

TFCompanion
Thin films analysis software
USER GUIDE
Version 3.0



Document History:

- Started November 9, 2005
- Update November 28, 2005 Added Linked layers and materials description (3.1)

Important Notice.

This manual describes functionality of TFCompanion ver.3.0

The evaluation copy of this software may have some limited functionality and intended **solely for evaluation/demo purposes**. Any use of evaluation/demo software for the other purposes is not authorized and constitute a breach of the license agreement.

After the purchase of this software, customer is provided with a **license key** that unlocks full functionality.

To evaluate this software – download and install a copy of the software (see installation instruction below in this manual) and request evaluation key at evaluation@semiconsoft.com

To license a copy of this software please contact leo@semiconsoft.com

To report a bug or problems please send email to bugs@semiconsoft.com

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System Requirements:

1. TFCompanion is Operating system independent – Windows, Linux, MacOS, Solaris (and other Unix OS) are supported. Java Runtime Environment (JRE) version 4.2 or higher is required.
2. VGA monitor – resolution 800x600 or higher (optimum resolution 1024x768)
3. CPU minimum 750MHz
4. Minimum 64MB RAM is recommended
5. 40MB free disk space

About this manual

This manual contains information about the features and options available in TFCompanion software. It is intended as an information resource for users of TFCompanion software. Several other information resources are available that may contain more up to date information:

- online help is included with TFCompanion distribution. Online help is updated periodically – the latest version can be downloaded <http://www.semiconsoft.com/html/Downlaod.htm>
- Tutorials are available at <http://www.semiconsoft.com/html/FaqTutorials.htm>

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About TFCompanion

TFCompanion™ is a powerful and user-friendly software application for thin film analysis and metrology.

Optical measurements are indirect in that they are measuring optical response of the physical properties not the properties themselves. One needs to solve an “inverse problem” in order to find the value of actual physical properties ((like thicknesses of the layers and optical properties of the materials) of interest. The “inverse problem” is solved numerically by finding the best fit between measured and calculated data. Physical properties are inferred from the model that gives the best fit. It is important to check the validity of the model, understand the sensitivity of the measured data to parameters of interest, and the correlation of these parameters in the context of specific measurement recipe, in order to get reliable results. TFCompanion simplifies this task by combining versatile analytical tools for interpretation of measured data. It allows simulation and sensitivity analysis to understand better complex dependencies and find optimal approach. TFCompanion gives the ability to estimate measurement/calculation errors, create and optimize measurement recipes. In research environment this allows to develop reliable and comprehensive measurement strategy; in production environment it helps mitigate tradeoffs between measurement accuracy and throughput.

TFCompanion provides flexible configuration of access level, feature set and capabilities. It supports both standalone and integrated (connected) mode. In integrated mode it can provide direct data acquisition and control of the measurements, in standalone mode - the measured data can be imported and analyzed off line. It supports Operator, Engineer and Administrator user levels with different access privileges and features available. TFCompanion is suitable for R&D and production environment.

TFCompanion family product matrix.

Several TFCompanion family products with different feature sets are available.

Product	Description	Standard level	Advanced level	Enterprise level
TFCompanion -E	Supports only ellipsometry parameters	✓	✓	NO
TFCompanion -R	Support only reflectance, transmittance, absorbance parameters (no ellipsometry)	✓	✓	NO
TFCompanion -RE	Supports all the parameters	✓	✓	✓

TFCompanion Feature matrix is presented in Appendix I.

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I. Software Installation, Configuration and Updates

1.1 TFCompanion Installation

TFCompanion software installer is available on CD or can be downloaded from Semiconsoft, Inc. website.

1. Download TFCompanion installer specific for your operating system (installers are available for Windows (win32), Linux, Mac (OSX10.x) and generic java installer for other systems). Installer can be downloaded from <http://www.semiconsoft.com/html/Download.htm> . Execute the installer and follow directions.

Note 1. TFCompanion requires Java Runtime Environment (JRE) installed on the target computer - JRE ver.1.4.2 or higher. Installer will try to locate Java installation on your computer; you will have an option to select the JRE to use. Bundled installer is available for Windows. On other OS please download and install JRE specific for this system. All MacOS have JRE preinstalled.

Note 2. If you have problem running the installer, try to download and install JRE first. If problem persist, hold CTRL key while starting and running installer – please copy the information in debug window (make a screen shot) and send to evaluation@semiconsoft.com

2. After installation is completed, you will need an evaluation key to start the application. Please send email to evaluation@semiconsoft.com. You will receive evaluation key – file “evaluation” that you will need to place in the `/init` directory of TFCompanion installation on your computer (**Fig. 1.1**).
3. You can now start TFCompanion. You will be asked to login (default user: Administrator; password: **psw**). Evaluation copy does not allow changing the password or creating a new user.

4. If you purchase a copy of TFCompanion – you need to register it to receive the license key. Select Help/Register from the main menu; fill the form and email created registration file “profile” to leo@semiconsoft.com. You will receive a temporary software license within 24 hours and a permanent license will be programmed and mailed to you shortly.
5. If you are using evaluation copy of TFCompanion – your evaluation key is valid for 30 days. Evaluation copy is TFCompanion –RE, Advanced version that is working in standalone mode. You can download a patch to allow integration with Ocean Optics hardware (see instructions below). Integration with other hardware is also available.

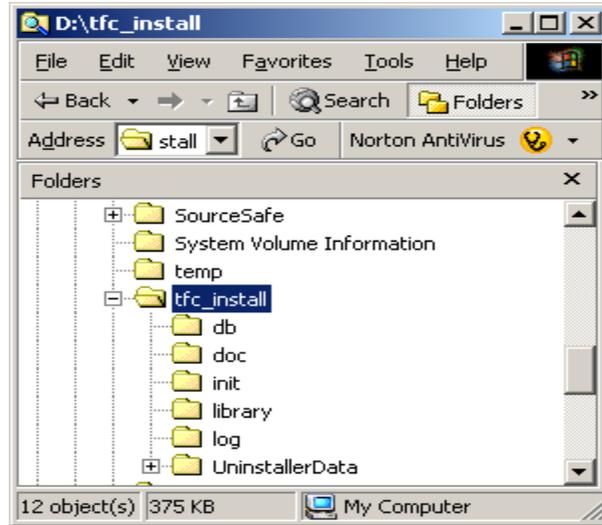


Fig. 1.1. TFCompanion installation directory structure
(in this case, tfc_install is the installation directory)

1.2 Integrating TFCompanion with hardware (optional).

TFCompanion can be integrated with hardware for complete data acquisition and measurement control of reflectance measurements. Integration is currently available for Ocean Optics (USB spectrometers) and Avantes spectrometers. Other hardware can be integrated on request.

 Currently, integration is only supported on Windows platform.

Following are details of integration with the Ocean Optics spectrometer.

1. You need to have Ocean Optics driver installed and OOIDRV32.dll library available. It is normally included with spectrometer; otherwise you need to request it from Ocean Optics.
2. Download the patch and unzip it in the installation directory of TFCompanion http://www.semiconsoft.com/html/oo_integration/unzip_oo_patch.zip

The patch contains following files:

- **//library/oo_io.dll** - connection library that communicates with the OOIDRV32.dll driver
- **/init/Hardware.xml** - XML configuration file that describes different hardware configurations. The default configuration is for Ocean Optics s2000 spectrometer
- **/db/mrecipes.db; db/mrecipes.idx** - database of default measurement and calibration recipes
- **/db/users.db; /db/users.idx** – database that contains different users (different capabilities and privileges). You will be asked to select the user and enter password (information is in the table below)

List of the Users:

User name	Password	Capability (all user have administrator level access)
Administrator	psw	Default account. Standalone operation: full capability
Admin_hw	psw	Integrated operations – full capability
Refl_user	refl	Standalone operations – only reflectance/transmittance capability
Refl_hw	refl	Integrated operations-only reflectance/transmittance capability
Ellips_user	ellips	Standalone operations – only Ellipsometry capabilities

3. Place Ocean Optics driver – file **OOIDRV32.dll** in the **//library** directory of TFCompanion installation (if you do not have the driver – please contact Ocean Optics)
4. Start TFCompanion and login as Refl_hw or Admin_hw user. Check the hardware configuration - select **Configure/Configure Hardware** from the main menu. The default-connected hardware is TFProbe_200 that corresponds to Ocean Optics s2000 spectrometer. You may want to check and change wavelength calibration coefficients for your hardware (save after change).
5. Connect computer to spectrometer using USB cable and make sure the driver is fully installed (please follow Ocean Optics installation instructions, you may also try run Ocean Optics data acquisition program that comes with spectrometer, to check that communication is working properly)

6. To check that TFCompanion communicating correctly with spectrometer: Select **Measure/Intensity Monitor** from the main menu. This should display continues data feed from the spectrometer (to adjust integration time, etc. – right mouse click on the plot).
7. TFCompanion uses measurement recipe to encapsulate measurement conditions. To review measurement recipes select: **Measure/Create Recipes** from the main menu. In the Measurements Recipes dialog select **Measurement recipes** database tab (side panel)- right mouse click and select **Review recipe**, select the record and select corresponding measurement (in the list of Measurements). Following build-in recipes are available:

Calib_refl – this recipe is used to make calibration before reflectance measurements (calibration sample is bare Si). You can review an example of calibration in the main window (Select Measure/Review Calibration/Refl) – the results (reflectance vs. counts) will be displayed.

Refl_raw – this recipe enables measurement of reflectance with selection of particular filmstack and calculation of the filmstack parameters. After measurement is completed, user can select filmstack and do data analysis

Refl_calc- this recipe enables integrated measurement and calculation of filmstack parameters. 2000A SiO₂/Si (calculated parameter is thickness) is associated with this recipe. Filmstack is loaded with the recipes – the thickness of the SiO₂ layer and measured vs. calculated data fit is displayed as a result of the measurement. User has an option to recalculate the results (without taking additional measurement, saving the measured reflectance, etc.)

1.3 Updating TFCompanion.

New TFCompanion updates are made available periodically (normally every month, or more frequently in case of bug fixes). One year of free updates and technical support is included with the purchase of the software. After first year, updates and technical support subscription is available at \$450/year (\$350/year academic).

1.3.1 Download and installation of updates.

There are several options available:

- use TFUpdater utility (recommended)
- download and install manually
- Check for updates and download from TFCompanion (install manually or using TFUpdater)

 It is strongly recommended to use TFUpdater utility for installation of the updates. Installation requires verification of subscription status (if information is missing the updated version will work only in evaluation mode) and check of TFCompanion.lax (configuration file). TFUpdater can be used with evaluation copy of TFCompanion as well.

 If you did not update TFCompanion since ~ March 2005 and have a valid subscription - you may need to update subscription information, please contact Semiconsoft, Inc.

a). *Use TFUpdater utility to download and install updates.*

TFUpdater is a separate program – the installer can be downloaded from <http://www.semiconsoft.com/html/Download.htm>

TFUpdater need to be installed in the same directory as TFCompanion (TFCompanion and TFUpdater executables should be located in the same directory).

TFUpdater will check if the new updates are available – it will prompt user to select Web update or select downloaded update file locally (**update.zip** file).

If new update is available the user will be prompted to download and install it.

b). *Use Help/Check Update option from the main menu.*

One can setup periodic updates check (every startup or every week, etc.) – this check will be performed in the background. If the new update is available – user will be prompted to download it. After download – exit TFCompanion and use either TFUpdater or manual installation.

c). *Manual installation*

Download new update (file update.zip);

Unzip file update.zip in the installation directory of TFCompanion

Check TFCompanion.lax file (back the current copy and open file in the text editor – Notepad, etc.).

Check that “library/jhall.jar” is on the class path. i.e. line “lax.class.path=” contains “library/jhall.jar” (add to the classpath if needed)

1.3.2 Materials database update

TFCompanion distribution includes a database of most commonly used materials. More extended materials database is available as a separate download from:

<http://www.semiconsoft.com/html/Download.htm>

After download one can unzip downloaded file in the **/db** directory of TFCompanion installation (in this case old materials database will be overwritten with the new database) or import selected materials from the new database (to import materials - unzip downloaded file in the new directory and use **Tools/Library Manager** from the main menu).

1.3.3 Optimizing TFCompanion configuration

TFCpanion can work with different versions of Java (1.4 – 1.5). Current version of TFCpanion (as of build 08.10.2005) is compatible with latest JRE 1.5. Most of configuration parameters of the Java Virtual Machine (JVM) that is used to run TFCpanion are defined in configuration file: **TFCpanion.lax**. This file is located in the installation directory of TFCpanion. TFCpanion.lax is a text file. Since build 02152006 special utility to change TFCpanion.lax settings is available at Configuration/ Launcher Configuration (from the main menu).

