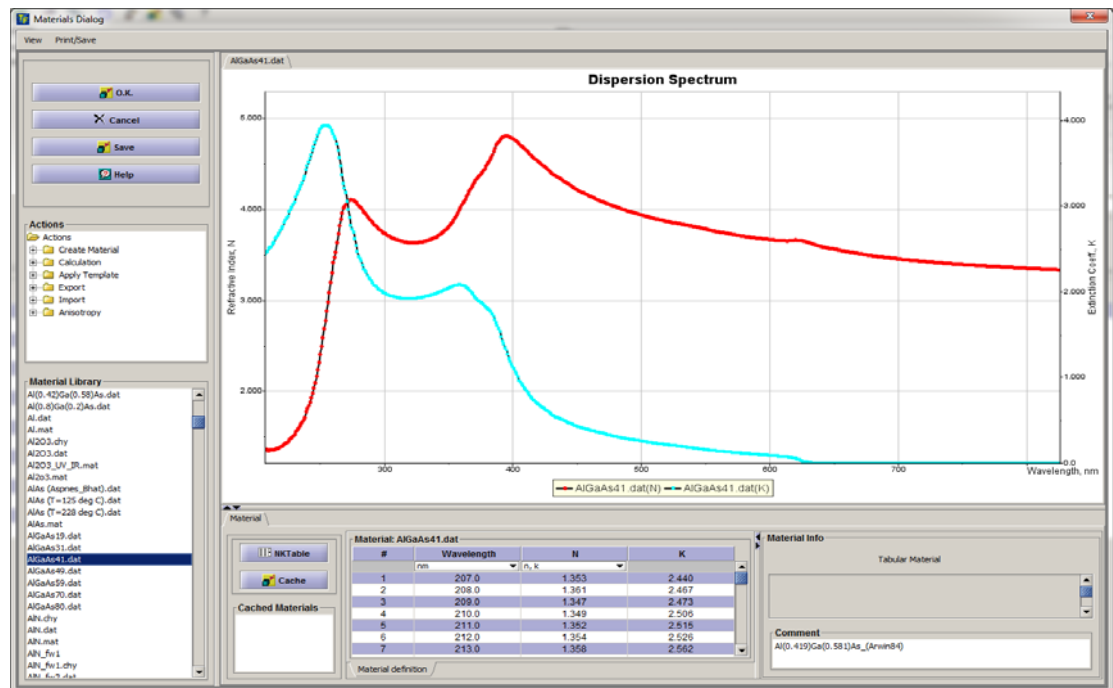


#### **2.2.4 Filmstack**

Measure and calculated (filmstack attached) is the only type of the measurement recipe that defines that filmstack is attached. In all other cases, filmstack is ignored. To attach the filmstack, select a record in the Filmstack database, right-mouse click and select *setFilmstack*. Filmstack needs to be created beforehand, calculation parameters selected and saved to the database. There is a full Filmstack panel (as in the main screen) in the Recipe Dialog that allows to review all the details of the filmstack. However, any changes entered here will not be saved – only the name of the filmstack is attached to the recipe, so filmstack is always loaded from the database.

## 2.3 Materials Dialog

Material is a basic building block of the filmstack model. For the purpose of MProbe measurement, material is defined by optical dispersion i.e. a set of optical constants ( $n$  &  $k$ ) at specified wavelengths. Optical dispersion can be defined as a fixed table of  $n, k$  values (Tabular materials) or as a wavelength dependent formulae with several variable parameters (Parameterized materials) or a physical mixture of 2 or 3 materials (Effective Medium Approximation – EMA material) or Compound material – a set of Tabular materials corresponding to different fixed compositions of the material (other compositions are interpolated). EMA and Compound materials are considered parameterized materials, as well. So two basic material type are **Tabular** and **Parameterized**.



**Fig. 2.3.1 Materials Editor Dialog**

To start Material Dialog, use *Tools/Materials Editor* from the main menu. Alternatively, right-mouse click on the material's record in the database and select "Review Selected Material"

**Note.** Layer Dialog has full functionality of the Material Dialog and can be started by clicking on the layer in the filmstack model.

**Material Dialog** allows performing the following functions:

- Save /Rename materials
- Edit existing materials
- Create new materials
- Fit parameterized material to existing Tabular (finding initial values);
- Render graphical representation of optical dispersion ( NK vs. wavelength)
- Calculate NK values for the parameterized materials (Cauchy, EMA etc.)
- Export and Import materials data in/to text format.

### **2.3.1 Saving material**

Saving materials to the database is a 2-step process. Use the Save button – you will be prompted to enter materials name. Material is temporary saved but not committed. Using O.K. button will commit material to the database and close the dialog. If Cancel button is used on the 2<sup>nd</sup> step – all changes will be rolledback (material is not saved) and dialog is closed

### **2.3.2 Editing existing material**

Material can be manually edited in the material definition table, all editable parameters can be edited/changed and comments added. In case of the parameterized materials there are two additional options available

- **NK Table** button allows to display parameterized material as a tabular material for more close review
- **Displayed OC** allows to define optical constants at specified wavelength as “displayed” during data analysis.

### **2.3.3. Create new material**

Select the material type from the **Create Material** branch of the Actions tree, set the name of the material, and an instance of the material initialized to default values will be created and displayed.

Now material's parameters values can be edited - dispersion plot data will be updated accordingly.

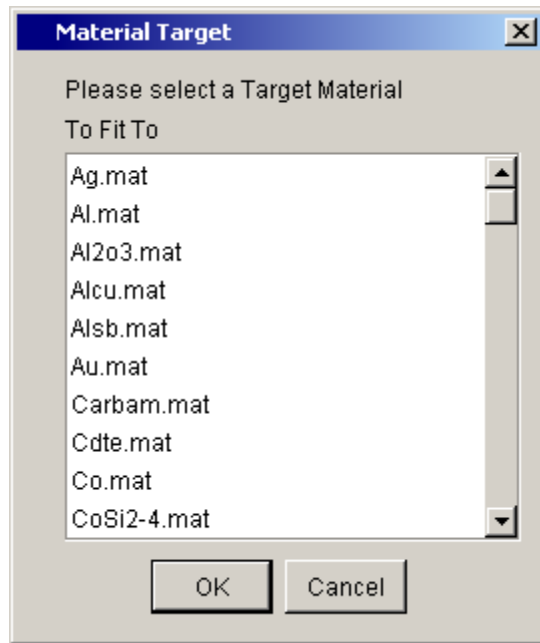
Following types of the materials can be created:

- Tabular material
- Compound Material
- Sellmeier material (2 versions)
- Cauchy material (3 versions)
- EMA (3 versions)
- Basic dielectric material (Hartman, Conrady, SchottBriot)
- Oscillator materials
  - Forouchi – Boomer amorphous model
  - Forouchi – Boomer amorphous & oscillator model
  - Adachi oscillator model
  - Afromovitz oscillator model
  - Drude –Lorentz oscillator model
  - Harmonic oscillator model
  - Tauc-Lorentz oscillator
  - Tauc-Lorentz Drude oscillator
  - CP Exciton oscillator
  - Cody-Lorentz oscillator
  - Cody-Lorentz-Urbach oscillator
  - Classical oscillator
  - Lorentz-Drude IR oscillator

#### **2.3.4 Fit parameterized material to existing material**

To set starting value of the parameters of selected or newly created Parameterized material, one can “fit” it to the known material’s optical dispersion. This process can be done in two steps:

- Select parameters that need to be fitted.  
In the Action tree, select *Calculation/Show Parameters*. Check the boxes next to parameters that need to be fitted.
- Select the target material. In the Action tree, select *Calculation/Fit To Material* – the list of available materials will appear. Select the target material from the list and click OK. This will start the fitting procedure.



**Fig. 2.3 2. A list of available “target” materials**

After the fitting procedure is completed, fitted parameters assume new values and dispersion curves (of the fitted and target material) are shown on the plot.

**Note.** Sometimes, fitting process need to be repeated couple of times to achieve the best fit.

### 2.3.5. Graphical representation of dispersion curves

Tabular and Plot sections of Material dialog are separated by a moveable border- use the mouse to drag it up/down and change the size of the visible section. The table is synchronized with the Plot. By default, both **n** and **k** dispersion plot are shown; one can select either **n**, or **k** or both dispersion plot(s) using **View** menu


### 2.3.6 NK values of parameterized materials.

To display NK values of the parameterized material select **NKTable** button. This will create a temporary tabular material calculated from the current parametric representation. To return back to the original parameterized representation, toggle the same button again.

To review NK values (without displaying them in the table) – move the mouse over the dispersion curve and corresponding values will be displayed in the popup.

### 2.3.7 Export and Import materials data in/to text format

Export/import of the materials in two text (ASCII) formats – SOPRA and TFCompanion are supported. Use Export/Import branches of the Action tree. The selection will invoke a File Chooser to navigate to the appropriate directory to save or read the file.

 Imported material is stored only in memory. To add it to the database use the Save button.

### 2.3.8 Loading another material

One can select another material without exiting Material Dialog. In order to do this – select material' record in materials database list (side panel) and use one of the options:

- **Set To Table** – this option loads selected material and sets it in **Material Dialog**
- **Add To Plot** – this option does not change the material displayed in **Material Dialog**; it only adds dispersion of the selected material to the plot – to compare with the current material

### 2.3.9 Printing and Saving dispersion plot

Use Print/Save menu to print plot or save it to image file.

### 2.3.10 Caching material data

To cache current material data use **Cache** button. A copy of the material is saved to memory and will be available during the current session. The record appears in the list box below the button. Double-clicking the record can retrieve cached material.

### 2.3.11 Parameterized materials

Parameterized materials allow to approximate spectral dispersion of the optical parameters as a smooth function of the wavelength and few parameters. This approach allows reducing the number of calculated parameters (in most cases) and better representing real life material properties. At the same time, Parameterized materials need to be used with caution; if filmstack is not accurate or too many parameters are calculated (or limited measurement data is available) – Parameterized materials may give unphysical results. This is especially true in the cases when empirical equations are used (e.g. Cauchy, etc.). TFCompanion supports most of the commonly used Parameterized materials and new materials are continuously being added. Following are the currently available material types:

1. **Cauchy** material type. Cauchy coefficients (N<sub>0</sub>, N<sub>1</sub>, N<sub>2</sub>) are selected using commonly used convention of Wavelength in um.

$$n(\lambda) = N_0 + \frac{N_2}{\lambda^2} + \frac{N_4}{\lambda^4}$$

N<sub>0</sub>, N<sub>2</sub>, N<sub>4</sub> are coefficients and λ is wavelength in um. The default Cauchy coefficients correspond to SiO<sub>2</sub> material.