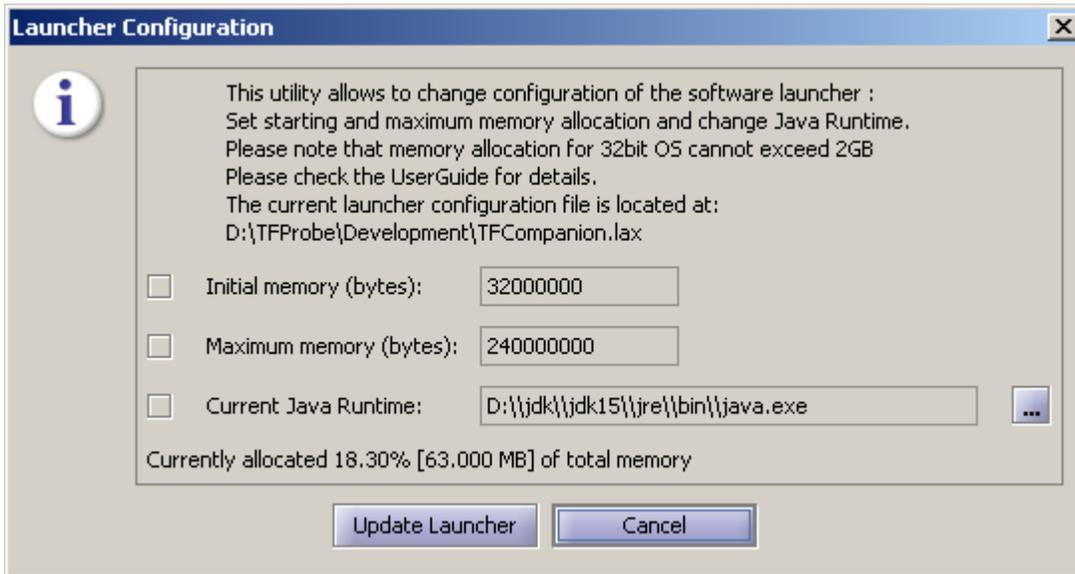


Fig. Launcher Configuration utility

To change parameter – check the box next to this parameter and edit the field. When Update Launcher button is selected – TFCpanion.lax file is updated (only parameter with enabled checked boxes will be updated). A copy of configuration file will be saved as TFCpanion.lax.org (backup copy). If TFCpanion.lax.org is already exist - TFCpanion.lax.org_1 file will be created, this way TFCpanion.lax.org file will always contain a copy of the original configuration.

a). Changing the Java version used to run TFCpanion.

Following is the snippet from TFCpanion.lax that defines JVM:

```
# LAX.NL.CURRENT.VM
# -----
# the VM to use for the next launch
```

```
lax.nl.current.vm=C:\Program Files\Java\jre1.5.0_03\bin\java.exe
```

Parameter "lax.nl.current.vm=" points to a JVM that is used to run TFCpanion

b). Changing memory allocation of TFCpanion process.

When TFCompanion is launched min and max memory allowed for this process is allocated. The default configuration does not set memory allocation explicitly and, instead, rely on default JVM configuration: normally min=64MB, max=64MB. This memory allocation is adequate in most cases. However, if TFCompanion is used heavily: for lengthy calculations, display of data and, especially, imaging applications- responsiveness and performance of the program can be improved by increasing memory allocation.

Following memory allocation is recommended:

1. Light to medium use (not imaging applications): min=64MB, max=120MB
2. Heavy use (imaging applications): min=64MB, max=400MB.

Please note that application will actually use only fraction of available memory (OS will not allocate memory until application request it)- so upper limit is more like insurance that program will not run out of memory.

Note1. Memory allocation is managed by OS, so if RAM memory is not adequate – paging (swapping of hard drive) will be enabled and this can slow execution.

Note2. In case of 32bit system max memory allocation cannot exceed 2GB.

Following is the snippet from TFCompanion.lax that defines memory allocation:

```

.....
# LAX.NL.JAVA.OPTION.JAVA.HEAP.SIZE.INITIAL
# -----
# the initial heap size for the Java VM
lax.nl.java.option.java.heap.size.initial=32000000

# LAX.NL.JAVA.OPTION.JAVA.HEAP.SIZE.MAX
# -----
# the maximum heap size for the Java VM
lax.nl.java.option.java.heap.size.max=240000000
.....

```

Memory in configuration file is defined in bytes.

1.3.4 Changing Color scheme.

Several color themes are available with TFCompanion and can be selected in **Help/Change Theme** (in the main menu). Selection of the color theme changes the matching set of colors that is applied to all visual components. The theme can be changed at any time. Selected theme is not currently saved, the setting is only valid during the session – default theme is always used at TFCompanion startup.

2. Starting TFCompanion

TFCompanion installer creates OS specific executable file and link (on desktop or startup menu). The executable file is located in TFCompanion directory (for windows TFCompanion.exe, Linux/Unix TFCompanion.bin). It is also possible to start TFCompanion from the command line using batch file (runTF.bat or runTF.bsh). Batch file startup can be normally used for debugging or experimenting with command line arguments (please batch file comments for details).

TFCompanion has two levels of password protection:

- License key password (optional). This password is assigned by the user and saved in the Hardware dongle or software license file (password can be changed or disabled at any time by the user). This password will apply to all users of software. If license key is password protected –TFCompanion will first request to input this password.
- User/password pair. Each user has specific password that is assigned when new user is created (default user is Administrator; password:psw).

During startup TFCompanion checks the registration (if it is evaluation copy then evaluation key is checked). After this TFCompanion loads configuration file TFComp_config.xml that should be in the **/init** directory; if file is not found - user is prompted to give its location. TFComp_config.xml defines all configuration properties of the program (locations of the databases, templates, defaults, etc.). After login, user can modify configurations properties using **Configurations** dialog.

TFCompanion will read configurations details from **TFComp_config.xml** and loads information from the database. If database is not found user is prompted to select the location of the database.

3. Using TFCompanion.

3.1 *Filmstack.*

Introduction.

Filmstack is an optical model of the sample that is measured - it consists of a substrate, collection of layers and an ambient. There is no limitation on the number of layers; they can be homogeneous or graded with specified profile. Substrate and ambient are infinite (do not have thickness), all layers have finite thickness. 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.

3.1.1 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 3.5)

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 can be linking 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.

Surface Roughness(random)

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 selected in Calculation dialog. 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 or oxide, etc. In addition, surface roughness can cause some depolarization and increase the noisiness of the data.

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

Incoherent layer

There is an upper limit on the thickness of the layer that can be measured using reflectance/ellipsometry methods at specific wavelength. 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 of light and its type (laser or lamp). In most cases, the thickness of few hundred μm 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”.

3.1.2 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 mean 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 need 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 (calculation recipe is stored in a separate database and may contains a reference to a filmstack record.)
 - Filmstack can be loaded as a part of a Measurement Recipe
 - 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).

3.1.3 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).

3.1.4 Creating Filmstack Directly

3.1.4.1 Adding a Layer.

Method 1:

Select **Layer Add** from the Filmstack menu (main menu) or Select  icon in the Toolbar. The list of materials available in the current material library will appear in a separate window. The name of the library, its location and creation date are shown in the status bar at the bottom of the window. Select (click on) the material you need. The name of the material and comments appear in the respective text fields. At this point you can **enter** selected material (button **enter**), **view/edit** material (button **View/Edit**) or **cancel** (button **cancel**).

- Select **Enter**. The dialog with a text field to input Thickness will popup. Thickness must be entered in Angstroms. Click **O.K.** button and the new layer will be added to the current filmstack. Click **Cancel** button if you changed your mind – the layer will not be added to filmstack.
- Select **View/Edit**. Material dialog is displayed. This option allows reviewing and/or editing of Material properties (any changes to the material need to be saved to the Database before closing Material dialog, otherwise they will be lost).

Method 2:

Use the left sidebar (select Materials tab to display the materials record) to select the material; right-click mouse to select (Add Layer or Review/Edit option as above)

3.1.4.2 *Deleting a Layer.*

Select **Layer Delete** from Filmstack dropdown menu or select  icon from the Toolbar. If there is only one layer - it is removed from the filmstack. If there is more than one layer a dialog with a list of layers is displayed. Layers are numbered from the substrate, i.e. if there are 2 layers the bottom layer is #1 the top layer is #2. Select the layer you would like to delete and click **O.K.** button. Selected layer is removed from the filmstack.

3.1.4.3 *Inserting a Layer.*

Method 1:

Select **Insert Layer** from the Filmstack dropdown menu or select  icon from the Toolbar. The list of materials available in the current material library will appear in a separate window. All the functionality is the same as for **Add Layer**. After material is selected and the thickness is set, a dialog will appear with a list of all available layer #'s where a layer can be inserted. These numbers correspond to the location of the inserted layer. For example, if filmstack has two layers Si3N4/Sio2/Si-substrate then the new layer (poly) can be inserted in position #1 (Si3N4/Sio2/poly/Si substrate) or position#2 (Si3N4/poly/Sio2/Si substrate). Note. If there is one layer, dialog will not appear and the new layer will be inserted to the only available position#1 (previous layer will move up correspondingly).

Method 2: Use the left sidebar (select Materials tab to display the materials record) to select the material; right-click mouse to select Insert Layer from the popup menu (the same action as in Method 1 above)

3.1.5 Using FilmstackCreator Dialog

Using *FilmstackCreator* allows one to quickly create or modify Filmstack. Select **Filmstack/ Filmstack Edit** from the dropdown Filmstack menu or select  icon from the Toolbar– FilmstackCreator dialog will appear. Current filmstack is listed in the Filmstack List There are two ways of editing creating filmstack in the Filmstack creator:

- Quick Filmstack -- for advanced users;
- Regular Filmstack – for novices.

RegularFilmstack and QuickFilmstack are interchangeable, i.e. filmstack created using Quick Filmstack Creator appears in the RegularFilmstack window as well as in the QuickFilmstack window.

Either way, after filmstack is created click **OK** button, program returns to the main window and filmstack is updated with new data. Selecting **OK** button commit all changes to the database, selecting **Cancel** button – rollback all the changes.

 If new or modified filmstack is not saved to the database (**Save** button) it will be available only during current session

3.1.5.1 *Quick Filmstack*

Quick Filmstack is designed for advanced users who know the available materials and their exact names. All filmstack can be typed in accordance with the common notation used in the printed materials. The signature is:
 <top layer></><next layer></>...</><bottom layer></>< Substrate material's name >.

Each layer has a following signature:

<Thickness in Angstroms><material's name>

Example: 100Gaas.mat/100Sio2.mat/Si.mat

After typing this String, click Enter. The string is parsed and filmstack is created – materials appear in the Filmstack window. If one of the materials is not recognized as a qualified name -- the error box appears and Quick Filmstack string is cleared. If the thickness value is missing or not recognized – dialog with the input field appears prompting to input thickness (in Angstroms) for particular layer.

The same way Quick Filmstack can be used to modify/edit existing filmstack. When the FilmStack Creator dialog appears, Quick Filmstack string corresponding to the current filmstack is set in the window. The user can manually modify materials, thicknesses, and insert or add new layers.

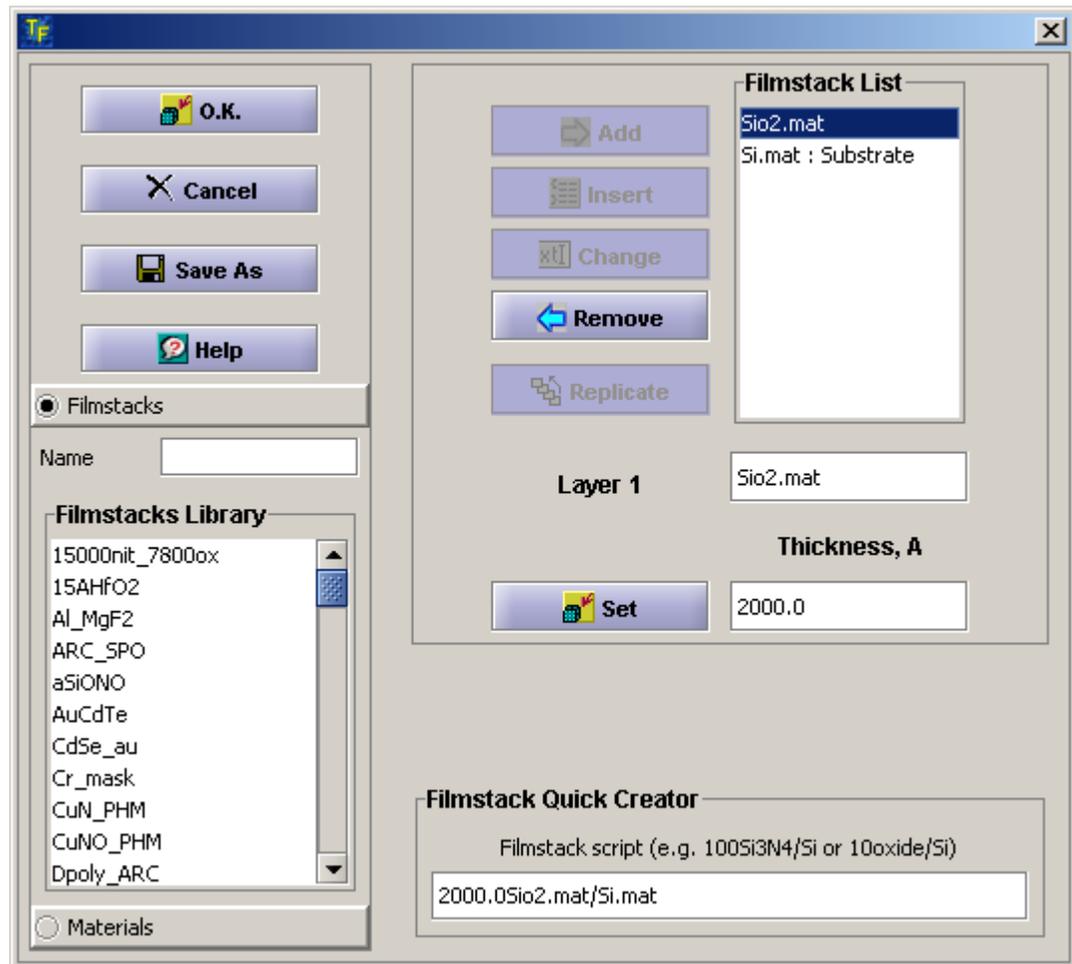


Fig. 3.1.5 FilmStack Creator Dialog.

3.1.5.2 Regular Filmstack

RegularFilmstack is designed for novices, who may not know the exact material names. All materials available in the database are listed in the left sidebar library.