2. **CauchyK** material type. CauchyK is extension of the Cauchy material type to support absorbing materials. It is frequently used for quasi-dielectric materials that have smooth and weak absorption e.g. due to doping or other impurities.

$$\begin{aligned} n(\lambda) &= N_0 + \frac{N_2}{\lambda^2} + \frac{N_4}{\lambda^4} \\ k(\lambda) &= K_0 + \frac{K_2}{\lambda^2} + \frac{K_4}{\lambda^4} \end{aligned}$$

N<sub>0</sub>, N<sub>2</sub>, N<sub>4</sub>, K<sub>0</sub>, K<sub>2</sub>, K<sub>4</sub> are coefficients and λ is wavelength in um

3. **CauchyExp** material type. CauchyK is extension of the Cauchy material type to support absorbing materials with sharper absorption edge then CauchyK can represent. In most cases, Tauc-Lorentz oscillator materials type gives a better solution then this approximation – it is used only in special cases, e.g. when the spectral range is limited.

$$\begin{aligned} n(\lambda) &= N_0 + \frac{N_2}{\lambda^2} + \frac{N_4}{\lambda^4} \\ k(\lambda) &= K_0 * \text{Exp}[-(\lambda - K_2) / K_4]^3 \end{aligned}$$

$N_0, N_2, N_4, K_0, K_2, K_4$  are coefficients and  $\lambda$  is wavelength in  $\mu\text{m}$

4. **Sellmeier** material approximation. Sellmeier approximation is traditionally used for representation of glass dispersion.

$$n = \sqrt{1 + \sum_{i=0}^k \frac{A_i \lambda^2}{(\lambda^2 - L_i^2)}}$$

$A_i, L_i$  coefficients  $i=0, \dots, k$  – number of nodes  $\lambda$  is wavelength in  $\mu\text{m}$

5. **Sellmeier2** material approximation. Extension of Sellmeier approximation to represent spectral dispersion of oxides in wide spectral range, introduced in

C.M. Herzinger, B. Johns, etc. "Ellipsometric determination of optical constants for silicon and thermally grown silicon dioxide via multisample multi-wavelength, multi-angle investigation" J. Appl. Phys. v. 83, No.6, 1998 pp.3323-3336

$$n = \sqrt{A_0 - C \lambda^2 + \sum_{i=0}^k \frac{A_i \lambda^2}{(\lambda^2 - L_i)}}$$

$A_0, C, A_i, L_i$  coefficients,  $i=0, \dots, k$  – number of nodes,  $\lambda$  is wavelength in  $\mu\text{m}$

6. **Harmonic Oscillator (HOA)** material approximation is used to represent dispersion of crystalline and polycrystalline materials e.g. Si, micro or polycrystalline Si, SiGe, AlGaAs, etc.

$$\varepsilon(E) = 1 + \sum_{n=0}^k A_n e^{-i\theta_n} * \left( \frac{1}{E + E_n + i\Gamma_n} - \frac{1}{E - E_n + i\Gamma_n} \right);$$

$A_n, E_n, \Gamma_n, \theta_n$  are coefficients,  $n=0, \dots, k$  is number of oscillators (maximum is  $k=9$ ),  $E$  is wavelength in eV,  $\varepsilon$  is dielectric constant

7. **Critical Point Exciton (CPE)** material approximation is an extension HOA model that is used to represent dispersion of various polymer materials (PMMA, F65, PFO, F8BT, Dow Red F, etc.)



$$\varepsilon(E) = UVterm - \sum_j A_j e^{i\theta_j} (E - E_j + i\Gamma_j)^n$$

**UVterm**,  $A_j$ ,  $E_j$ ,  $\Gamma_j$ ,  $\theta_j$  are coefficients,  $j=0,...,k$  (maximum  $k=9$ ),  $n$  –determines the type of the critical point (selected by the user);  $n$  represents dimensionality of the critical point;  $n=-1$  corresponds to discrete excitons,  $n=-1/2$  corresponds to 1D critical points,  $n=0$  corresponds to 2D critical point (logarithmic),  $n=1/2$  corresponds to 3D critical point.  $E$  is wavelength in eV,  $\varepsilon$  is dielectric constant. CPE model sometimes also called “Phase relaxed Lorentzian” when  $n=-1$ ,  $k=1$  (e.g. H.Arwin, R. Jansson Electrochimica Acta, 39:211-215, 1993)

8. **Tauc-Lorentz oscillator (TLO)** materials approximation is widely used to represent dispersion of amorphous materials, especially in the areas near absorption edge(e.g. SiN, aSi, HfO<sub>2</sub>, etc.).

$$\varepsilon_2(E) = \frac{AE_0C(E-E_g)^2}{((E^2-E_g^2)^2+C^2E^2)E},$$

for  $E > E_g$

$$\varepsilon_1(E) = \varepsilon_{inf} + \frac{1}{2} \frac{A}{\pi} \frac{C}{\xi} \frac{a_h}{\alpha E} \ln \left[ \frac{(E_0^2+E_g^2+\alpha E_g)}{(E_0^2+E_g^2-\alpha E_g)} \right] - \frac{A}{\pi \xi} \frac{a_{tan}}{E_0} \left[ \pi - \alpha \tan \left( \frac{2E_g+\alpha}{C} \right) + \alpha \tan \left( \frac{-2E_g+\alpha}{C} \right) \right] +$$

$$2 \frac{AE_0C}{\pi \xi \alpha} E_g (E^2 - \gamma^2) \left[ \pi + 2\alpha \tan \left( \frac{\gamma^2 - E_g^2}{\alpha C} \right) \right] - 2 \frac{AE_0C}{\pi \xi} \frac{E^2 + E_g^2}{E} \ln \left( \frac{|E-E_g|}{E+E_g} \right) +$$

$$2 \frac{AE_0C}{\pi \xi \alpha} \frac{E^2 + E_g^2}{E} E_g \ln \left[ \frac{|E-E_g|(E+E_g)}{\sqrt{(E_0^2 - E_g^2) + E_g^2 C^2}} \right], \text{ where}$$

$$a_h = (E_g^2 - E_0^2)E^2 + E_g^2 C^2 - E_0^2(E_0^2 + 3E_g^2);$$

$$a_{tan} = (E^2 - E_0^2)(E_0^2 - E_g^2) + E_g^2 C^2;$$

$$\xi = (E^2 - \gamma^2)^2 + \frac{\alpha^2 C^2}{4};$$

$$\alpha = \sqrt{4E_0^2 - C^2};$$

$$\gamma = \sqrt{E_0^2 - C^2}/2;$$

Adjustable parameters:  $A, C, E_0, E_g, \varepsilon_{inf}$ .

Reference: G.E.Jellison and F. Modine "Parameterization of the optical functions of amorphous materials in the interband region., Appl.Phys.Lett. 69(3),1996

9. **Tauc-Lorentz-Cody oscillator (TLC)** material approximation is an extension of TLO that mitigates the problems of representing sharp absorption edge in deep UV The model was introduced in A.C. Ferlauto et. al J.Appl. Phys. 92, 2424 (1994)

$$\begin{aligned}\varepsilon_2 &= G(E) * L(E) \\ G(E) &= \frac{(E - E_g)^2}{(E - E_g)^2 + E_p^2}; \\ L(E) &= \frac{AE_0 CE}{(E^2 - E_0^2)^2 - C^2 E^2}\end{aligned}$$

10. **Tauc-Lorentz-Cody-Urbach oscillator** is an extension of TLC to represent weak absorption in the band-gap region using Urbach tail. A.C. Ferlauto et. al J.Appl. Phys. 92, 2424 (1994)

$$\begin{aligned}\varepsilon_2 &= \begin{cases} \frac{E_t}{E} \exp(\frac{E - E_t}{E_s}); 0 < E \leq E_t (\text{Urbach tail}) \\ G(E) * L(E); E > E_t (\text{Cody-Lorentz}) \end{cases} \\ G(E) &= \frac{(E - E_g)^2}{(E - E_g)^2 + E_p^2}; \\ L(E) &= \frac{AE_0 CE}{(E^2 - E_0^2)^2 - C^2 E^2}\end{aligned}$$

11. **Lorentz-Drude oscillator** material approximation is an extension of HOA model to represent absorption in the IR part of the spectrum. Specifically, it takes into account the impact of the free-carriers using Drude approximation.

$$\begin{aligned}\varepsilon(E) &= 1 - \frac{E_p^2}{E^2 - iE/\tau} + \\ &Ae^{-i\theta} \left( \frac{1}{E + E_0 + i\Gamma} - \frac{1}{E - E_0 + i\Gamma} \right);\end{aligned}$$

A, E<sub>0</sub>, Γ, θ, E<sub>p</sub>, τ are coefficients, E – wavelength in eV

12. **Effective-Medium Approximation** (EMA) material is used to represent dispersion of heterogeneous materials using dispersions of its components. This approximation is accurate when heterogeneous material can be described as a physical mixture of its components and components particles are small enough (smaller than wavelength). EMA is used very widely for representing poly-crystalline materials e.g. polySi. TFCompanion supports 2 and 3-components EMA .

$$\sum_{n=0}^3 \frac{\varepsilon_n(\lambda) - \varepsilon(\lambda)}{\varepsilon_n(\lambda) + 2\varepsilon(\lambda)} * VF_n = 0;$$

VF<sub>n</sub> (volume fraction of the components) coefficient  $\varepsilon_n$  is dielectric constant of the nth component (up to 3 components).

13. **Compound Binary Approximation** (CBA) material is used to represent dispersion of binary materials e.g. SiGe. It is based on the linear approximation of optical parameters spectra for specific composition. Interpolation is based on the dispersion spectra defined for specific compositions (nodes). The accuracy of the approximation obviously depends on the number of nodes. This approximation is especially useful in the cases when composition is changing in a small range where enough nodes are accurately defined, e.g. in production monitoring environment.

14. **Form Birefringence Approximation** (FBA) material is used to represent optical properties of high-spatial frequency surface grating. Approximation is normally valid in the case when grating pitch is significantly smaller than wavelength of measurement (pitch < 10 \* wavelength). Implementation is based on S.M. Rytov "Electromagnetic Properties of a Finely Stratified Medium" \* Soviet-JETP, vol. 2, No.3, 1956 pp.466-475

15. Adachi oscillator approximation is used to represent dispersion of II-V compound semiconductors (InGaAs, GaP, etc.,) especially in the interband region

$$\begin{aligned}\varepsilon &= \varepsilon_{\infty} + \varepsilon_1 + \varepsilon_2 + \varepsilon_3; \\ \varepsilon_1 &= A_0 \left( \frac{f(x_0)}{x_0^2} + \frac{f(x_1)}{2(x_0 + x_1)^{1/2}} \right) \\ x_0 &= \frac{E + i\Gamma_0}{E_0}; \quad x_1 = \frac{E + i\Gamma_0}{E_0 + \Delta_0}; \\ f(x) &= \frac{2 - \sqrt{1-x} - \sqrt{1+x}}{x^2}; \\ \varepsilon_2 &= A_x \left( \frac{1}{Y - G_0} + \frac{1}{8(Y - G_0/4)} + \frac{1}{27(Y - G_0/9)} \right); \\ Y &= E_0 - (E + i\Gamma_0); \\ \varepsilon_3 &= -\frac{B}{\xi^2} \ln(1 - \xi^2); \quad \xi = \frac{E + i\Gamma_1}{E_1};\end{aligned}$$

Sadao Adachi "Physical Properties of III-V semiconductor compounds", J. Wiley Interscience Publication, 1992, ISBN 0-471-57329-9

16. Afromovitz oscillator approximation is used for GaAlAs and some other compound semiconductors dispersion approximation

$$\begin{aligned}\varepsilon &= 1 + \frac{E_d}{E_g} + \frac{E_d}{E_g^3} (E + i\Gamma)^2 + \\ &+ \frac{E_d}{2E_g^3(E_g^2 - E_g^2)} (E + i\Gamma)^4 \operatorname{Ln} \left( \frac{2E_g^2 - E_g^2 - (E + i\Gamma)^2}{E_g^2 - (E + i\Gamma)^2} \right) \\ k &= \begin{cases} \operatorname{Im}(\sqrt{\varepsilon}) & E < E_g \\ \operatorname{Im}(\sqrt{\varepsilon}) + A(E - E_g) + B(E - E_g)^2 & \end{cases}\end{aligned}$$

17. Farouchi-Bloomer approximation for amorphous materials can be used for similar application as Tauc-Lorentz approximation. Although, TL approximation is, typically, preferable.