The Current filmstack is listed in the Filmstack List window and in the QuickFilmstack window.

User has full control over filmstack, he can add, insert, remove or change any layer or substrate, set or change the thickness of any layer.

- **Add Layer** Select material in the list and use **Add** button.
- **Insert Layer** Select material in the list, select the place to insert in Filmstack list (new layer will be inserted under select layer) and use **Insert** button.
- **Removing Layer** Select the layer you want to remove in the Filmstack List use **Remove** button and the layer is removed from the filmstack.
- **Changing Layer** Select material in the list, select the layer you want to change/substitute, use **Change** button – new material will be set to selected layer
- **Replicate layers** Select the layers you want to replicate, use **Replicate** button; you will be prompted to select the number of replication. Selected group of layers will be replicated specified number of times (added on top of select group)
- **Set thickness** Select the layer in the Filmstack List – selected layer and its current thickness is displayed. Edit the data in the Thickness text field and use **Set** button to update the thickness.
- **Review layer** Double-click on the layer in the **Filmstack** List – the Layer dialog with all the information about the layer is displayed. You can edit Layer using - all the updates are carried back to filmstack after Layer dialog is closed.

3.1.6 Caching Filmstacks and Filmstack History

While working on the project user may change the original (starting filmstack). Each new change to the filmstack is done directly on the object not on the copy; as result-previous versions of the filmstack, unless saved to the database, are lost and cannot be recovered. User has two options either save filmstacks to database or save it to cache (memory). The difference between these two options is that database will allow using filmstack during future session for all the projects; caching saving filmstack to a current project and allows returning to this filmstack only during the current session (user can also save the Project to the database and reload it during next session). It may be useful to save intermediate filmstacks to cache and, perhaps, later save some selected filmstacks to persistent storage.

Cached filmstacks can be reviewed during the session and user can return to them at any point. To cache current filmstack use **Filmstack/Cache Filmstack** menu item (or use  toolbar icon). To review cached filmstacks use **Tools/History** menu item (or use  toolbar icon). The **FilmstackHistoryDialog** appears and displays all currently cached filmstacks. User can review filmstacks and make any of filmstacks “current”.

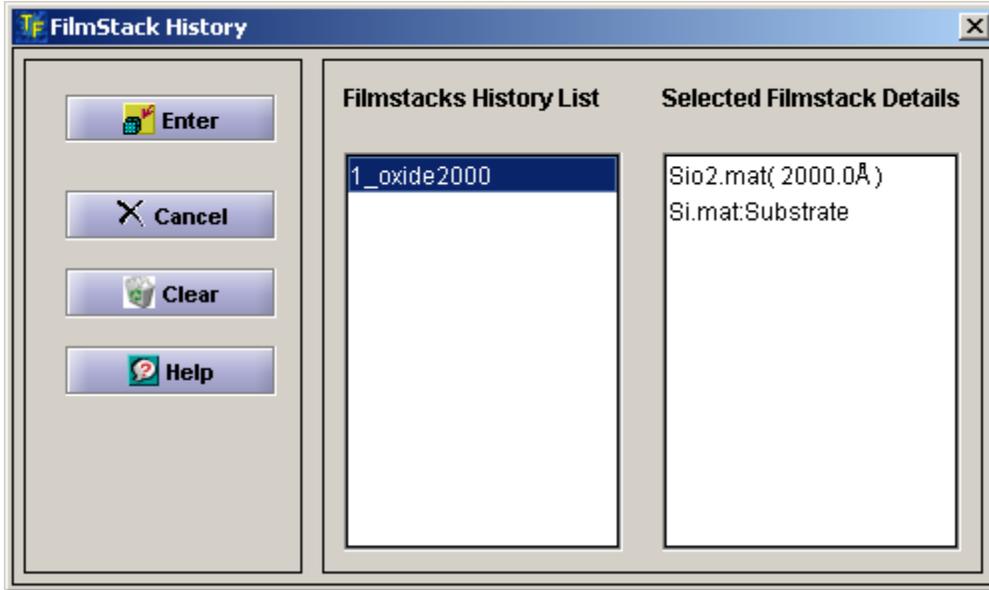


Fig. 3.1.6 Filmstack History dialog.

Section 3.2 Parameters Calculation

Optical measurements are indirect and filmstack parameters are inferred from the best fit of the measured data to the data generated (simulated) from the selected optical model of the filmstack. This process of finding parameters of the filmstack based on the measured data (target) is mathematically known as solution of inverse problem. This problem can be solved analytically only in limited number of simple cases. General solution is achieved by numerical methods of minimizing the difference between measured (target) data and simulated data, using selected optical model of the filmstack. Selected parameters of the filmstack are adjusted until the minimum is achieved.

$$\chi^2 = \frac{1}{N-M+1} \sum_{i,j} \left(\frac{p_{ij}^{meas} - p_{ij}^{calc}}{\sigma_{ij}} \right)^2 w_{ij},$$

where index i indicates the type of the parameter

(e.g. in the case of ellipsometry measurements

$i=0,1$ with 0 - corresponding to Delta, 1 - corresponding to Psi)

index j indicates the point in the data set;

P_{ij}^{meas} is a measured parameter i at point j ;

P_{ij}^{calc} is calculated (or generated) parameter i at point j ;

σ_{ij} is standard deviation of the measurement parameter i at point j ;

w_{ij} is weight of parameter i at point j ;

N is number of measurement parameters*points;

M is number of calculated filmstack parameters;

χ^2 is a merit function that is being minimized

TFC Companion uses modified Marquardt-Levenberg minimization that gives fast and robust convergence. However, this method is sensitive to the starting values of the minimization (that is initial values of the filmstack). If a starting value of a parameter is relatively “far away” from the correct value, minimization can be trapped in the local minima, and global minimum –real solution—will not be found. It is especially an issue when the films in the filmstack are thick – thickness more than one cycle for the wavelength of measurement. (The optical cycle is a thickness of a film corresponding 360 deg. change of a phase. Actually, many commercial ellipsometers are measuring phase (i.e. DELTA) in the 0-180 degree range, so practical cycle thickness is twice thinner in this case).

There are several methods that can be used to improve chances of better convergence and avoid the local minima:

- Check before starting calculation. Use **SimulateFit** option in the main screen to check how close (or far away) is your initial filmstack model to the correct result. **SimulateFit** generates the data set using your filmstack model, the data set is matching the measured data (parameters, wavelength, angle ranges, etc.); it does NOT do minimization. The source of discrepancy is normally easy to see and fix in the simple filmstacks.
- Use **Order Search** (sometimes called Grid search) if thickness of some layers is not known reasonably accurate. Order Search can be done on one or several layers. In a nutshell, the idea of the Order Search is to perform minimization with different starting values, compare the Goodness-of Fit (GOF) of the results and select the result with the best GOF as a solution. Order Search can be set in the Layer dialog. Details of the OrderSearch implementation are discussed below.
- Use **constraints** on the calculated parameters. Constraints allow limiting permitted range of the calculated parameters. In general, minimization program works best without constraints or with very loose constraints. However, there are situation, e.g. correlation between calculation parameters is strong, when the use of constraints is necessary. **Note**. Do not set constraints too tight

In the majority of practical cases calculation can be done quickly and the results are reliable and unambiguous. However, in the complex cases or during the development of the model one may need to be patient. Calculation dialog provides full control over minimization process and all available information and tools to make the process as convenient as possible.

The following steps need to be performed in order to do the calculation:

1. Create the filmstack
2. Load the measurements
3. Select calculated parameters and set calculation conditions (constraints, order search, etc.), if necessary.
4. Calculate

Note. In the integrated version of TFC Companion several steps are encapsulated in the “measurement recipe”. In this case, user loads measurement recipe and select Measure.

3.2.1 Create a Filmstack

Creating of the Filmstack is discussed in the previous section **3.1 Filmstack**

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After filmstack is created, its graphical representation as a stack of layers (buttons) is displayed on the main screen (Filmstack tab in Filmstack panel). More details about filmstack are displayed in the Parameters and Records tabs of the Filmstack panel. Clicking on the layer or substrate brings **Layer Dialog** with all details of material and layer parameters.

3.2.2 Select parameters that should be calculated or/ and displayed

Any filmstack parameter can be selected as calculated, displayed or both:

- Calculated parameters are, well, calculated – their value is “adjusted” during the fitting process.
- Displayed parameters are not adjusted directly during fitting process but are displayed at the end of the calculation. For example, photoresist layer dispersion can be represented using Cauchy model. Calculated parameters will be Cauchy coefficients. However, the user is interested in n, k values at specific wavelength. N, k at specific wavelength can be selected as a displayed parameters. At the end of the calculations, the program will calculate selected n, k values using Cauchy coefficients and display them.

In most cases parameters selection can be done in the **Parameters** tab (**Filmstack panel** in the main dialog screen): select thickness calculation using **Solve** check boxes in **Filmstack Details** table and **Solve for** panel n, k related parameters.

Note. **Solve for** can be used for selection of “direct” n, k calculation and for “indirect” n, k calculation in case of parameterized materials. For example, in case of the Cauchy material n calculation selection (at specified wavelength) will prompt user to select “actually” calculated Cauchy coefficients (n value at specified wavelength will a “displayed parameter”. One can select **all** keyword instead of wavelength – in this case all the n, k values matching measured data wavelengths will be calculated, e.g. this can be used to calculate optical properties of a substrate material, etc.

Full access to all parameters is available in the Layer Dialog that can be started by clicking on the layer. Parameter can be marked as calculated and/or displayed. Selected parameters are displayed in the **Selected Parameters** panel (click on Calculated or Displayed tab to view respective parameters).

3.2.3 Select Order Search Option (optional)

Order Search option can be selected in the **Layer Dialog**. By default OrderSearch is set to *None*. There are two OrderSearch option available: *Restricted* and *Standard*.

Standard OrderSearch automatically selects a span of two cycles: one cycle up and one cycle down from the current thickness. If current thickness is less than a cycle thickness – only one cycle (up) is selected.

Custom OrderSearch allows custom selection of the *Minimum Thickness*, *Maximum Thickness* and *Number of Points* in the grid.

3.2.4. Setting constraints (optional)

Every calculated filmstack parameter can be constrained, i.e. the range of allowed values can be limited. Constraints can be set in the Calculation Dialog, which displays a table of all the calculated parameters; minimum and maximum constraints values can be

edited directly in the table. In addition, layer thickness can be constrained directly in the main screen (Parameters tab in Filmstack panel).

3.2.5. Load the Measured data

Measured data can be read from a file or input manually from the keyboard.

3.2.5.1 Reading From the File.

From the main menu select File-Import Measured Data, you can also use **M** icon in the toolbar – user is prompted to select the measured data file (alternatively, drag-and-drop the file directly to the table (Measured data table)). Generic measurement file Reader will detect automatically the format and read the file appropriately. If the format is not supported or file is corrupted an Exception is thrown and appropriate error message is displayed.

Currently supported measured data formats are Rudolph (data format used for FE, SpectraLaser and Matrix series by Rudolph Technologies, Inc.), Woollam (data format used for SpectraEllipsometers by J.A.Woollam, Inc), SOPRA (data format used for Spectroscopic Ellipsometers (EG and GESP) by SOPRA), BIL (data format used by Beaglehole Instruments), JY (data format used for Spectroscopic Ellipsometer by Jobin-Yvonne (Horiba)), Nanofilm data format and TFComp format (data format generated by the simulation engine of this TFCompanion product). Detailed specification for TFComp format is included in Attachment II. The latest version is available at http://www.semiconsoft.com/html/download/docs/Import_data_fomat_for_TFCompanion.pdf

Several data sets (different data in one or several files) can be loaded and used in one calculation (calculation using same filmstack). When user attempts to load new data and there is already data in the table (case of several measured files) – user is prompted select to either Add new data to existing or discard the old data.

After measured data file is read - the data is displayed in the **Measured Data** Table. Each row of the table represents one measured point, Delta, or Psi or CosDelta or TanPsi or Reflectance.

First column (**Use**) contains checkboxes. Selected checkbox indicates that the measured point (row) is selected otherwise it is ignored in optimization. By default all measured points are selected. This gives a fine-grained control of what points are used or ignored. The data is also displayed in the graphical form, the chart of each measured parameter – in a separate tab.

Measured Data panel can be zoomed to full screen – right-mouse click on the panel border (top border) and select **full screen** (you can also right-mouse click on Table and select Full Screen from the popup menu). Full screen mode also enables additional capabilities to manipulate the charts.

3.2.5.2 Manual Input.

By default **Measured Data** table is not editable. Right click mouse on the table and select **Edit Table**.

After you entered or modified the data – right mouse click and select **Set Data** this will enable checking and parsing of the input. In general, it is recommended to use a text file to input the data in all but very simple cases.

3.2.5.3 *Levels of Measured Data Control (optional)*

There are three levels of measured data control that have different granularity and functional goals:

1. *Measured point level control*

This has the finest level of granularity and is implemented using checkboxes in the **Measured Data** table. When measured data is loaded, all points are selected (checkboxes are checked). User can uncheck the box, in this case corresponding measurement point is removed from the data set. This control is intended to use for de-selecting some points that are clearly erroneous.

2. *Weight coefficient and standard deviation (s.d.) control*

Weight coefficients setting has also measured point level control. It allows setting of relative weight of measured points in the minimization process. These weight coefficients may be based on measurements accuracy or other consideration. It is generally more flexible mechanism than removing inaccurate points all together. Standard deviation is another, more natural, way of setting relative weight to different measurement points. In fact, reasonably accurate estimate of s.d. helps a lot to improve convergence and make minimization process more reliable. It also ensures that χ^2 is unbiased estimator with expected value ~ 1.0 and the confidence intervals of calculated parameters make sense. In some cases s.d. is included with the measurement data. One can also set s.d. manually the same way as the weight. The most convenient way to do this is to use **Data Selection Dialog/Spectrum View Dialog** that can be accessed from the **Calculation dialog**.