$$n(E) = \sqrt{\epsilon_{\infty}} + \frac{E_0 * E + C_0}{E^2 - B * E + C}$$

$$k(E) = \begin{cases} \frac{A(E-E_g)^2}{E^2 - B * E + C} & E > E_g \\ 0 & \end{cases}$$

$$E_0 = \frac{A}{B} \left( -\frac{B^2}{2} + E_g * B - E_g^2 + C \right);$$

$$C_0 = \frac{A}{B} \left( (E_g^2 + C) \frac{B}{2} - 2 * E_g * C \right);$$

$$Q = \frac{1}{2} \sqrt{4C - B^2}$$

18. Farouchi-Bloomer oscillator approximation ads support to crystalline material in addition to amorphous

$$n = n_{\infty} + \frac{B(E-E_i)+C}{(E-E_i)^2 + \Gamma_i^2}$$

$$k = \begin{cases} \frac{A(E-E_i)^2}{(E-E_i)^2 + \Gamma_i^2}, & E > E_g \\ 0 & \end{cases}$$

$$B = \frac{A}{\Gamma_i} (\Gamma_i^2 - (E_i - E_g)^2);$$

$$C = 2A\Gamma_i(E_i - E_g)$$

19. Schott- Briot dispersion is , primarily used for glasses.

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

$$k = 0;$$

20. Hartman approximation is used for dielectric materials, primarily glasses

$$n = A + \frac{C}{\lambda - B};$$

$$k = 0;$$

20. Conrady approximation is used for dielectric materials, primarily glasses.

$$n = A + \frac{B}{\lambda} + \frac{C}{\lambda^{3/2}};$$

$$k = 0;$$

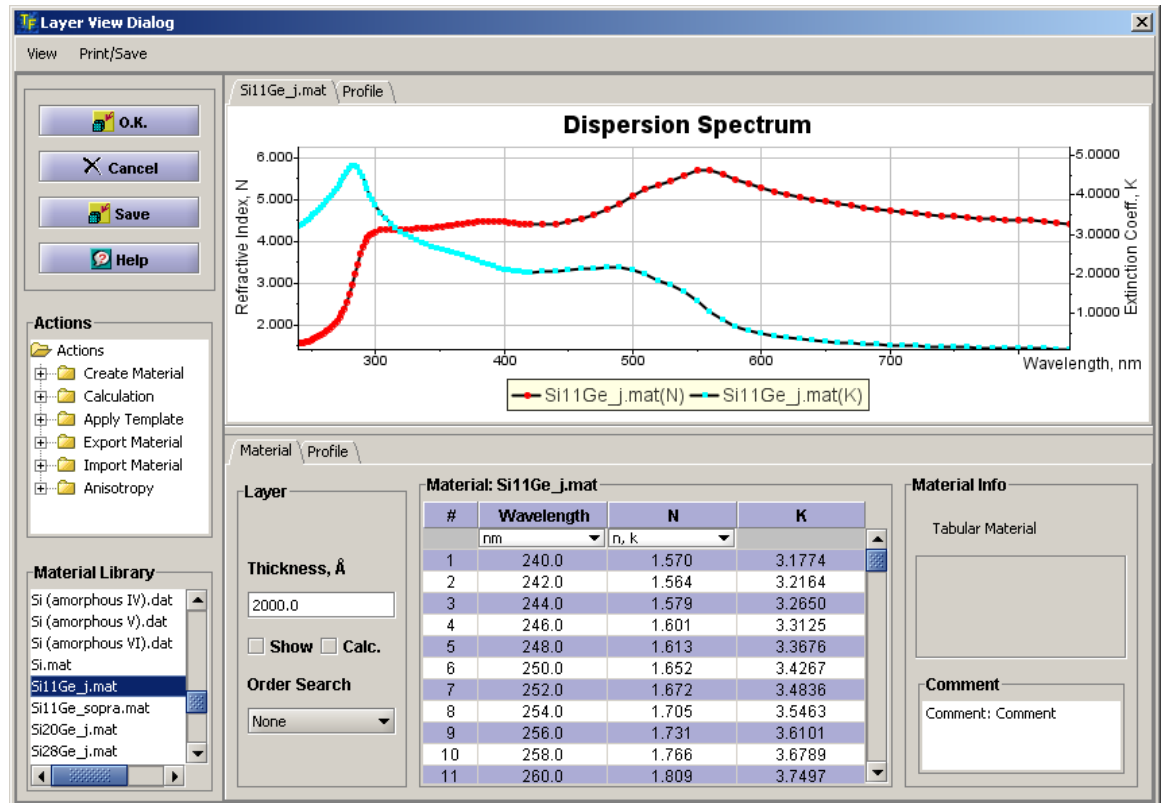
21. Classical oscillator approximation is similar but a bit extended form of the Harmonic oscillator. It can be used for various materials.

$$\varepsilon = \varepsilon_{\infty} + \frac{(\varepsilon_s - \varepsilon_{\infty}) E_t^2}{E_t^2 - E^2 + i \Gamma E} + \frac{E_p^2}{-E^2 + i \Gamma_D E}$$

$$+ \sum_{i=0}^1 \frac{A_i E_{oi}^2}{E_{oi}^2 - E^2 + i \Gamma_i E}$$

## 2.4 LayerView Dialog

**Layer View Dialog** shows full information about the selected layer. It is similar to **Material Dialog** and has the same layout but provides additional information about layer's thickness and profile. This dialog is invoked by selection of the layer in the filmstack – clicking on a layer “button” on the main screen filmstack or double-clicking the layer record elsewhere in the program. This dialog can be used to review and edit all parameters of selected layer.



**Fig. 2.4.1 LayerView Dialog**

### 2.4.1 Setting Measured parameters (Calculate and/or Display)

For material or profile parameters: select *Calculation/Show Parameters* in the Action tree. Check the boxes next to parameters that need to be calculated/displayed.

For thickness parameters: Check the box(s) next to Thickness value.

### 2.4.2 Setting Order Search

OrderSearch or GridSearch is used to overcome local minimum problem characteristic to minimization methods used to solve inverse problem (i.e. finding physical parameters of the filmstack by optical response – measured optical data). Results of the calculations, especially in the case of the thick films, depend on the starting thickness. The idea of the *Order Search* is to perform calculations with different starting values of thickness and select the result that has the best fit. These calculations are done in parallel (in the separate threads of execution) to speed up the process.

There are two *order Search* options: **Custom** and **Standard** search.

**Standard orderSearch** is two cycle thicknesses range: one cycle thickness up and one down from the nominal thickness value.

**Custom orderSearch** prompts user to select minimum, maximum thicknesses and the number of starting points.

### 2.4.3 Layer profile.

*Measuring layer profile, typically, require oblique reflectance or ellipsometry measurement. Using normal reflectance in MProbe measurement does not give enough information calculate profile.*

Layer profile can be Uniform or Graded. Default layer profile is Uniform. Several profile type are supported: Uniform, Linear, Gaussian and Polynomial. The following are exact equations for profiles:



Uniform (default);

$$C(x) = C_0 = C_d$$

Linear

$$C(x) = C_0 + (C_d - C_0) \frac{x}{d}$$

Gaussian

$$C(x) = C_d * \exp\left(\frac{\alpha}{d^2}\right)$$
$$\alpha = 4 \log\left(\frac{C_0}{C_d}\right) * \left(x - \frac{d}{2}\right)^2$$

Polynomial

$$C(x) = C_0 + \sum_{i=0}^n A_i x^i + \left( C_d - C_0 - \sum_{i=0}^n A_i x^i \right) * \left( \frac{x}{d} \right)^n$$

In equations C stands for a graded parameter: n or k or composition; x is the position along the layer's thickness ( $0 < x < d$ );  $C_0$  is a value of the parameter at the bottom boundary and  $C_d$  is a value of the parameter at the top boundary.

User can edit profile parameters and mark them as Calculated. User also needs to select the Number of Grades (sub layers to approximate the profile).

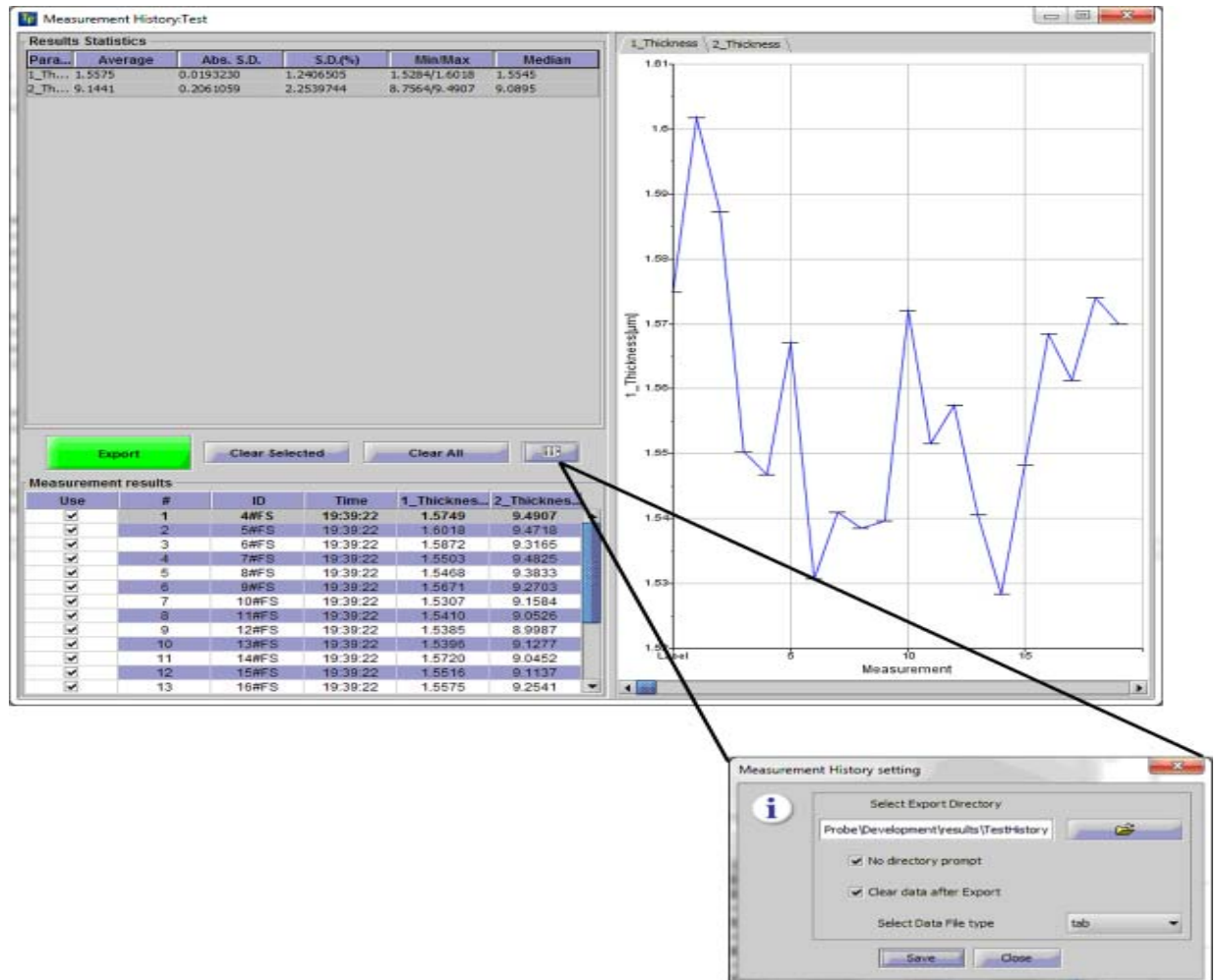
**i** Only layers with EMA and Compound Materials types support Non-Uniform profile. Other material types are converted to a two-component EMA material when user selects profile type other than Uniform.

## 2.5 . Measurement History Dialog

Measurement history utility allows review, selection and export of the measurement results. All measurement results are automatically cached and available during the session. Results are grouped by the filmstack models used i.e. by measured sample types.

Measurement results and basic statistics are displayed.

To start Measurement History Dialog, select Data/Measurement History from the main menu

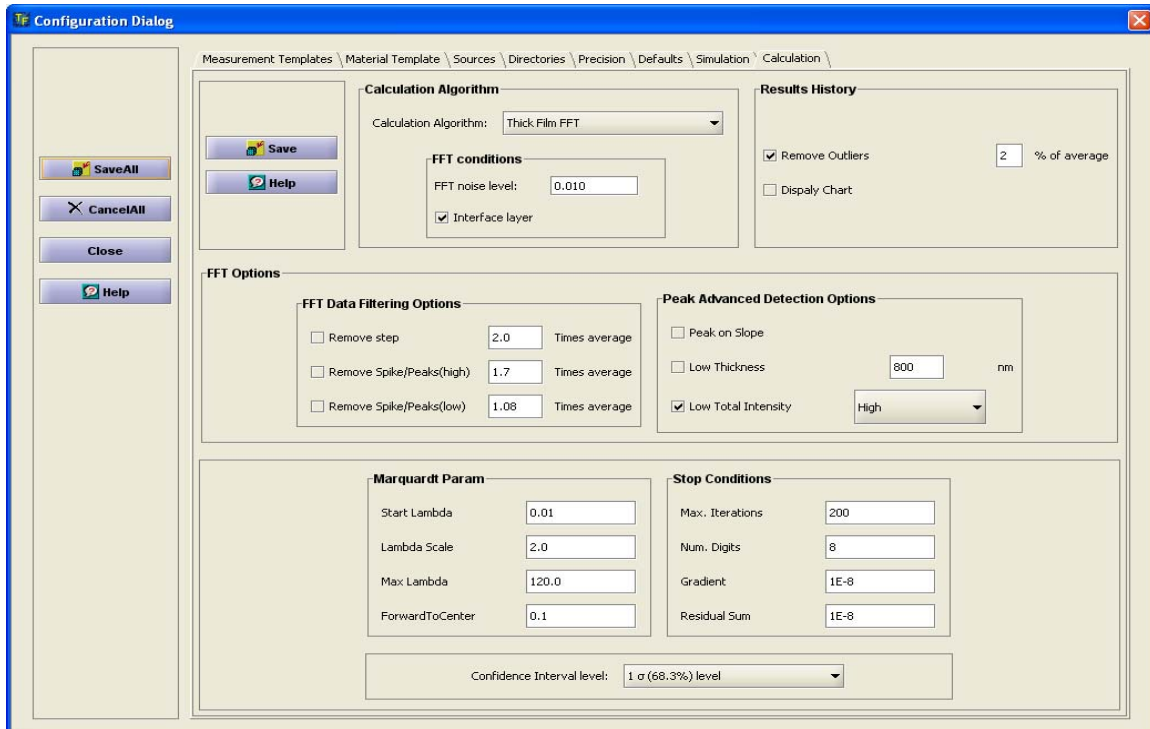


**Fig. 2.5.1 Measurement History Dialog**

Statistics Table displays measured Parameter name, average value, s.d., relative s.d., Min/Max values, Median

Results table displays sample ID, measurement time and parameters values for each measurement. These results are also displayed in the chart (Chart is enabled by default but can be disabled in configuration)

Bad points/outliers can be manually excluded by checking off a record in the table.. Alternatively, outliers can be automatically excluded. Outliers removal can be setup in Software Configuration



**Fig. 2.5.2 Setting Outliers removal in configuration.**


Rejection limit is set in % of the mean value, all measurement that fall outside this limit will be rejected. The limit is calculated as  $\text{limit} = 100 * |p - \text{avg}| / \text{avg}$ , where p is the value of the measured parameter, avg – average value of this parameter value calculated from all measurements.

## 2.6 Configuration

TFCompanion supports flexible configuration of software properties, templates, etc. and selection of connected hardware configuration. Both software and hardware configurations are saved in XML files located in /init directory of TFCompanion installation: software configuration is saved in the file TFComp\_config.xml; hardware configuration is saved in the file Hardware.xml.

To start software **Configuration Dialog** - select **Configure/Configure Software** from the main menu.

To start Hardware **Configuration** - select **Configure/Configure Hardware** from the main menu.

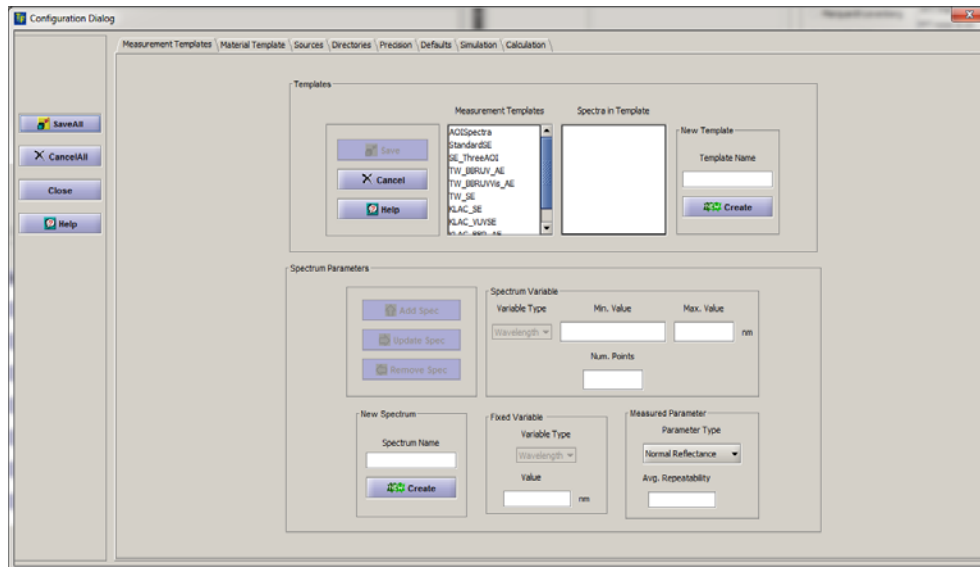
 Hardware configuration is accessible only when login user has hardware privileges.

### 2.6.1 Software configuration.

To start software **Configuration Dialog** - select **Configure/Configure Software** from the main menu. **Configuration Dialog** allows setting defaults (including units and calculation conventions), databases location and templates. Templates are used throughout TFCompanion to streamline data input – it allows loading specified configuration with one click instead of filling the form each time. Templates will normally describe configuration or conditions that are frequently used e.g. measurement template may describe properties of specific hardware that is frequently used, etc.

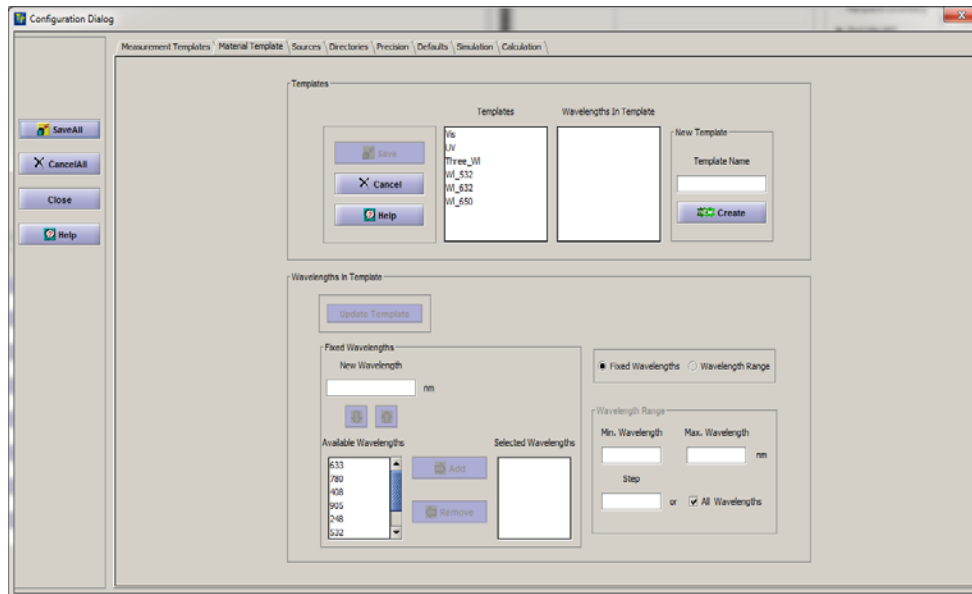
**Software Configuration Dialog** contains several tabbed panels:

- *Measurement templates.* This panel allows creating measurements templates. These templates encapsulate specifics of the hardware properties e.g. measured parameter, spectral range, measurement precision, etc. Several spectra of different type can be combined in one template. These templates are used in Error Estimation dialog. Several templates are included with TFCompanion distribution and can serve as an example.



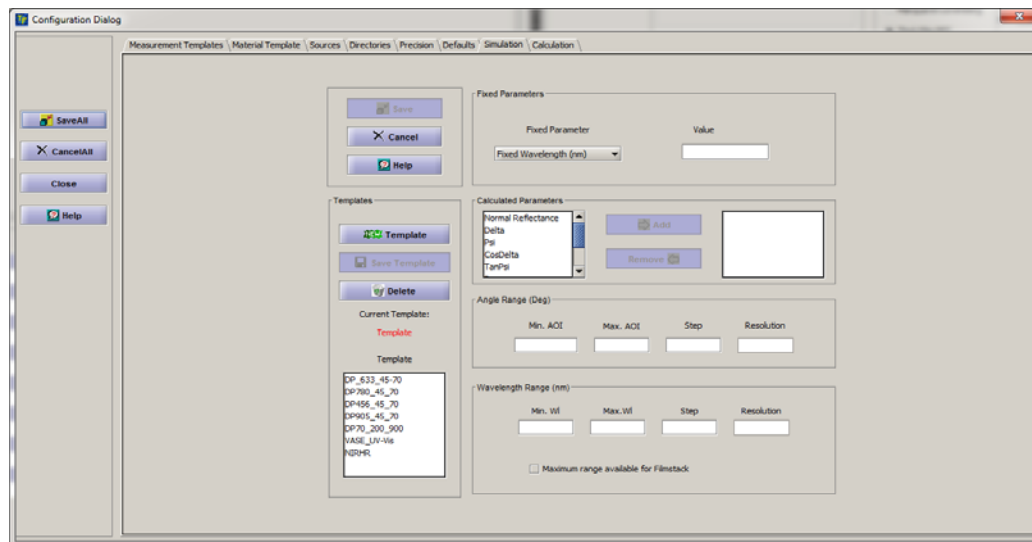
**Fig. 2.6.1 Measurement templates panel**

- **Material templates.** This panel allows creating tabular material template. The template encapsulates wavelength range or discrete wavelength(s). Applying template to existing material (this can be done in Materials Dialog) will modify materials e.g. limit the range or interpolate optical constants for specific wavelengths.



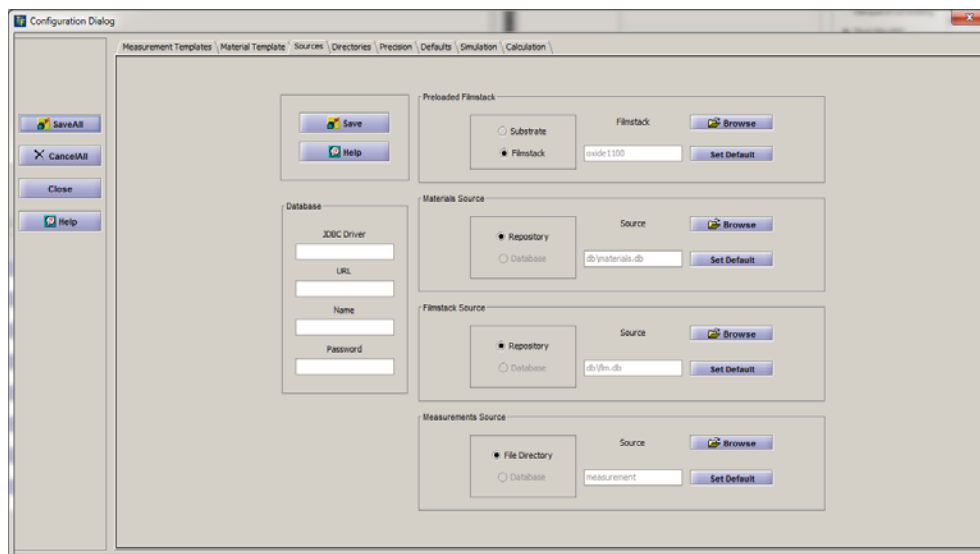
**Fig. 2.6.2 Material template Panel**

- **Simulation.** This panel allows creating simulation templates. These templates can encapsulate typical configuration used in simulation e.g. variable parameters range (wavelength or angle), simulated parameters, etc. Templates can be used in Simulation dialog and allow loading full configuration required for simulation. In this case simulation is reduced to two steps: load template, calculate results.