3. *Spectra level control*

TFC Companion group measured data sets in spectra. A spectrum is a set of measured points that has the same type and value of the fixed parameter, the same type of variable parameter and the same type of the measurement type. For example, Normal Reflectance spectrum will have angle-of-incidence 0 (fixed parameter), variable parameter – wavelength, measurement type – reflectance. Ellipsometry spectrum can be a collection of Delta, Psi pairs measured at the same condition. Actual measurement from the instrument can correspond to several spectra, e.g. in VASE measurements measurement taken at each of the angles of incidence will correspond to one spectrum. Different measured parameters supported by TFC Companion are described in Appendix III. The most recent version is available at

http://www.semiconsoft.com/html/download/docs/Parameters_conventions_TFCopanion.pdf

This control allows selecting or de-selecting (ignoring) different spectra of the measured data. It is implemented in the **Data Selection Dialog** that is called from the **Calculation dialog** (see next section for more details).

3.2.6 Starting Calculation.

There are two calculation options:

- Select Calculate in the main dialog the results of the calculation will be displayed and fitting plot will be displayed in the main dialog. In the case the default setting of the calculation options is used and results are cached automatically.
- Select Actions/Calculate or  icon to start Calculation Dialog. Use of the Calculation dialog gives more options to select the data, set parameters properties and review the results

Calculations can be repeated with different calculation conditions, etc., as needed.

3.2.7 Select Calculation Conditions and Options (optional)

Calculation Dialog allows full control over calculation process and conditions.

To start *Calculation Dialog* - select **Actions/Calculate** in the main menu. *Calculation Dialog* allows selection of a subset of the measured data to use in the calculation, change display/calculate flag of the parameters and select optimization conditions.

3.2.7.1 Selecting Measured Data

Measured data can frequently be grouped in spectra e.g. measured data can contain 2 or more wavelength spectra each taken at different AOI. This option allows Spectrum level control of the data i.e. using subset of the measured data in optimization. Clicking **Select Data** button will show **Data Selection Dialog** page. This dialog shows a list of spectra (each spectrum is identified by spectral variable – wavelength or angle- and icon indicating the type of the data). Clicking on the spectrum in the list will display additional information about the spectrum: range, value of the fixed parameter. By default all spectra are selected. CheckBox **Select Spectrum** shows whether current spectrum is selected or not. To change the status of the spectrum check/uncheck this checkbox. To select/deselect all the spectra check/uncheck the **selectAll** checkbox.

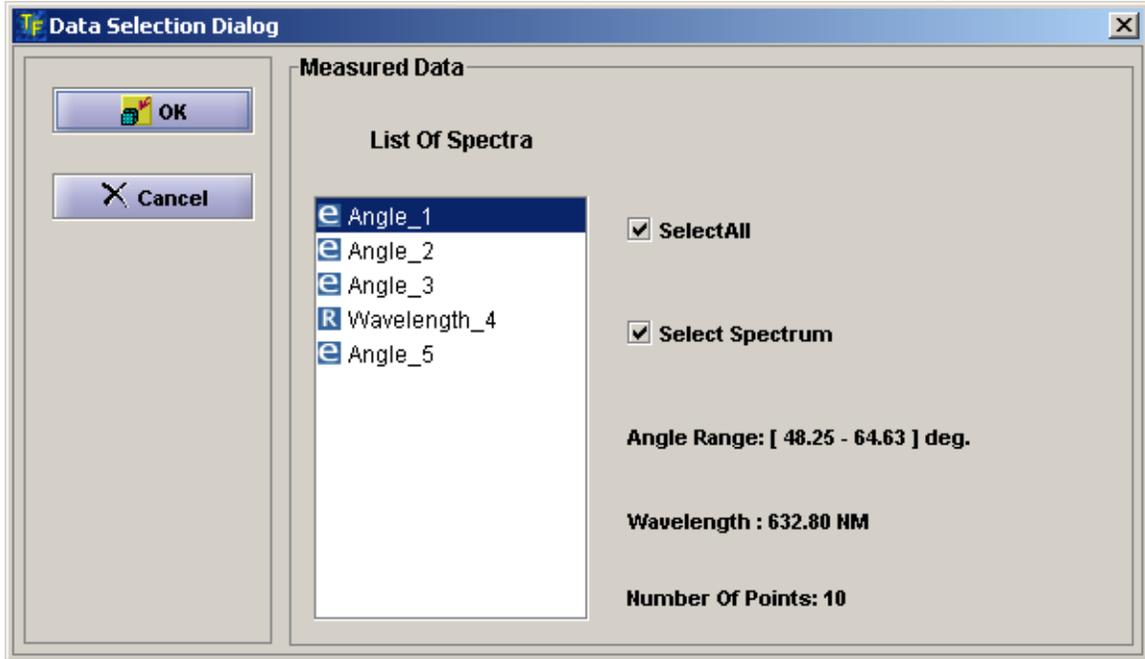


Fig 3.2.7.1 Review measured data in Data Selection Dialog.

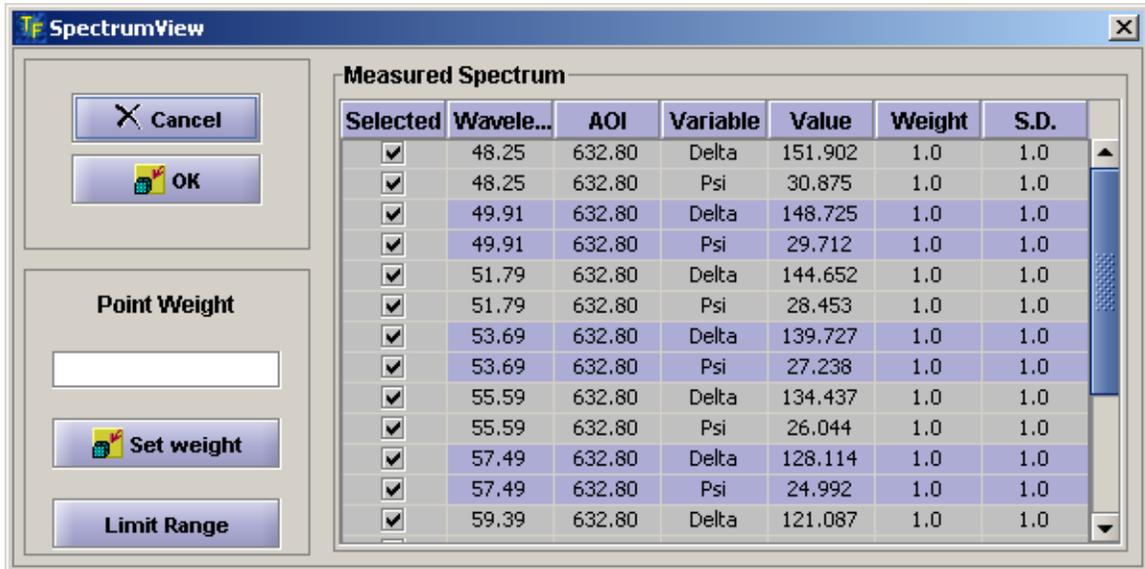


Fig 3.2.7.2 Review measured data of selected Spectrum in Spectrum View Dialog (double click a record in Data Selection Dialog).

3.2.7.2 *Change Parameters properties.*

All the parameters that are selected as Displayed or Calculated are listed in the Parameter table. All the parameters properties displayed in the table can be changed directly:

- Checking/unchecking check boxes in the Iterate or Display columns change the status of the parameter in the relevant row.
- Edit the parameters constraints directly in the table.
- Edit the starting value of the parameter

3.2.7.3 *Confidence level.*

Allows to select different levels of confidence (from σ to 3σ , default is 90%). Confidence intervals are calculated using standard statistical methods. Confidence intervals are displaying for all the calculated parameters. These data is displayed in the parameters table in a separate column after calculation is completed.

3.2.7.4 *Plotting Options.*

There is a choice of three options of displaying a plot of Calculated vs. Measured data fit:

- *No plot (None checkbox)*. Plotting is disabled.
- *Displaying after the last iteration (AtTheEnd checkbox)*. The plot is displayed after the end of calculation.
- *Displaying after each iteration (Continuously checkbox)*. The plot is displayed after each iteration as calculation progresses. This option is not available with OrderSearch. This option is recommended only in research mode, as it slows down calculations – user can review the results of the calculation after each iteration step.

3.2.7.5 *Calculation Conditions.*

These set of parameters are related to optimization termination conditions (maximum number of iterations and Goodness of Fit (GOF)) and Advanced Controls – parameters to customize Marquardt-Levenberg minimization process.

In majority of cases default optimization parameters are quiet good and no adjustment is needed. In a rare occasion, when it may be useful to customize some of the parameters full access to these parameters is provided in the **Advanced Controls** dialog page. Advanced Controls buttons starts this dialog with appropriate text fields pre-populated with default values of the parameters. Access to following parameters is provided: starting value of Lambda (startLambda), Lambda scaling coefficient (LambdaScale), maximum value of Lambda (Max. Lambda), Number of Significant Digits (NumSignDigit), value of a Gradient (Gradient), value of Residual Sum of Squares (ResSumSquares), value of Forward to Center derivative calculation condition.

There are several stop conditions that are implemented in minimization procedure to address finite numerical precision. Minimization stops if the point is close enough to the minimum or cannot find minimum as demonstrated by:

- a). Gradient is smaller than specified value;
- b). Residual sum squares is not changing between iterations (changing less than precision);
- c). Number of significant digits (calculated from covariance matrix) is more than specified value;
- d). Marquardt parameter is bigger than specified value (in most cases means -can not find minimum);

Advanced control parameters very seldom have any effect of the calculation results. Detailed description of the Marquardt-Levenberg minimization can be found in William H. Press et al. "Numerical Recipes in C", Cambridge Univ. Press, 1992 (ISBN 0-521-431-8-5) pp. 683-689.

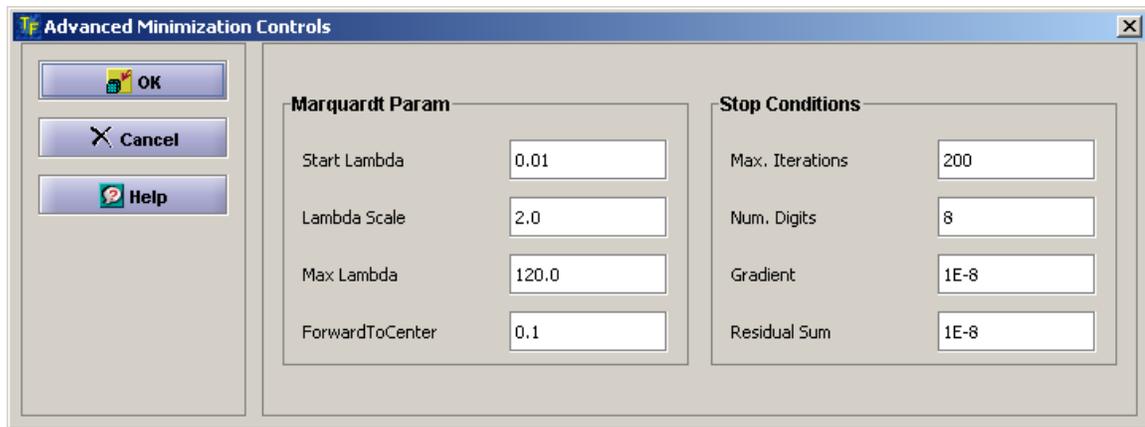


Fig 3.2.7.3. Advanced Minimization Control

Note. The default calculation conditions are set for the general case of a biased minimization (s.d. of the measurements is not known – set to 1.0). If the s.d. deviation is known some of the stop conditions can be relaxed (gradient and residual sum – increased, Num. Digits - decreased). However, these changes are advised only in the case when calculations take a long time and reduction of the number of iteration may make sense.

3.2.8 Using Calculation Results.

After calculation is completed the results and a fit plots are displayed. The results can be exported in the text file. Calculation dialog offer additional options of caching results (to memory), for later review; review of the detailed calculation results, e.g. correlation coefficients, etc.

If calculation is performed directly from the main dialog – the results of calculation are cached automatically.

Cached results can be reviewed in Compare Data dialog (Data/Review Data from the main menu). Compare Data dialog offer different options to compare results and save charts.

To export the results of the calculations:

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- In *Calculation Dialog* – use **Export** button
- In case calculation were done from the main dialog (results were cached in *Calculation Dialog*) – use **File/Export Calculation Results** from the main menu;

Note. In case of Beaglehole Instruments data. The original measured data file is updated with the calculated data (backup copy of the original file is automatically created). In other cases, the data is exported in the new text file.

3.3 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.

Two basic functions can be performed in Simulation dialog:

- Calculation of the selected parameters as a function of the selected variable (e.g. Delta vs. wavelength) or two variables (e.g. Delta vs. wavelength and AOI (Angle-Of-Incidence));
- Calculation of the sensitivity of selected parameters to selected variable as a function of another variable (e.g. Delta to AOI ($\partial\Delta/\partial\varphi$) vs. wavelength) or two variables (e.g. Delta to AOI ($\partial\Delta/\partial\varphi$) vs. wavelength and layer thickness);

Simulated parameters are: Ellipsometry, Reflectance and Transmittance parameters (see http://www.semiconsoft.com/html/download/docs/Parameters_conventions_TFCompanion.pdf)

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.