**Fig. 2.6.3 Simulation configuration panel**

- **Sources.** This panel allows selection of materials and filmstack databases, default filmstack that is loaded when TFCompanion started, measurement data directory. Databases and measurement data directory are selected relative to TFCompanion installation directory.



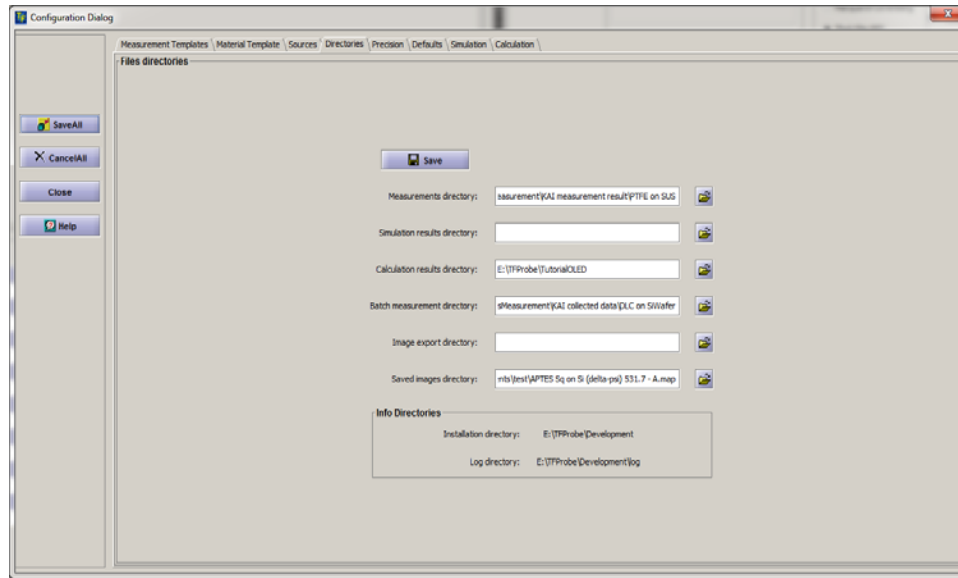
**Fig. 2.6.4 Sources configuration panel**

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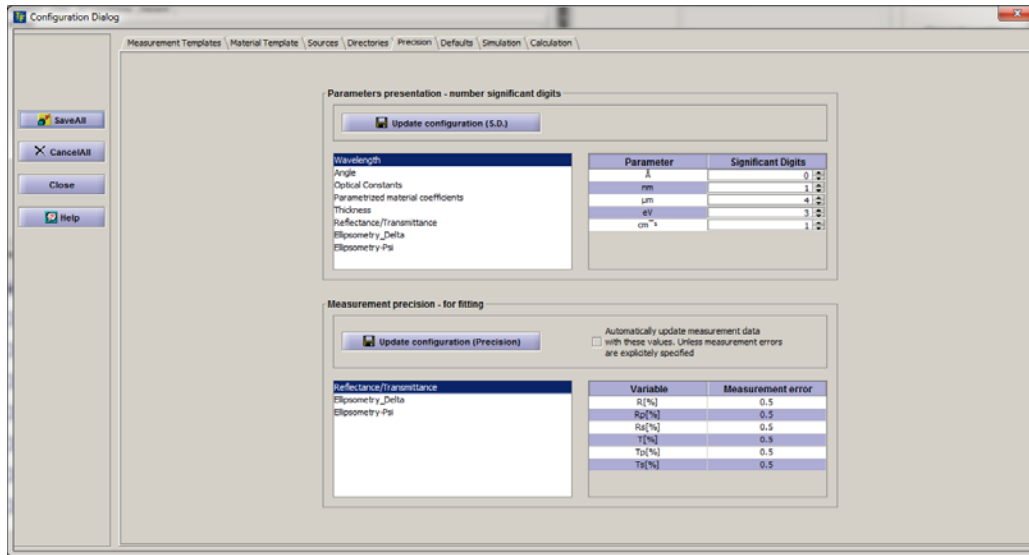
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- **Directories** This panel shows location of the default export directories: Measurement results, Simulation results, Calculation results, Batch Measurement results, Image export, saved Images. The directory is automatically updated based on user export action. For example, last measurement export directory becomes default measurement export directory. Directory can be manually changed



**Fig. 2.6.5. Export directories configuration panel**

- **Precision Configuration Panel** has two types of precision setting: number of significant digits to display the values in the software and measurement error. Measurement errors, if check box is checked are automatically added to the measured data and used in data analysis. The measurement error value affects the Goodness –of- Fit value that can be used to decide on the quality of fit.




**Fig. 2.6.6. Precision Configuration panel**

*Defaults.* This panel allows setting of unit and several important conventions that are used throughout the program.

- *Conventions (General and Delta).*

Both general and Delta conventions are related to ellipsometry measurements – they have no effect of reflectance or transmittance results.

*Delta* can be defined in the range 0-360deg or 0-180 deg. Some hardware, e.g. rotating-analyzer or rotating polarizer ellipsometers, are able to determine Delta only in 0-180 deg range. Other hardware, e.g. rotating compensator ellipsometers, can measure Delta in 0-360 deg. Range.

 If loaded measured data has Delta in 0-360 deg range TFC Companion will use 0-360deg. convention during calculations automatically.

*General convention* allows selection either of two conventions Azzam or Beaglehole (BIL). Azzam convention defines  $\Delta = 180^\circ$  for bare substrate ( $R_p = -R_s$ ) while BIL convention defines  $\Delta = 0$  for bare substrate ( $R_p = R_s$ ).

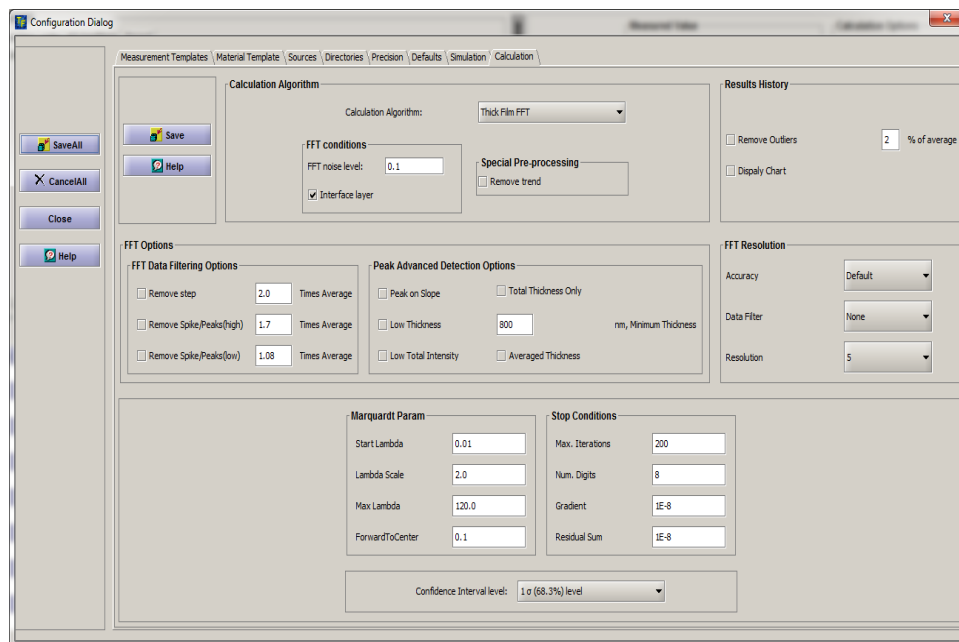
- *Default material units and resolution.*

User can select optical properties units that will be used to display optical constants. Wavelength resolution setting is used in interpolation decisions.

- Wavelength range and number of points for parameterized materials. This setting is used in creating new parameterized materials



- Default spectrum variables and ranges define parameters used to create default simulations conditions (unless template is used).
- **Calculation.** This panel defines default calculation conditions. It includes several panels related to FFT and Marquardt (curve fit) parameters:
  - **Calculation Algorithm** panel is similar to Calculation Options panel in the main dialog and other places in the program and allow to default algorithm. In addition it has a special pre-processing option for FFT. Typically, FFT is best applied to a leveled spectrum – if the spectrum has a trend, it need to be removed. In most cases, it is done automatically by the software. Selecting “Remove trend” option make it a default for all data.
  - **Results History** defines defaults for the History dialog. If Remove Outliers option is selected – all results exceeding selected % value will be unchecked in the table and not shown in the chart. If Display chart is selected – chart is automatically displayed when History Dialog is opened.



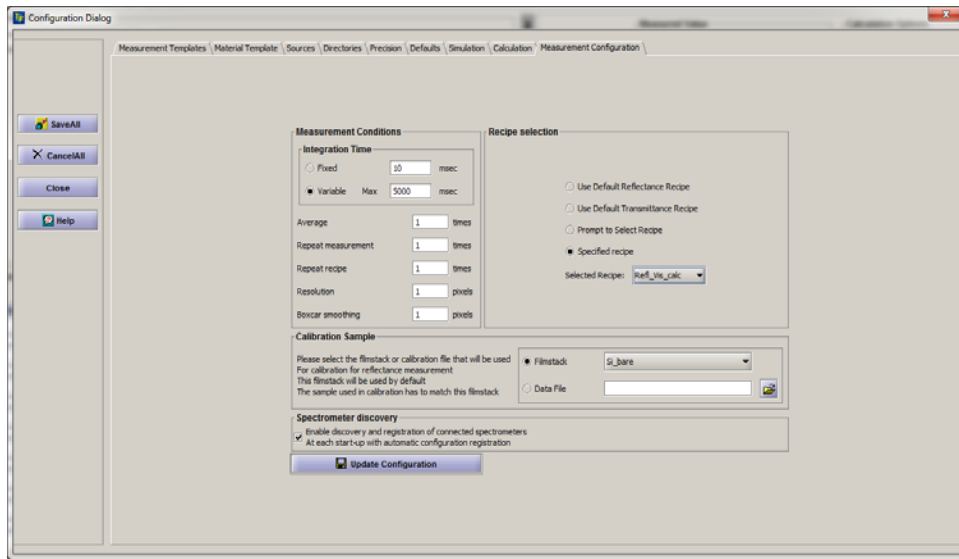
**Fig. 2.6.7 Calculation Configuration Panel**

- **FFT Resolution** panel defines Accuracy, Data Filter and Resolution that can be selected from the drop-down boxes. Default accuracy relies on the resolution to determine the peak position, High-accuracy uses interpolation and Maximum accuracy using a Gaussian fit to a peak.
- **Peak Advanced Detection Options** panel defines several hint option “Peak on the slope”, “Low thickness” and “Low total

Total thickness instructs software to measure only total thickness and ignore everything else.

*Averaged thickness* is used for measurement on the non-uniform surface when several thicknesses can be present within a measurement spot. Normally, several measurements are taken using this option and automatically averaged for stability.

- FFT Data filtering options is used process the spectrum before applying FFT. These options are used is to remove features that are exceeding average value by specified amount.
- *Marquardt Parameters* panel defines default values used in curve fitting. They are almost never need to be changed and intended for advanced user only.
- *Measurement Configuration* panel defines default Measurement Conditions that are used in the newly created measurement recipes, Recipe selection strategy, Calibration sample and Spectrometer discovery
  - Measurement conditions are defining parameters that are used in the measurement recipes. It does not effect existing measurement recipe.
  - Recipe selection panel has several options. The default option is “Specified recipe” that is setup when software is first used during installation of the MProbe. This recipe is automatically loaded during software startup.
  - Calibration sample defines what is used during calibration/Baseline measurement. In vast majority of cases Filmstack option is used. Filmstack corresponds to a calibration sample that is used during the calibration procedure. Data File option can be used if a reflectance standard (with known calibrated reflectance is used).
  - Spectrometer discovery should be always enabled except in special cases.



**Fig. 2.6.8 Measurement Configuration**

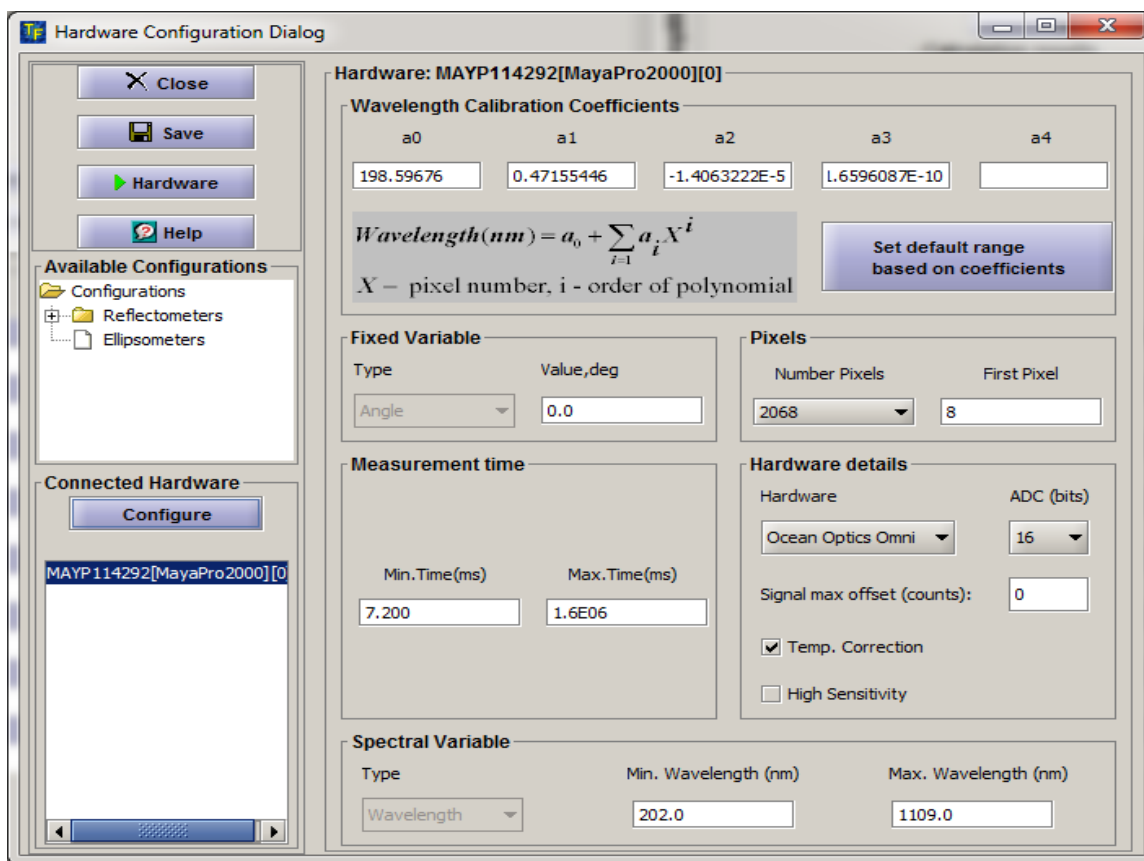
- i** To save configuration changes – user needs to select **Save (or Update Configuration)** in particular panel (this saves selected changes to memory) and select **SaveAll** – this updates xml configuration file with all the changes made in different panels

## 2.6.2 Hardware configuration

**Hardware configuration** dialog allows review and editing of the hardware properties and selection of the currently connected hardware. Hardware configuration dialog can be started by selecting **Configure/Configure Hardware** menu item in the main menu.

- i** Hardware configuration dialog and **Configure/Configure Hardware** menu item in the main menu are not available in the standalone mode.

MProbe system automatically detects spectrometers, read relevant information from the spectrometers and configure hardware, when spectrometer is enabled in configuration (default). Editing of the hardware configuration was used in the older version of the software (before ver. 4.5) or when third party spectrometers used (not MProbe)

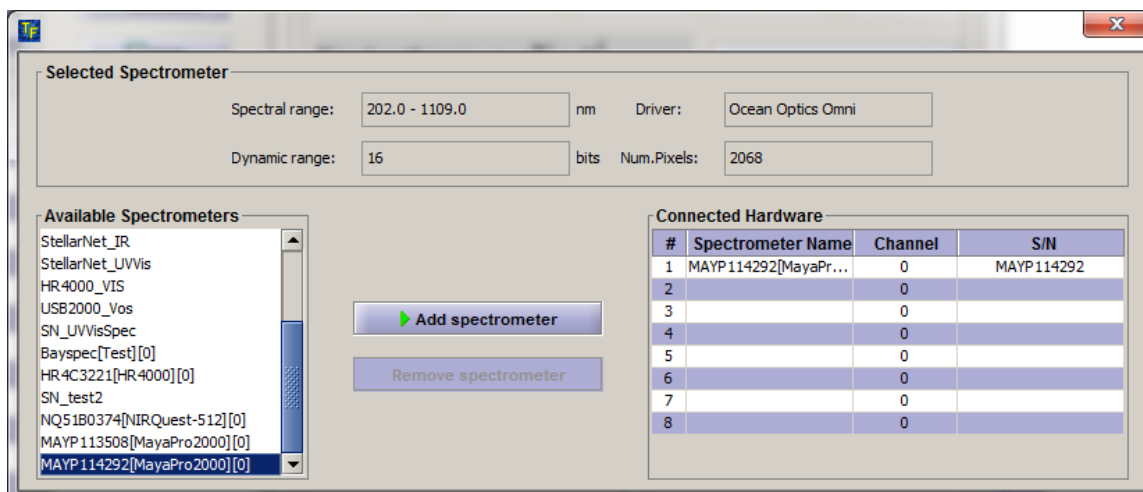


### 2.6.9 Hardware configuration dialog

All hardware profiles are displayed in the **Available Hardware** side-panel window. Displayed hardware properties are updated as user selects any of the available hardware profiles. Depending on access privileges user can edit the properties and also select currently connected hardware. **Currently connected** hardware properties are used for all the interactions with the hardware.

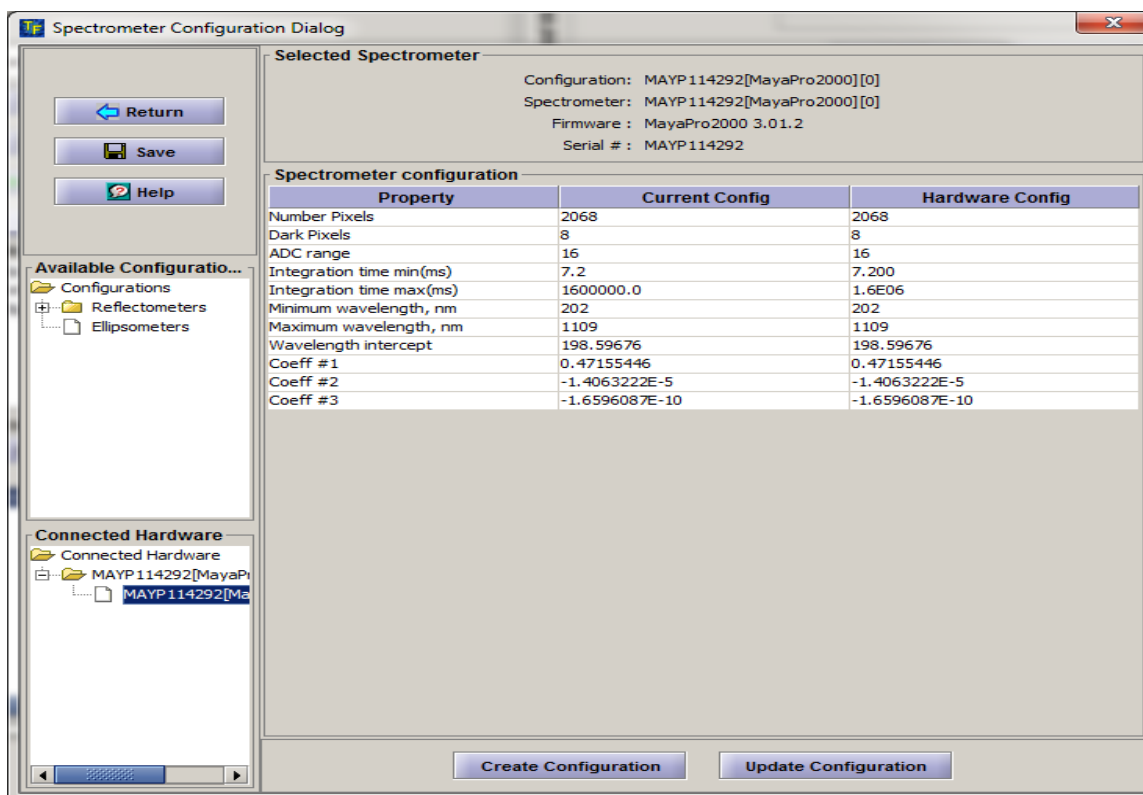
Wavelength calibration coefficients and wavelength range are read directly from the spectrometer. Strictly speaking there maybe small discrepancy between them due to rounding that does not affect functionality. Using “Set default range based on coefficients” button user can exactly match wavelength range to coefficients.

Hardware can be removed from or added to the current configuration using dialog activated by Configure button.



**Fig. 2.6.10 Configure dialog (activated by Configure button)**

To manually edit spectrometer properties use Spectrometer Configuration dialog (activated by *Hardware* button). Parameters can be directly entered/edited in the table and current hardware configuration updated.



**Fig. 2.6.11 Spectrometer configuration dialog**

The ability to edit hardware properties depends on the user access level privileges: Administrator level user can edit any property; Operator can only see properties of the selected hardware; Engineer can edit some of the properties (e.g. wavelength calibration).

All the hardware profiles data is stored in the xml file: **Hardware.xml**, located in the **/init** directory of software installation. This file is supplied with the software and contains information relevant to specific hardware options available. It is expected that user never tries to change xml file directly. **Hardware configuration** dialog allows creating and adding new profiles as necessary.

## 2.7 FILMSTACK

### What is Filmstack?

Filmstack is an optical model of the sample that is measured - it consists of a substrate, a collection of layers and an ambient. Filmstack can also have properties. There is no limitation on the number of layers. Substrate and ambient are infinite materials i.e. do not have thickness - all layers have finite thickness, material and properties. In the cases, when physical substrate is transparent and one need to measure transmission or backside reflectance need to be taken into account – physical substrate need to be represented as a “layer” in the filmstack model (substrate will be Air or other material if the sample is immersed). Thick transparent layers are supported – software will detect automatically if the thickness exceeds typical coherency length of light and give an option to the layer to “incoherent type”. As an example, glass slide with roughened backside is a substrate (no reflection from the back side); however, the same slide with the polished backside is an “incoherent type” layer. The key factor is whether reflectance from the backside need to be taken into account (measured by detector) or it does not.

Any element of the filmstack can be edited (ambient, substrate, layers). One can create filmstack (add/insert/remove layers). One can also modify parameters of the existing filmstack (e.g. change material of the layer or thickness, etc.). By default all layers and materials in filmstack are independent; however, one can explicitly “link” layers and /or materials.

Filmstack can be created and all elements edited in two places in the program:

- Filmstack Panel (in main window)
- Filmstack Editor

### Layer types and properties

Layer is a convenient optical model abstraction of a physical film. Layer always has a finite thickness and material associated with it. TFCompanion supports two types of the layers:

- Homogeneous layer. Optical properties have “uniform profile” along the thickness (z) coordinate.
- Graded layer. Optical properties have specified profile along the thickness (z) coordinate. This profile is represented by dividing layer on sub-layers (grades) with specified optical properties.(see section )

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### **2.7.1 Layer properties.**

#### ***Independent and linked layers.***

By default all layers and materials in filmstack are independent; however, one can explicitly “link” layers and /or materials. Linking layers and materials is inter-related and one needs to exercise care when mixing them together. Linking of layers automatically links corresponding materials (one cannot unlink materials of the linked layers), i.e. linking of materials supersedes linking of layers. For example, linking two materials does not link corresponding layers but linking two layers does link respective materials. Linking two objects (layers or materials) means that all the parameters (properties) of these objects are linked; consequently only two equal layers can be linked (must have the same thickness and material, in case of the graded layer also the same profile, etc.). When linking layers, one needs to select a node (master layer) and link other layers to this master (there can be several nodes each with its dependent layers). The node is the layer that is “visible” to calculation routine and displayed calculated parameters have this layer designation. Material of the node (master) layer becomes itself a node of the related linked materials. It is possible to link layers and link another material without linking corresponding layer. One example one can link two oxide layer and adding oxide material of the third layer to the link (e.g. material can be a part of the EMA).