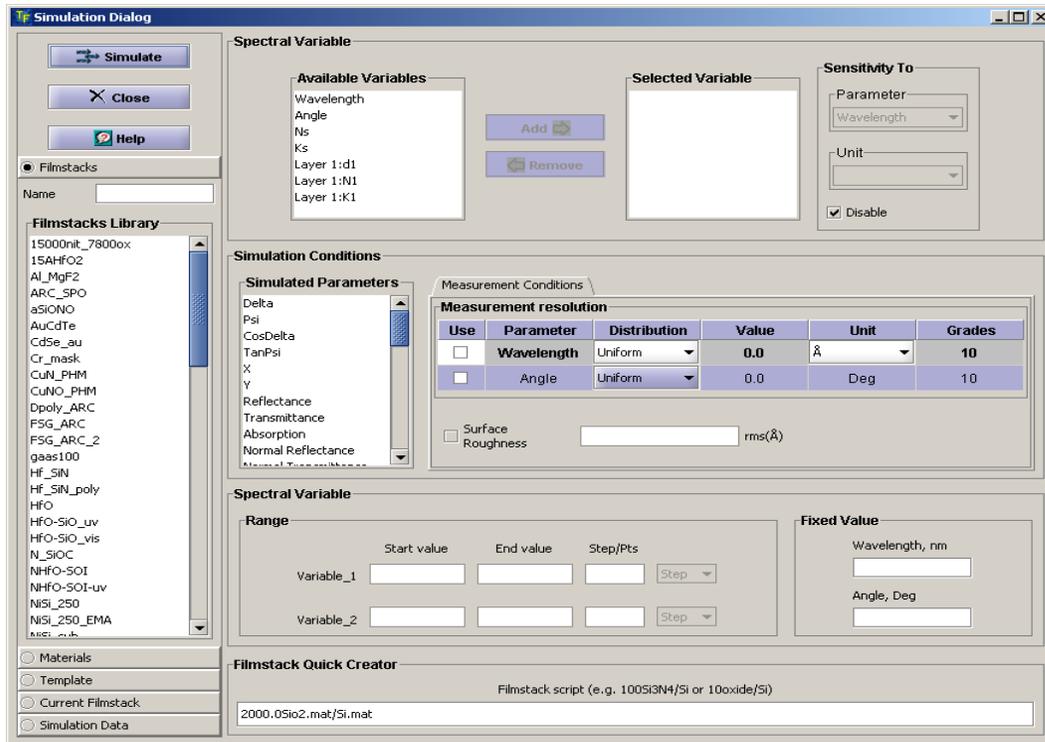


Fig. 3.3.1 Simulation dialog

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*

3.3.1 Selecting Variable

To select an appropriate variable record in the **Available Variables** List and use the **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.

3.3.2 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.

3.3.3 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.

3.3.4 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)

3.3.5 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.

To calculate Sensitivity click **Evaluate** button

3.3.6 Presentation of Data and Saving

In the case of one variable, the results of the simulation are presented in the **Simulation Results 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 **Simulation Results Dialog** are using following default units:

- For reflectance, transmittance and absorbance -- %;

- For ellipsometry 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.

a) 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/docs/Import_data_format_for_TFCompanion_software.pdf.

This file can be imported as a “measured data” in TFCompanion. For details see Optimization (section).

Plot can saved in JPEG format. User is prompted to select the name and location of the file. Default location is **<installation directory>\simulation\<>name>.jpeg**

b) Printing or Saving results in HTML format .

Select **Print** button to preview and edit Table of the data in HTML format or print a plot. HTML document is created and rendered in the internal browser (**HTMLPreviewDialog**). User can edit the title of the Table (use **setTableTitle** button to reset the title). HTML formatted table can be printed (use **Print** button) or save to a file (use **saveHTML** button). Saved HTML files can be imported to your favorite word processor or displayed in the browser.

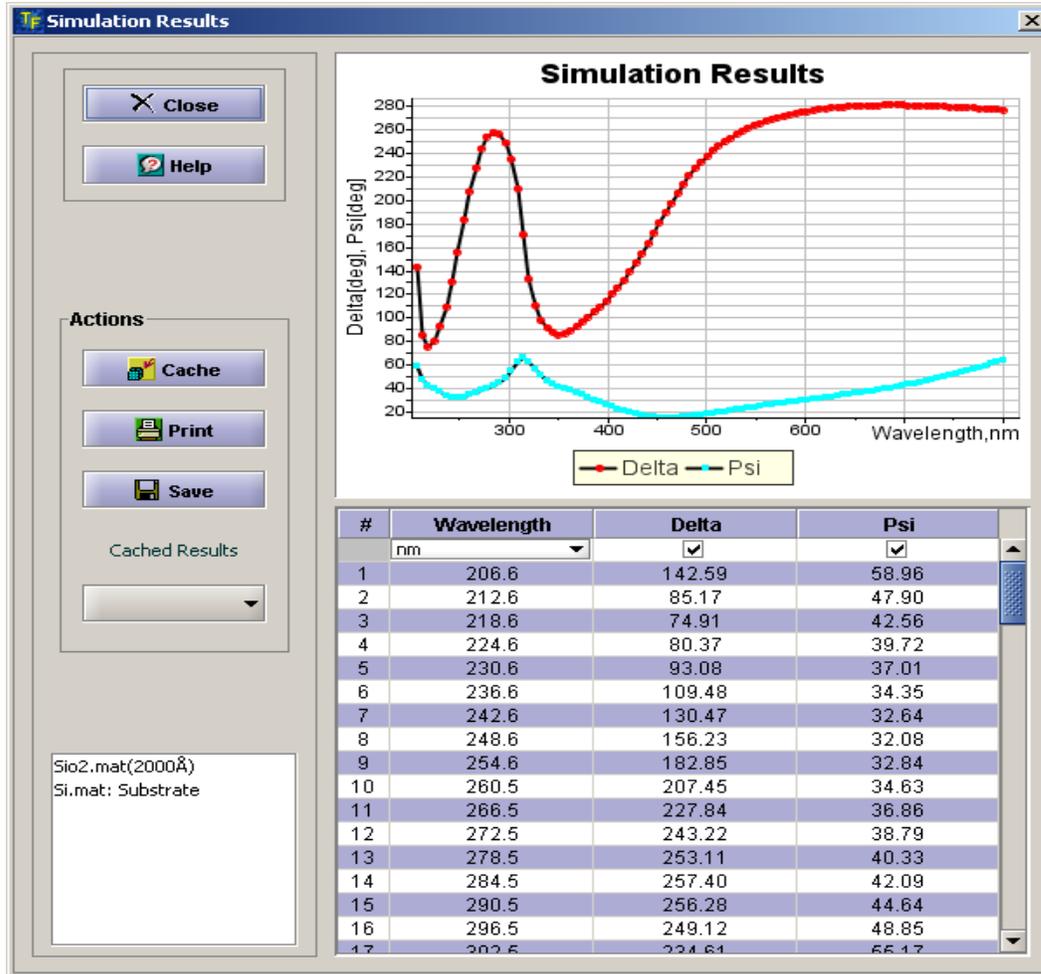


Fig. 3.3.2 Simulation Results dialog

c). 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 reviewed in several places:

- **Simulation Results** dialog **Cached Results** drop-down. Only one record in time can be selected results are shows
- **Simulation Dialog – Simulation Data** sidebar –allows comparing 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).

d). 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**

i If ambient is not mentioned – void is assumed implicitly

e). 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.

f).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.

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

g) 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)

3.4 Creating and Modifying Materials

TFC Companion software comes with the extensive database of commonly used materials; additional materials database is available for download free of charge. User can import materials from the text file (SOPRA or TFC Companion materials format are supported) and export materials from the database to a text file. User can also create new materials and manually input specific parameters.

TFC Companion supports two types of the materials: Tabular and Parameterized.

a). *Tabular materials* – materials properties are represented as a table of Optical constants vs. wavelengths. Optical for other wavelengths within the range are found using linear interpolation. Extrapolation outside the defined range is not supported.

b). *Parameterized materials* – optical properties are represented using parameterized mathematical equations. Parameterized materials are representing, in most cases, more accurately the dispersion of real materials. Some parameterized materials are using empirical equations (e.g. Cauchy, Sellmeier) others are consistent with Kramer-Kronigs relations and rigorously derived (e.g. Tauc-Lorentz and Harmonic oscillator).

New materials can be created or imported and existing materials modified using **Materials dialog** or **Layer Dialog**. When material is imported, created or modified in **Layer Dialog** – this material is becoming a part of this Layer (and relevant filmstack).

i All the materials imported, created or modified in the **Material** or **Layer Dialog** should be explicitly saved to Materials database (use **Save** button) lest they will be lost in case of **Material Dialog** or available only as part of the relevant layer in case of **Layer Dialog**.

Material Dialog allows performing the following functions:

1. Create new materials
2. Save /Rename materials
3. Fit parametric material to a Tabular (finding initial values);
4. Render graphical representation of the NK vs. wavelength;
5. Calculate NK values for the parametric materials (Cauchy, EMA etc.)
6. Export and Import materials data in/to text format.

Materials dialog can be started using *Tools/Material Editor*. **Layer Dialog** can be started from various locations in the program (where filmstack is displayed) by clicking on the relevant filmstack layer (double click if displayed in the list).

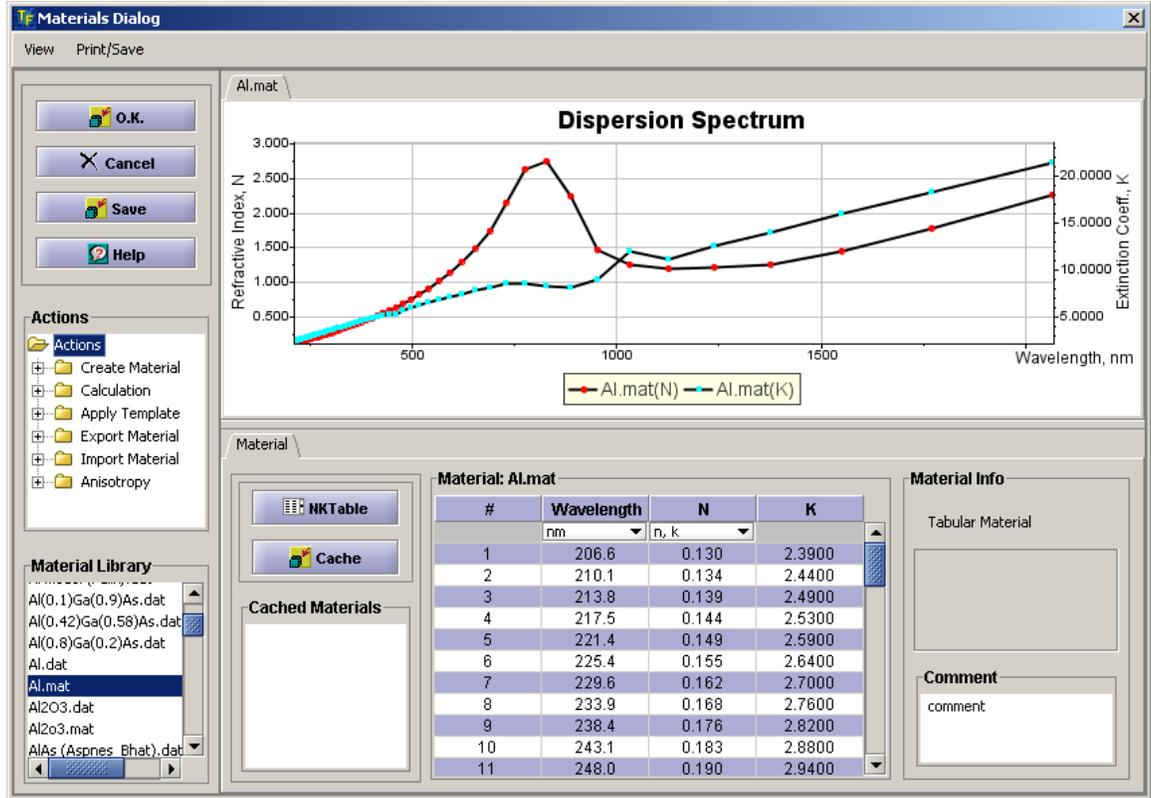


Fig. 3.4.2 Material Dialog

Most of the **Material Dialog** functionality is concentrated in the **Actions** tree.

3.4.1 Creating New Materials

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 the user can edit material's parameters values (dispersion plot data will be updated accordingly).

3.4.2 Saving Material

Use **Save** button to save material to the database.

i Saving to the database is a two-step process. **Save** button initiate the process by saving material to repository. The second step is completed when user exits Material Dialog. If **Cancel** button is selected – all changes are rolled-back; if **O.K.** button is used to exit the dialog – all the changes are committed (physically saved to the database).

3.4.3 Fitting parametric 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 (Fig.16). Select the target material from the list and click OK. This will start the fitting procedure.

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.

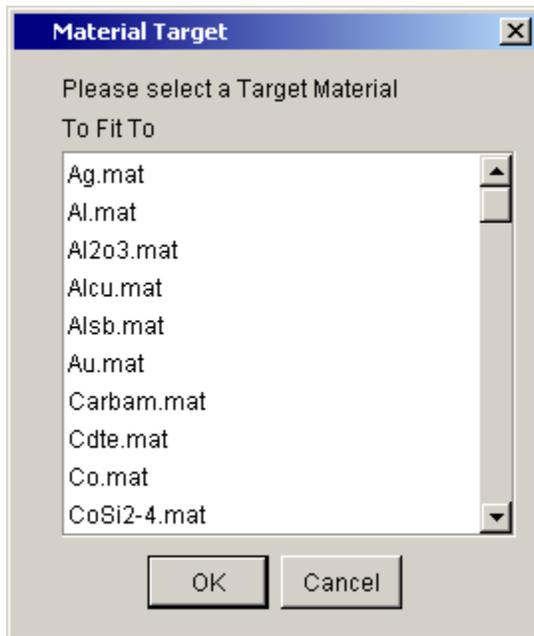


Fig. 3.4.2 A list of available “target” materials

3.4.4 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.