The link map of layers and materials is displayed in the Links panel (Filmstack panel in the Main window). Linking and unlinking can be also done at that place. (see ..)

#### ***Incoherent layer***

There is an upper limit on the thickness of the layer that can be measured using reflectance/ellipsometry methods given finite wavelength resolution. When thickness of the layer exceeds coherence length of the light used for measurement – the phase is undetermined, consequently there is no “interference” between front and backside reflected light. This thickness depends on the wavelength and wavelengths resolution of light. In most cases, the thickness of few hundred  $\mu\text{m}$  makes layer “incoherent” in visible spectral range. By default, all layers are “coherent”. When thickness is set (Parameters table in Filmstack panel – main Window) the coherence length is estimated and if the layer is thick enough – user is prompted to select “incoherent” layer type. If the thickness is decrease and layer is “incoherent” – user is prompted to set layer “coherent”.

### **Filmstack Properties**

There are several properties that are defined for filmstack. These properties include various correction factors that account for filmstack artifacts or non-ideal setup/measurement conditions.



## ***Surface Roughness***

Effect of random surface roughness is manifested differently depending on the measured parameter. Reflectance and transmittance measurements are affected directly and the effect can be estimated using Kirchoff scalar model. Roughness value (rms in Angstroms) can be set . At the same time, ellipsometry is affected by roughness in a different way. The best way to model roughness effect on ellipsometry measurement is to represent it as a separate layer, perhaps EMA of material void + oxide, etc. In addition, surface roughness can cause some depolarization and increase the noisiness of the data.

**Note.** Using rms roughness setting will have effect only on reflectance /transmittance data and no effect on ellipsometry data.

**Note.** Roughness should always be constrained with minimum value>0. Roughness=0 will cause exception.

## **Scale**

Scale simulates the effect of the light intensity change. It can be used for correction of the distance change between the probe and the sample and light intensity drift during long term measurement.

## **Offset**

Offset parameter corrects for a large offset of reflectance due calibration or distance issues

## **Dullness**

Dullness parameter is somewhat similar to Roughness but it is not wavelength dependent. It can be used to correct the measurement of the samples that have extra light attenuation without scattering. For example, unpolished metal.

## 2.7.2 Creating Filmstack

### LOADING EXISTING FILMSTACK

Filmstack objects are stored in a database. Filmstacks are self-consistent, i.e. they are not relaying on external references/links. This means that it contains copies of all the materials that it uses – there is no link between materials database and filmstacks database.

There are several ways to load filmstack:

- **Loading from the database:** Filmstacks database (along with other databases) is displayed in the left-sidebar of the main dialog. One needs to select the record, right-mouse click and select **Set Filmstack** from the pop-up menu.
- **Loading from the cache:** Filmstacks can be cached in memory at the various stages of a project. To load filmstack from the cache one needs to select Tools/History (from the main menu), select the filmstack record and click Enter.
- **Indirect loading.**
  - Filmstack can be loaded as a part of a Calculation Recipe
  - Filmstack can be loaded as a part of a Measurement Recipe (if option “attached filmstack” is used)
  - Default filmstack loading as start-up of the application. User can select a filmstack that is loaded at application start-up in configuration dialog (Configure/Software Configuration select Sources tab, select browse in Pre-loaded filmstack panel and select a filmstack from the database and save a new configuration).


**Note.** In case of indirect loading, only a link to filmstack record is saved. If filmstack record is not present in the database – the error will occur during loading.

### CREATING FILMSTACK

There are two ways to create/edit filmstack:

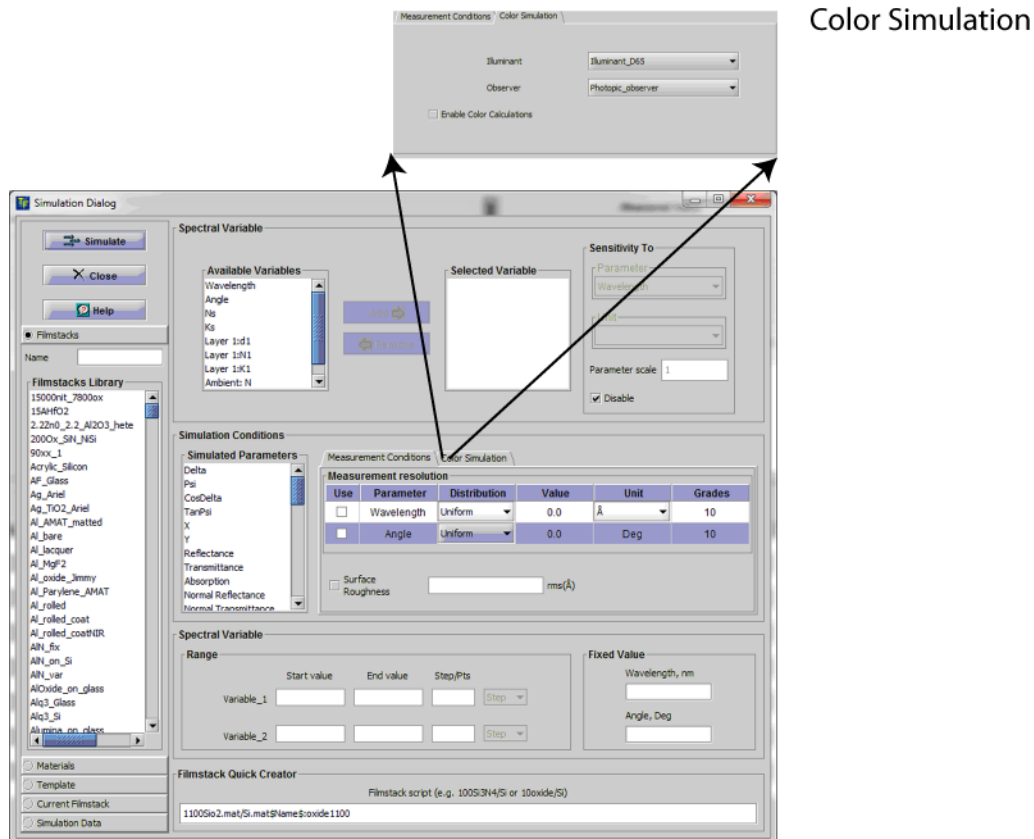
- Directly in the main dialog by either using **Filmstack** menu (Layer Add, Layer Insert, Layer Delete) or toolbar options or materials database in the sidebar. This method is recommended for small changes of the filmstack (e.g. changing (adding, deleting, inserting one layer).
- Using **Filmstack** dialog page. Select **Filmstack/Edit Filmstack** from the main menu. This method is recommended in case of significant changes of the filmstack (e.g. creating multilayer filmstack)

## 2.8 DATA SIMULATION

Data Simulation is performed in Simulation Dialog. This dialog can be started from the main menu (**Action/Simulate**) or using button **Simulate** or using  icon in the toolbar. The current filmstack in the main screen is inherited by the Simulation dialog.

Following functions can be done in Simulation dialog:

- Calculation of the selected parameters as a function of the selected variable (e.g. Reflectance vs. wavelength) or two variables (e.g. Reflectance vs. wavelength and AOI (Angle-Of-Incidence)). Correction for wavelength and angle resolution and surface roughness can be added to simulation.
- Calculation of the sensitivity of selected parameters to selected variable as a function of another variable (e.g. Delta to AOI ( $\partial\Delta/\partial\phi$ ) vs. wavelength) or two variables (e.g. Delta to AOI ( $\partial\Delta/\partial\phi$ ) vs. wavelength and layer thickness)
- Calculation of the color coordinates based on reflectance or transmittance



**Fig. 2.8.1 Simulation Dialog**

Available simulation parameters depend on the version of TFCompanion. Reflectance/Transmittance parameters are listed in the –R version (used with MProbe system), ellipsometry parameters are listed in –RE and –E versions. Available variables are wavelength, angle-of-incidence, thickness (of any layer), optical constant -n or k (of any of materials in filmstack). Simulation results are presented in tabular and graphical form.

Before starting the simulation one needs to define simulation conditions:

- Select variable(s);
- Edit variable's range parameters and unit;
- Select fixed variables values;
- Select simulation parameters;
- Select measurement conditions (optional);

**Available Variables** list is populated based on the current filmstack. Four variables—Wavelength, AOI (Angle-of-Incidence), Ns (n of substrate), Ks (k of substrate) – are always present. In addition, each layer has 3 variables: thickness, n, and k. The layer variables are listed in the following format:

Layer [#]: d [#] for thickness;

Layer [#]: N [#] for the n;

Layer [#]: K [#] for the k; where [#] stands for the number of the layer.

e.g. thickness of the layer 1 is listed as *Layer 1:d1*

### 2.8.1` Selecting Variable

To select an appropriate variable record in the **Available Variables** List and use *Add* button - selected variable is added to the **Selected Variables** List. At the same time, variable's range will be displayed in the text fields - **Variable Range** in the bottom part of the dialog. Each variable has *Start Value*, *End Value* and a *Step*. The default step is calculated assuming 30 points i.e.  $\text{Step} = (\text{Ending Value} - \text{Starting value}) / 30$  (configuration default that can be changed). A default range for wavelength is based on the wavelength range of the respective material's spectrum. Default ranges of the other variables are determined from 0 (Start Value) to the Current value (End value).

Up to two Variables can be selected. Highlight a variable in the **Selected Variables** List to edit its range.

### 2.8.2 Editing Variable Values.

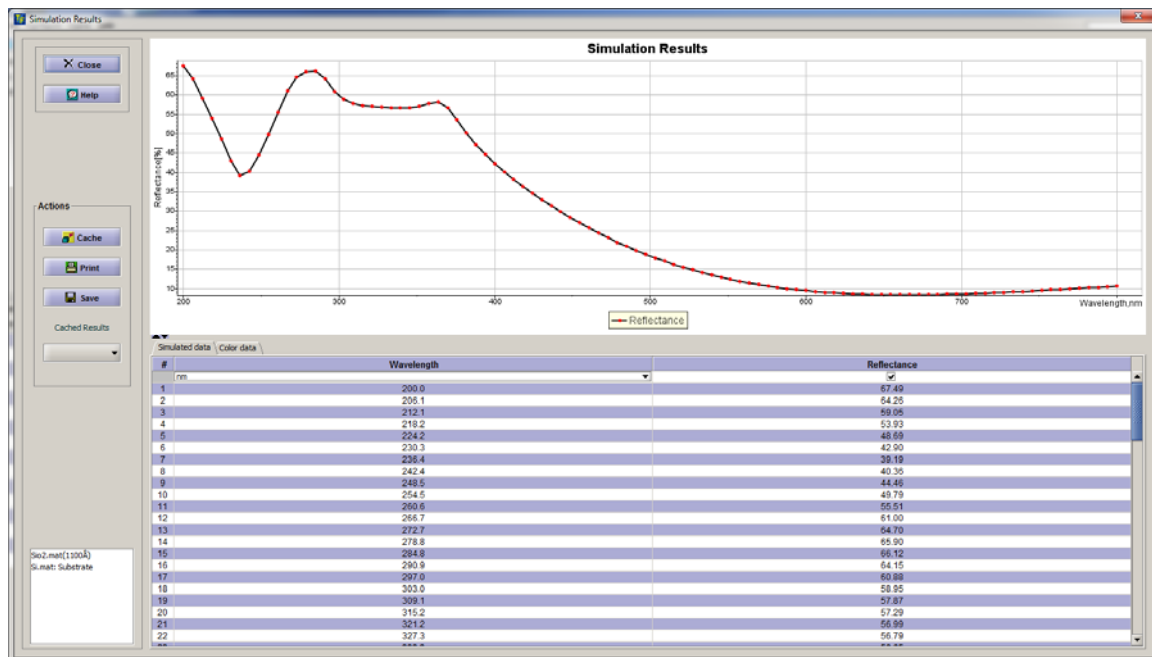
All the values can be edited as needed. The changes to edited values are committed as soon a cursor leaves the respective text field or Enter key is used. Number of points or step size can be used interchangeably.

### 2.8.3 Selecting Fixed Variables Values.

Unless both Wavelength and AOI are selected as variables- one of them is fixed. Default wavelength is 632.8 nm and default AOI is 70 deg.(defined in configuration). Fixed value can be easily edited. For example, if wavelength is selected as a Variable – only AOI fixed value can be edited. If AOI value is not changed – default is used in the calculations.

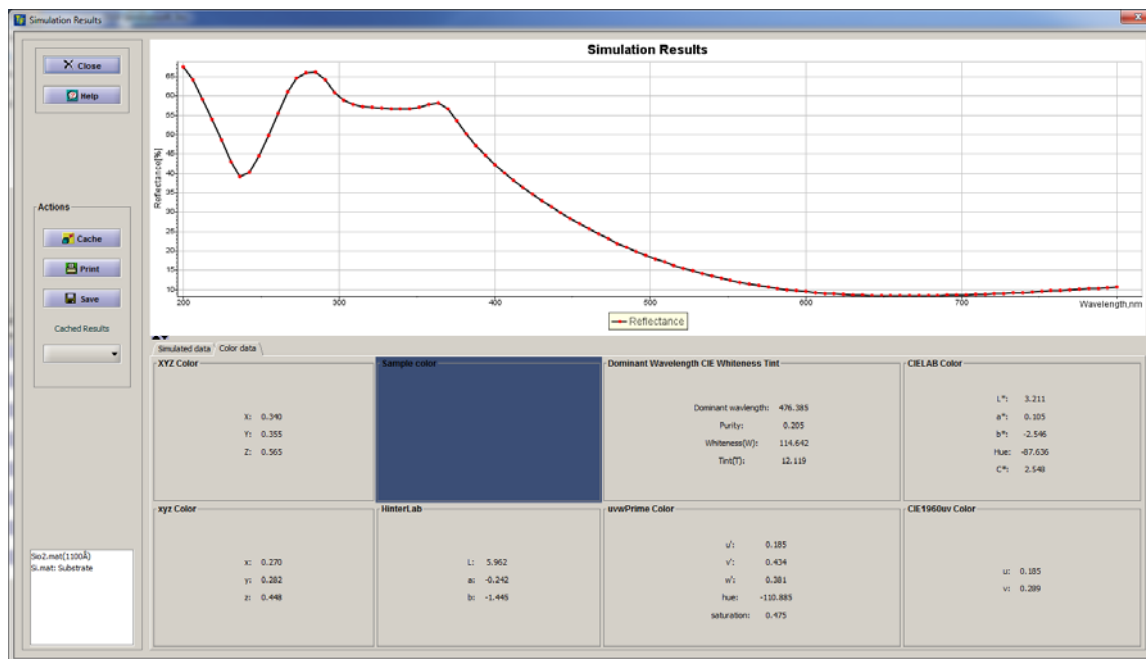
### 2.8.4 Selecting Simulation Parameters

All parameters are listed in the **Simulation Parameters** List. Selection can be done by clicking on the parameter record in the list (check mark appears next to parameter)



**Fig. 2.8.2 Result of simulation displayed.**

If Color coordinates calculation is selected – it is displayed along with reflectance/transmittance data



**Fig. 2.8.3 Color coordinates calculation displayed along the simulation results**

## 2.8.5 Sensitivity Calculation.

Preparations for the Sensitivity calculations require one additional step - selection of a “second”, sensitivity variable. For example, if one wants calculate Sensitivity of the selected parameters to the Angle-Of-Incidence (AOI) as a function of the Wavelength. In this case Wavelength is the “first” variable selected for Simulation and AOI is a “second” variable selected specifically for Sensitivity calculations. Note that “first” and “second” variables can be the same, i.e. one may calculate sensitivity to Wavelength as a function of the Wavelength. This “second” variable should be selected from the **Sensitivity To** list. By default this list is disabled, to enable it– uncheck **Disable** checkbox located next to this list. Once Sensitivity parameter is selected, relevant fields on **Parameter** panel are activated. The user can easily change its the unit of the sensitivity parameter.

## 2.8.6 Presentation of Data and Saving

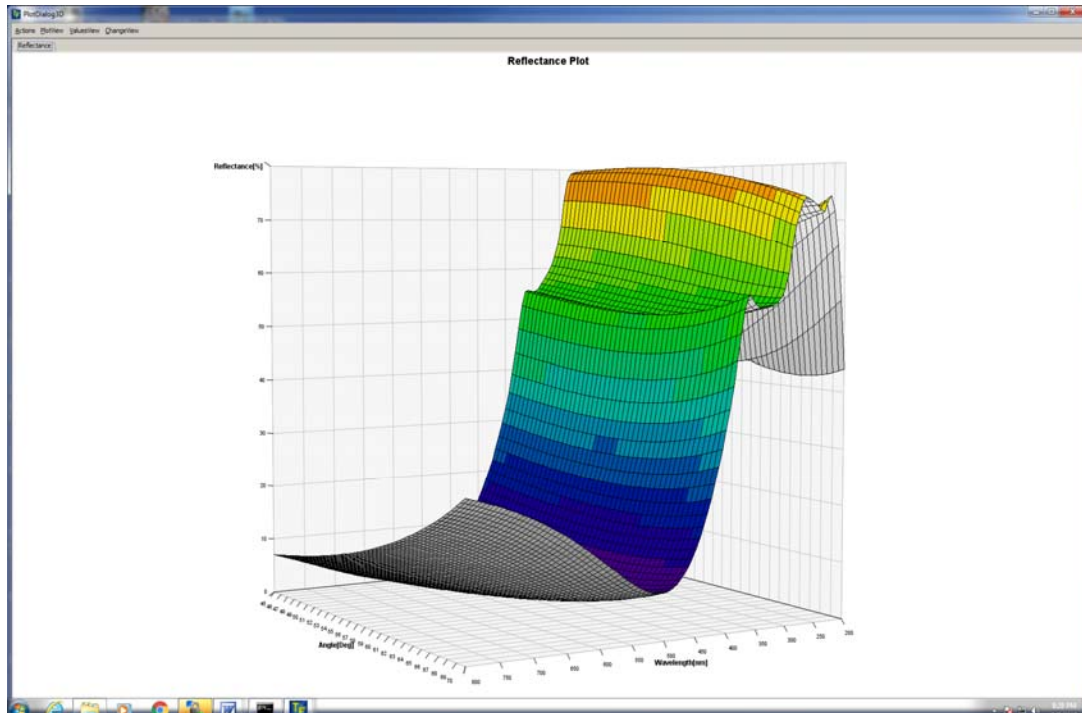
In the case of one variable, the results of the simulation are presented in the **SimulationResults Dialog** that combines a data table and the plots. In the case of the two variables the results are always presented in the form of the 3D Plot.

Results displayed in the **SimulationResults Dialog** are using following default units:

- For reflectance, transmittance and absorbance -- %;

- For ellipsometric angles (Delta, Psi, Rp-Rs\_Phase) – degrees;  
Unit of the variable: wavelength, angle, thickness, optical constants can be changed using drop-down menu in the table.

Results are displayed in the table and in the plot. The table and plot are synchronized so that the change of variable's unit or checking/unchecking parameter box will be reflected in the plot (unchecking the box removes the plot of the respective parameter). Results can be saved, printed or cached. Saving and printing is available separately for the plot and table data using the same **Print** and **Save** buttons. After clicking the button user is given the choice to select either Plot or Data.



**Fig. 2.8.4 Simulation results displayed as 3D plot.**

### **2.8.7 Saving Results to File.**

Results of the evaluation (table data) can be saved to an ASCII text file. Default location is **<installation directory>\simulation\<name>.dat** file. Default name is *test*. User is prompted to select the location and name of the file. TFCompanion measured data format is used to save the data; detailed description:

[http://www.semiconsoft.com/html/download/Import\\_data\\_format\\_for\\_TFCompanion\\_software.pdf](http://www.semiconsoft.com/html/download/Import_data_format_for_TFCompanion_software.pdf).

This file can be imported as a “measured data” in TFCompanion.

Plot can be saved in JPEG format. User is prompted to select the name and location of the file.

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Default location is <installationdirectory>\simulation\<name>.jpeg

### 2.8.8 Caching results

Results of the simulation can be cached in memory for further review and comparison with other data. Cached results are only available during the current session unless they are saved. Cached results are automatically a part of a Project that can be saved and loaded during the future session. Use the **Cache** button in **Simulation Results** dialog to cache the results. Cached results can be reviewed in several places:

- **Simulation Results** dialog **Cached Results** drop-down. Only one record in time can be selected results are shown
- **SimulationDialog – SimulationData** sidebar –allows to compare the results of different simulations. Select a record, right-click mouse and select Show Plot from the popup menu. (Hide Plot to remove the plot). The plot is displayed in a separate window (the user can return back to Simulation Dialog).
- **Compare Data Center** (select Data/Compare Data from the main menu, select simulation tab).

### 2.8.9 Modify/Review current filmstack

There are several options that allow to modify or change the current filmstack directly in Simulation Dialog:

1. Select Filmstacks Tab in the sidebar, select filmstack record in the list, right-click mouse and select **Set Filmstack** from the pop menu;
2. Select Current Filmstack tab in the sidebar, select element you would like to edit, right-click mouse and select **Edit** from the popup menu. Layer or Material dialog is displayed; it allows to change any parameters
3. Use **Filmstack Quick Creator** (bottom of the dialog). This option allows to type in directly the structure of the filmstack. The format of the input is similar to standard notation used to describe filmstack in literature:

**thickness2MaterialName2\thickness1  
MaterialName1\MaterialNameSubstrate**

where thickness1 & thickness2 are thickness of corresponding layers  
MaterialName is the name of the Layer or Substrate material. Example:

**2000.0Sio2.mat/Si.mat**

-  If ambient is not mentioned – void is assumed implicitly



### 2.8.10 Using templates

Templates can be used to streamline the process of selecting simulation conditions (they can though off as scripts). Custom templates can be defined in Configuration Dialog (Configure/Configure Software from the main menu). Applying templates is simple: select **Template** in the sidebar, select a template record, right-click mouse and select **Apply Template** from the popup menu. All the simulation conditions will be set – only need to select Simulate button.

### 2.8.11 Setting measurement conditions

Sometimes it may be useful to estimate the effect of resolution and or surface roughness on optical response. One can select Wavelength and Angle-of-Incidence resolution and estimate their effect on the results. In case of ellipsometry parameters simulations – the degree of polarization will be also shown.

- ❗ Surface Roughness has no appreciable effect on ellipsometry parameters – it should be used only for reflectance/ transmittance parameters

### 2.8.12 System specific parameters simulation

TFCompanion allows to simulate system specific parameters for RAE/RPE and RC E ellipsometry system. These simulations require additional information about the system (Analyzer/Polarizer azimuth angles, compensator parameters). When relevant parameter(s) (Alpha) is selected – additional tab panel

**Hardware configuration** is added to Measurement conditions. User can select appropriate conditions. In case of RCE system – information about compensator is also required. There are two options is setting compensator parameters:

- Load calibration from the file (space separated Wavelength[nm] retardation [deg] - one pair on each line);
- Select the type of the compensator and retardation at specified wavelength (retardation at other wavelength will be calculated assuming zero order plate)