3.4.5 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.

3.4.6 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.

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

3.4.7 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.

3.4.8 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** or **Add To Plot**:

- **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.

3.4.9 Printing and Saving dispersion plot

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

3.4.10 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.). TFC Companion 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 (N0, N1, N2) are selected using commonly used convention of Wavelength in um.

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

N₀, N₂, N₄ are coefficients and λ is wavelength in um. The default Cauchy coefficients correspond to SiO₂ 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.

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

$$k(\lambda) = K_0 + \frac{K_2}{\lambda^2} + \frac{K_4}{\lambda^4}$$

N₀, N₂, N₄, K₀, K₂, K₄ 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.

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

$$k(\lambda) = K_0 * \text{Exp}[-(\lambda - K_2) / K_4]^3$$

N₀, N₂, N₄, K₀, K₂, K₄ are coefficients and λ is wavelength in um

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,..k – number of nodes λ is wavelength in um

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, λ is wavelength in μm

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, ε is dielectric constant

Introduced in: F. L. Terry, Jr., A Modified Harmonic Oscillator Approximation Scheme for the Dielectric Constants of $\text{Al}_x\text{Ga}_{1-x}\text{As}$, *J. Appl. Phys.*, 70, pp. 409-417 (1991).

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.)

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

UVterm, $A_j, E_j, \Gamma_j, \theta_j$ are coefficients, $j=0, \dots, k$ (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, ε 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, HfO2, etc.).

$$\varepsilon_2(E) = \frac{AE_0C(E-E_g)^2}{((E^2-E_0^2)^2+C^2E^2)E}$$

for $E > E_g$

$$\varepsilon_1(E) = \varepsilon_{inf} + \frac{1}{2} \frac{AC}{\pi \zeta} \frac{\alpha_h}{\alpha E} \ln \left[\frac{(E_0^2+E_g^2+\alpha E_g)}{(E_0^2+E_g^2-\alpha E_g)} \right] - \frac{A}{\pi \zeta} \frac{\alpha_{atm}}{E_0} \left[\pi - \alpha \tan \left(\frac{2E_g+\alpha}{C} \right) + \alpha \tan \left(\frac{-2E_g+\alpha}{C} \right) \right] +$$

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

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

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

$$\alpha_{atm} = (E^2 - E_0^2)(E_0^2 - E_g^2) + E_g^2 C^2;$$

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

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

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

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)
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)
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.

$$\varepsilon(E) = 1 - \frac{E_p^2}{E^2 - iE/\tau} +$$

$$Ae^{-i\theta} \left(\frac{1}{E + E_0 + i\Gamma} - \frac{1}{E - E_0 + i\Gamma} \right);$$

A, E₀, Γ, θ, E_p, 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 polycrystalline materials e.g. polySi. TFC Companion supports 2 and 3-components EMA .

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

VF_n (volume fraction of the components) coefficient ϵ_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-JETF, vol. 2, No.3, 1956 pp.466-475

3.5 Filmstack Layer View.

Layer View Dialog shows full information about the selected layer. It is similar to **Material Dialog** (section 3.4.) 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.

3.5.1 Setting Iteration (Calculate and Display Parameters)

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.

3.5.2 Setting Order Search

OrderSearch or GridSearch is used to overcome local minimum problem characteristic to minimization methods used to solve inverse problem of ellipsometry (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: **Restricted** 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.

3.5.3 Layer profile.

TFCompanion support inhomogeneous layer that have graded composition. The profile is represented by a sublayers (user can select the number of grades).

Default layer profile (compositional) is Uniform. Several profile type are supported: Uniform, Linear, Gaussian and Polynomial. The following are the 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

$$C(x) = C_d * \text{Exp}\left(\frac{\alpha}{d^2}\right)$$

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

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.

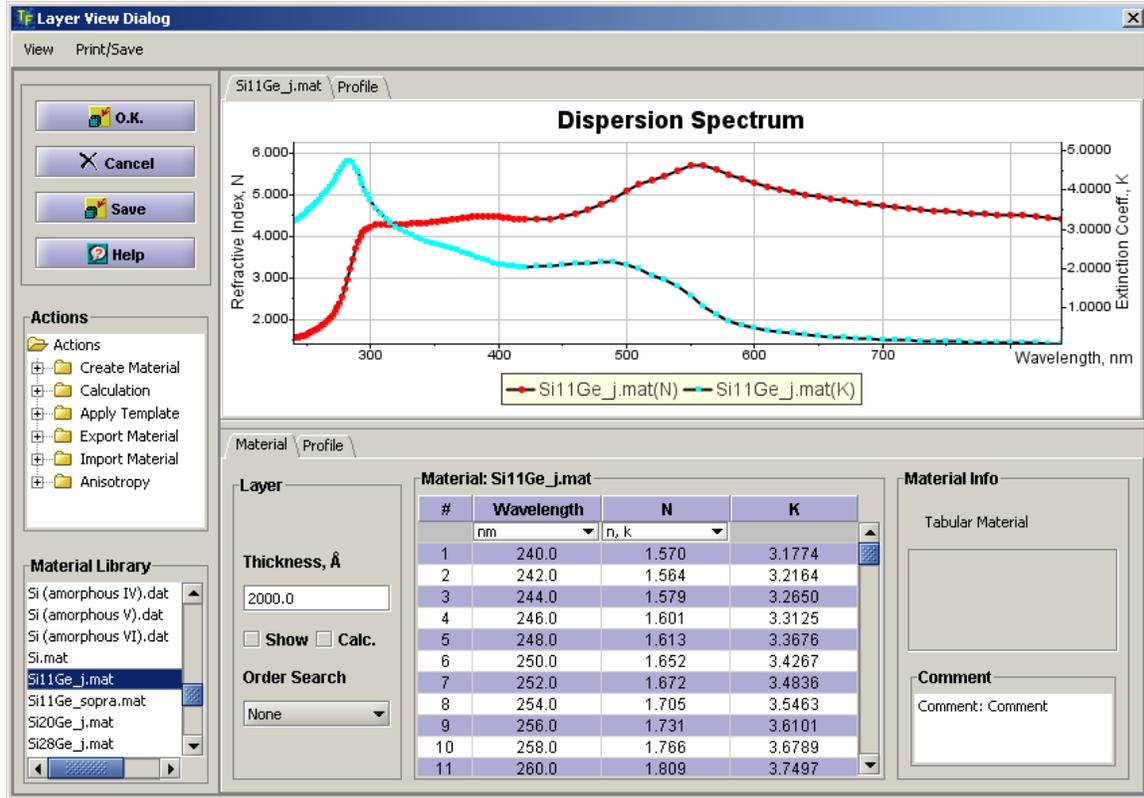


Fig. 3.5.1 Layer View Dialog

3.6 Comparing Data

Introduction.

TFC Companion supports graphical comparison of different data sets:

1. Comparison of spectral dispersion of different materials (available in Materials Dialog – see section 3.4);
2. Comparison of the measured data and calculated results fit. (Displayed after calculation or use of the **Simulation Fit** option – see section 3.2);
3. Comparison and review of different cached data sets (described in this section)

To compare/review cached data select **Review/Compare data** (in the Data menu) from menu on the main screen – this starts **Compare Data Center** dialog.

Compare Data Center is a dashboard that lists all available cached data in different tabs (Simulation, Calculation, Batch results) and also the content of the measurement database (Measurement tab), one can also load measurement data from a text file (use **Load** button). Red icon () indicates that the tab is empty, green icon () indicates that that tab has records.

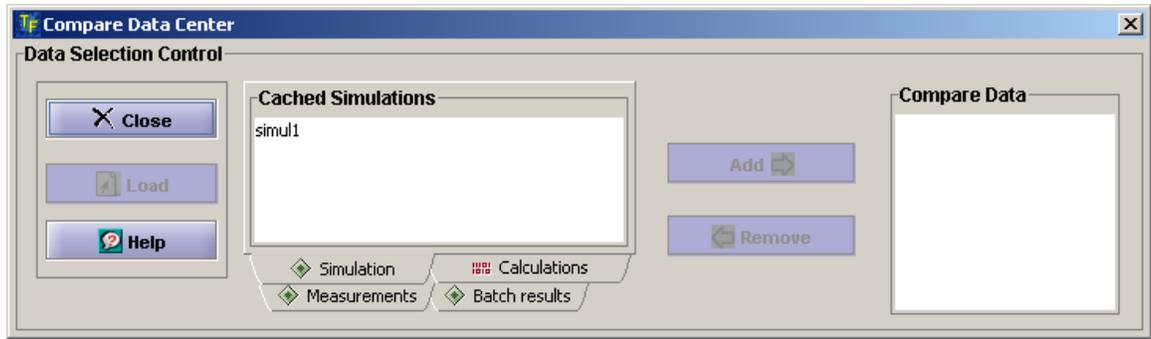


Fig. 3.6.1 Compare Data Center dialog

3.6.1 Using Compare Data Center

Compare Data Center is a simple dashboard dialog that displays the records of all available cached data plus Measurement database records. One can compare different data sets by selecting a record and using **Add** button to put it in **Compare Data** list. Once record is added - the corresponding plot is displayed in the separate window (**Compare Data dialog**); both dialogs are displayed at the same time (user can toggle between the screen by holding ALT key and using TAB on the keyboard).

a). Comparison conditions.

In order to be displayed on the same chart data sets need to be compatible i.e. represent the same parameter as a function of the same variable.

Example 1. Measured, calculated and simulated reflectance as a function of wavelength can be compared on one plot.

Example 2. Measured Delta and measured/calculated/simulated Psi will be displayed on different charts

Example 2. Measured Delta vs. wavelength and Delta vs. angle will be displayed on different charts.

b). Comparing and Reviewing Calculation data.

User can review all the details of the cached calculation data. When the record is selected – additional panel with relevant information are displayed in **Compare Data Center** dialog (Fig. 3.6.2). When user selects Add button – Calculated vs. Measured data plot is displayed

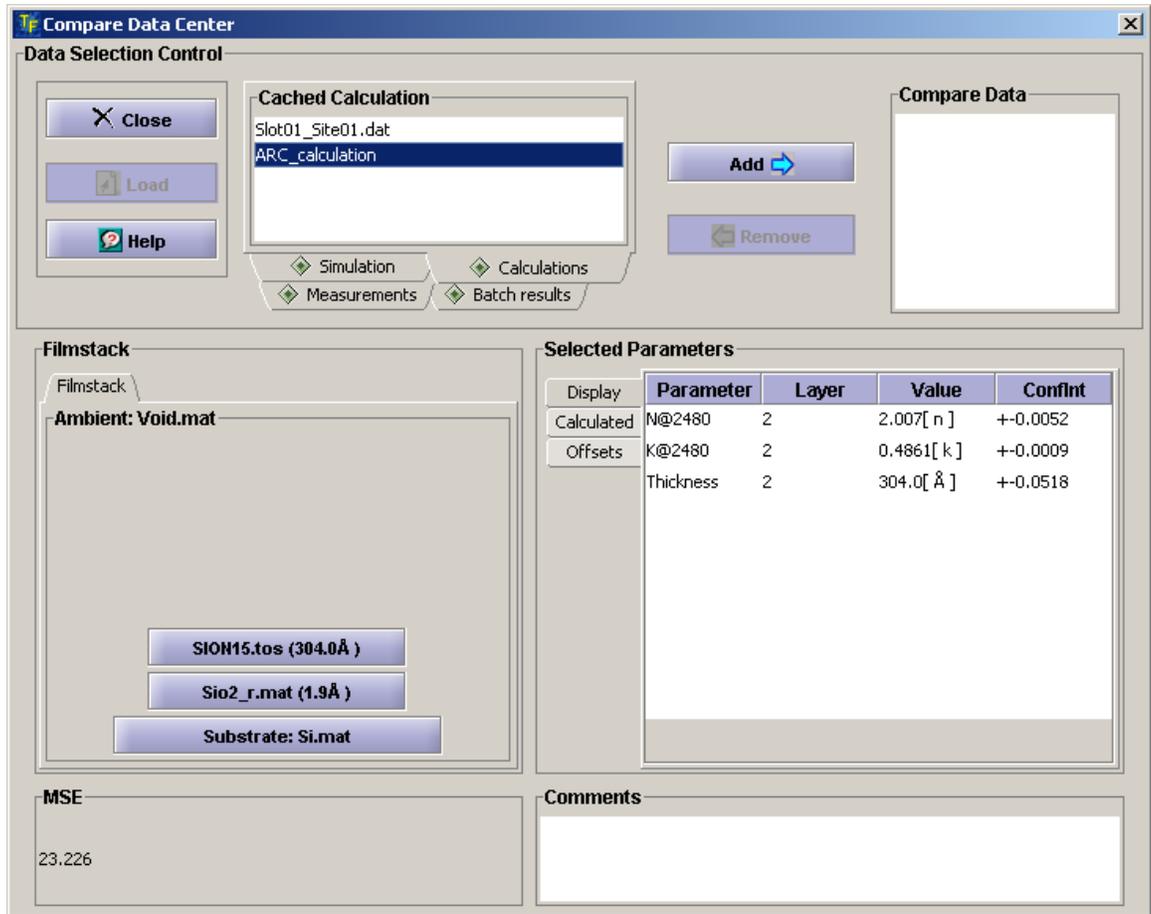


Fig. 3.6.2 Reviewing calculation results (selected record ARC_calculation is cached calculation results, Slot01_Site_01.dat record corresponds to original measurement data)

3.6.2. Compare Data Dialog

All the plots are displayed in Compare **Data** dialog (Fig. 3.6.3). The plots are displayed in tabbed panel based on parameter. All plots are interactive – area can be zoomed by holding SHIFT key and dragging mouse to outline the area (to zoom-out hold SHIFT key and click the mouse). Several analysis options are available in Compare **Data** and **Analyze Data** menus (Difference, average, derivatives, Limit, smoothing, etc.). Use Control Plot menu to control plot properties and select/hide series.

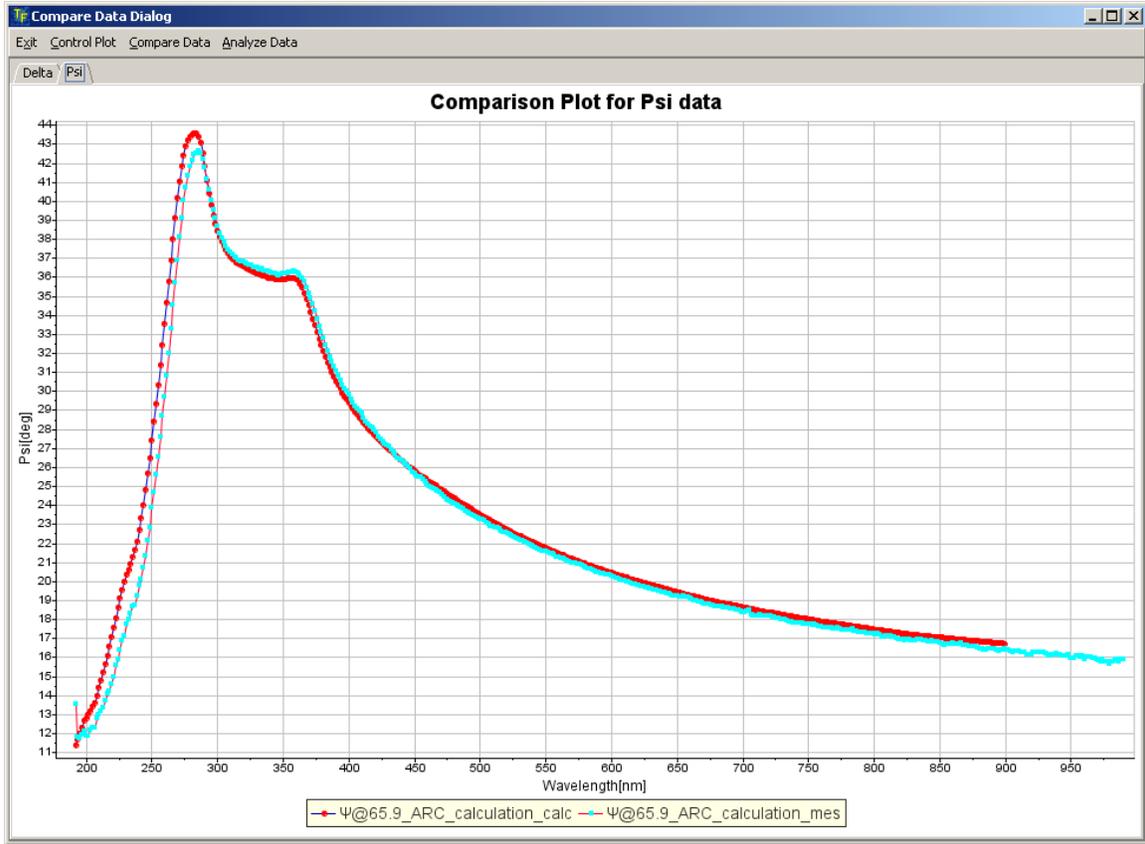


Fig. 3.6.3 Compare data dialog

3.7 Error Estimator

Error Estimator is a simplified version of Performance Spec Estimator. It can be used to quickly estimate measurement precision while working on fitting the measured data, selecting filmstack or deciding what measurements are required in particular sample.

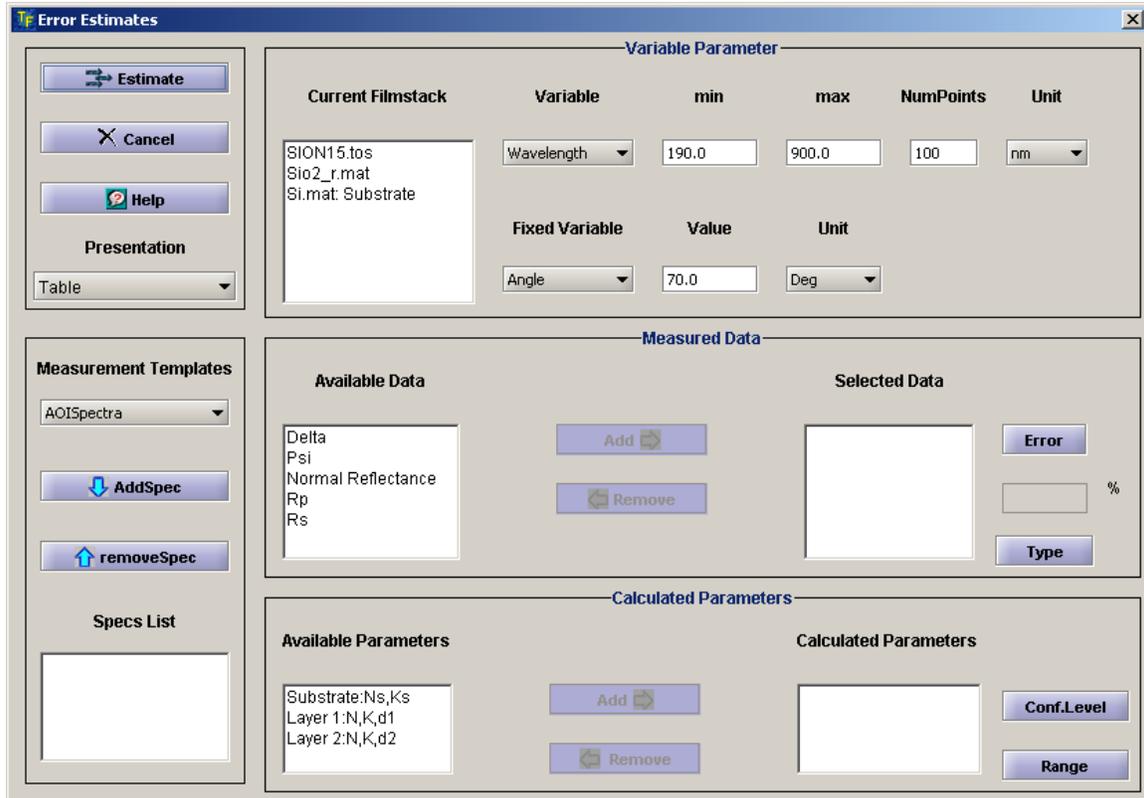


Fig. 3.7.1 Error Estimator Dialog.

Error Estimator allows to estimate measurement precision for different “*What if Scenarios*” – basically propagate precision of measured parameters (Delta, Psi, Reflectance) to precision of calculated filmstack properties. User selects “Measured Parameters” from the list of available parameters (Delta, Psi, Normal Reflectance, Rp, Rs) and sets the measurement errors of these parameters (in %). Then, spectral range, number of points and a value of the fixed variable (Wavelength or Angle) are selected. Unlimited amount of “Measured” spectra can be created and added. (Some typical measurement configurations are already set in templates and can be loaded directly. User can also create custom template to represent specific measurement instrument). Next, user selects calculated parameters in the Film Stack and sets a range of the calculated parameter (if calculation for more than one point is desired). Estimated errors for all the selected parameters are calculated as one half of the confidence interval (Confidence interval is user selected from σ to 3σ) and displayed in Tabular and Plot form in absolute or relative units.

The results can be cached and reviewed. These estimates are considered “Optimistic” because it assumes perfect fit between measured and calculated data i.e. selected filmstack accurately represent the sample. Degradation in fit will negatively affect actual precision.

To start **Error Estimator** create desired filmstack and select **Action/Error Estimates** from the main menu. Error Estimates dialog will appear (3.7.1).

Error Estimation process consist of following steps:

1. Preparing measured Spectrum:
 - Defining “measured” Spectrum;
 - Setting “measurement errors”;
2. Setting calculated Parameters
 - Selecting Calculated Parameters;
 - Setting a range for one of filmstack’s parameters;
3. Evaluation

3.7.1 Preparing measured Spectrum

Several Spectra can be prepared and added sequentially as needed. Spectra preparation and setting of the calculated parameters are totally independent and can be done in any order.

i Several standard measurement templates that describe typical SE, multiangle measurement, etc. are available. User can create custom measurement templates to represent the measurement corresponding to specific hardware configuration. Selecting template – loads all the needed properties and makes the process much quicker.

i Once spectrum is prepared and added to the list, no changes can be done. The only way is to remove the spectrum and add another one with desired changes.

3.7.1.1 Defining “measured” Spectrum

Spectrum is defined by **Variable** and **Fixed Variable**. Variable sets the range of the measurements (minimum Value, maximum Value and number of points). Variable and Fixed Variable can be either Wavelength or Angle-Of-Incidence (AOI).

After Variables are set, measured data should be selected from available parameters listed in the **Measured Data** list. Delta, Psi, Normal Reflectance, Rp and Rs are currently available. Use **Add** button to add selection to **Selected Data** list.

3.7.1.2 Setting “measurement errors”

To set measurement error -- select parameter in **Selected Data** list and click **Error** button. Input error dialog will appear. Measurement Error should be set to every Selected parameter. If the error is not set - default value is used. Currently default values are hard coded (Reflectance-1%, Delta and Psi-0.1%).

After errors are set select **AddSpec** button to add current Spectrum to a list.

3.7.1.3 Setting error type (one per spectrum)

Select **Type** button next to error textbox. Select a type of the random error distribution from the list. This distribution is used to create a synthetic data set (to mimic actual measured data). The type of the distribution depends on the specifics of the metrology instrument. In most cases, Normal with correlation is a good approximation. The notion

of a correlated noise is significant for correct estimation of repeatability - it is very rare to have completely uncorrelated noise. Noise correlation is easy to understand if one considers the sources of noise, e.g. in Spectroscopic Ellipsometry measurements light source and detector noises are contributed to the entire wavelength spectrum, clearly this portion of the noise is correlated (typically 10-20%). Of course, if one uses multi-angle measurements with the laser light source – correlation will be even higher (typically 50-70%)

3.7.2 Setting Calculated Parameters

3.7.2.1 *Selecting Calculated Parameters*

Select a layer or substrate that contains parameters that need to be calculated and click **Add** button. Layer/Material View dialog will be displayed. Mark all the desired parameters as calculated by checking a CheckBox next to it. All the checked parameters will be added to the calculated parameters list box.

3.7.2.2 *Setting a range for one of the (filmstack) parameters*

Frequently, it is desirable to calculate error estimates as a function of one of the filmstack's parameters (e.g. thickness of the one of the layers). This variable parameter has to be set as calculated (if in fact this parameter does not need to be calculated it can be unchecked later). Select variable parameter in the **Calculated Parameters** list – **Input Range** dialog will be displayed. Set minimum and maximum values of the range and number of points. If variable parameter does not need to be calculated uncheck a checkbox to disable calculation.

3.7.3 Presentation

Results of the Error Estimation can be presented in a Table and Plot form. Type of the presentation can be selected in the **Presentation** drop-down. Plotting can also be done after results are presented in the Table form.

3.7.3.1 *Plotting.*

Direct plotting (from the Error Estimation dialog) can be used for quick review of the data. However, this data cannot be saved and exists only while the plot is displayed.

If caching, reviewing and comparing of the data is desired—user should select Table form of the presentation and Plot data from there. User can toggle between Absolute and Relative presentation of error.

3.7.3.2 *Table Presentation(fig 3.7.2)*

When results are displayed in the Table format they can be cached (use **Cache** button) or plotted (use **Plot** button). When the data is cached, the name of the cached record is displayed in the **Cache** list. Cached data is maintained

during the current session and all the records cached during the session will be displayed in the Cache list. To review the cached record, double-click on it and the data will be displayed in the table. It can be plotted the same way as current Error Estimation results. User can toggle between Absolute and Relative presentation of error.

Estimated Absolute Errors

Estimated Errors of Meeasured Parameters

Variable (2_Thickness...)	2_Eg_err 2.630 Max (Avg)	2_Eo_err 3.900 Max (Avg)	2_A_err 87.870 Max (Avg)	2_C_err 7.900 Max (Avg)	2_Thickness... 313.000 Max (Avg)
100.00	0.08 (0.0783)	0.33 (0.3097)	8.87 (8.3605)	0.69 (0.6503)	0.51 (0.4781)
147.37	0.05 (0.0442)	0.17 (0.1639)	4.92 (4.6542)	0.36 (0.3445)	0.53 (0.4988)
194.74	0.03 (0.0273)	0.11 (0.1000)	3.23 (2.8425)	0.24 (0.2100)	0.61 (0.5332)
242.11	0.02 (0.0185)	0.07 (0.0697)	2.06 (1.9192)	0.16 (0.1463)	0.62 (0.5771)
289.47	0.01 (0.0134)	0.06 (0.0530)	1.50 (1.4019)	0.12 (0.1113)	0.65 (0.6047)
336.84	0.01 (0.0102)	0.05 (0.0425)	1.22 (1.1101)	0.10 (0.0892)	0.69 (0.6288)
384.21	0.01 (0.0071)	0.03 (0.0277)	0.91 (0.8420)	0.06 (0.0578)	0.66 (0.6129)
431.58	0.01 (0.0057)	0.02 (0.0202)	0.72 (0.6953)	0.04 (0.0426)	0.61 (0.5913)

Fig. 3.7.2 Results of Error Estimator calculation (Table Presentation).

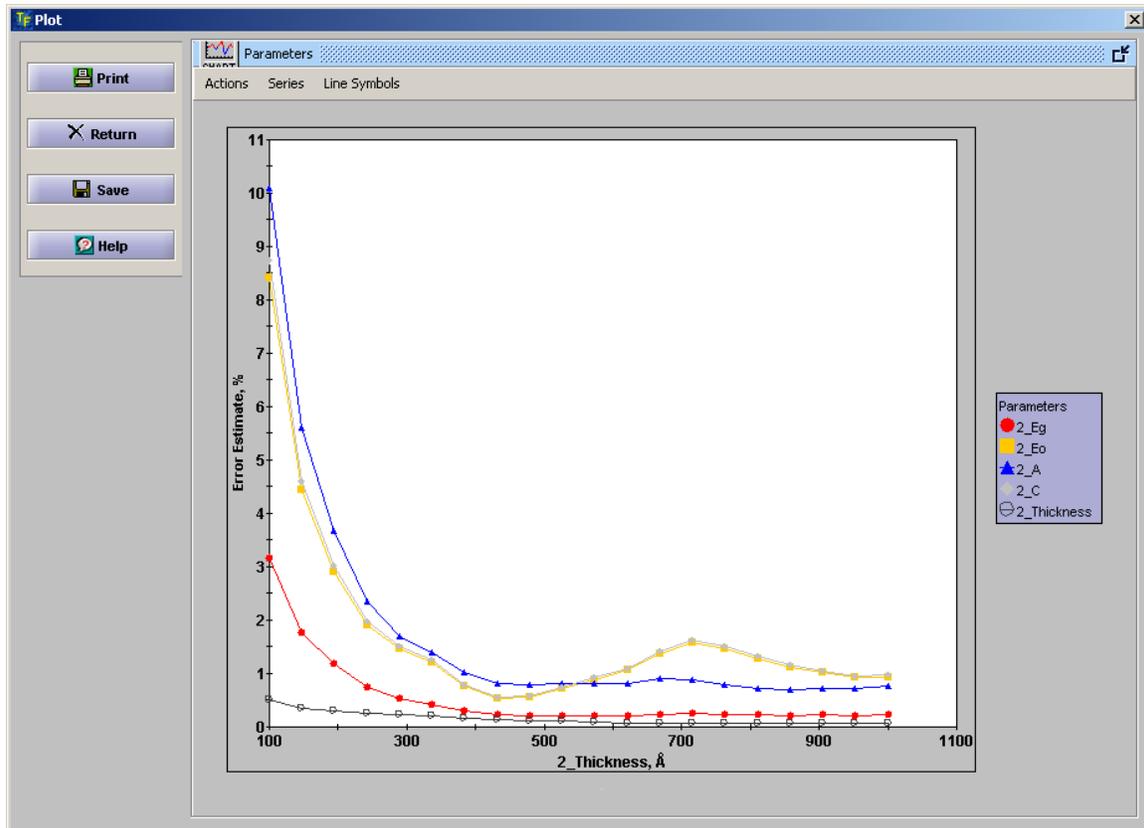


Fig. 3.7.3 Results of Error Estimator calculation (Plot Presentation).

3.8 Projects, Sessions, Caching data

TFCCompanion supports the persistence of intermediate data/results that are aggregated in the Project. Each time the new TFCCompanion session is started (the program is executed) the new default project is created. The user can load any existing project and retrieve all the data from the previous session. All the data cached by user (materials, filmstack, simulation, calculations, batch results, error estimation results, etc.) while working with TFCCompanion is aggregated in the Project (current project is used, i.e. default project or user loaded project). Before exiting TFCCompanion user can save the project to database. If the project is saved – it can be loaded during other session and all the data will be available to continue the work on the project, otherwise the project is disposed and all the data is lost.

i Current filmstack is saved by default with the project. Cached simulation, calculation, error estimation and batch calculation data include relevant filmstacks as well.

It is a good practice to save all the filmstacks and materials you have created during the session, and may need to use later, to a relevant repository (filmstack or material) independently of the project.

i When filmstack loaded from cache and this filmstack is not available in the database – user is given an option to save filmstack to the database or continue without saving.

To Save/Load a project, use File/Save Project or File/Load Project from the main menu.

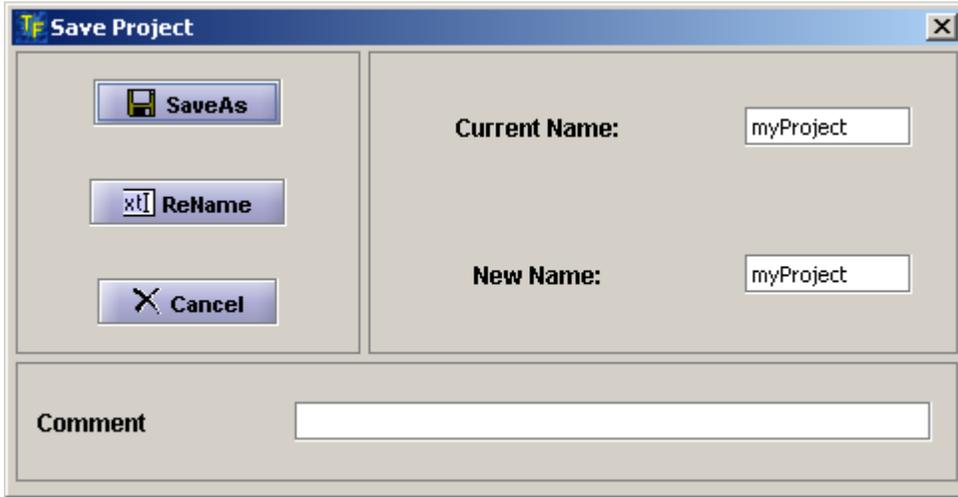


Fig. 3.8.1 Save Project dialog.

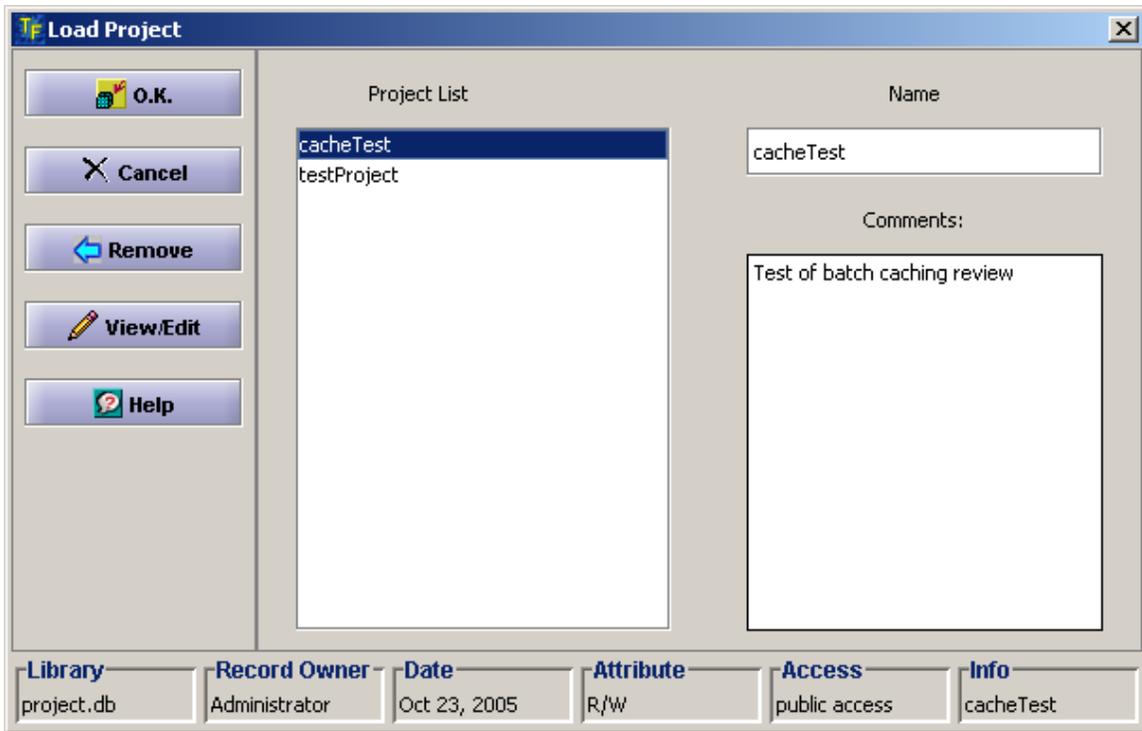


Fig. 3.8.2 Load Project dialog.

3.9 Configuration

3.9.1 Introduction

TFC Companion supports flexible configuration of software properties, templates, etc. and selection of connected hardware configuration. Both software and hardware configuration is saved in XML files located in /init directory of TFC Companion installation: software configuration – in file TFCComp_config.xml; hardware configuration – in 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.

3.9.2 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 TFC Companion 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.

Configuration Dialog contains several tabbed panels:

- *Measurement templates.* This panel allows to create 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 TFC Companion distribution and can serve as an example.
- *Material templates.* This panel allows creating tabular material template. The template encapsulates wavelength range or discrete wavelength. 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.
- *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.
- *Sources.* This panel allows selection materials and filmstack databases, default filmstack that is loaded when TFC Companion started, measurement data directory. Databases and measurement data directory are selected relative to TFC Companion installation directory.

 TFC Companion monitors user action and updates location of measurement, batch and result files during the session. This information is persisted between the

sessions and saved in session.data file. However, configuration file is not changed and serve as repository of default locations.

- **Defaults.** This panel allows selecting the setting of several important conventions and properties 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 either 0-360deg or 0-180 deg range. 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.

i If loaded measured data has Delta in 0-360 deg range TFCompanion will used 0-360deg. convention during calculations automatically.

General convention allows selection either of two conventions Azzam or Beaglehole (BIL). Azzam convention defines Delta=180deg. 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.*

Use 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.

i To save configuration changes – user needs to select **Save** 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

3.9.3 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 available only for users that have Operations = "integrated" in their user profile.

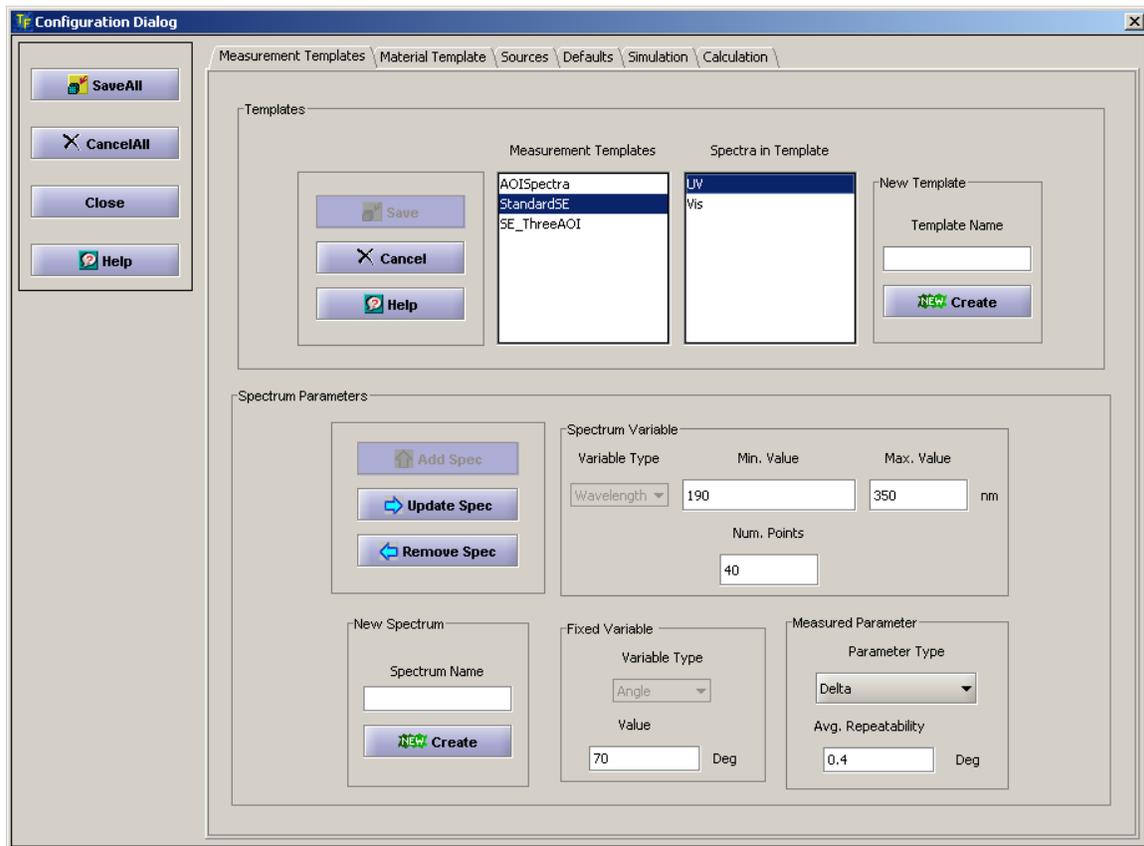


Fig. 3.9.2.1 Software configuration dialog.

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.

All the 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.

i In most cases, there is no additional check of whether currently connected hardware is selected correctly and actually matches the connected hardware. Please use caution when using selection.

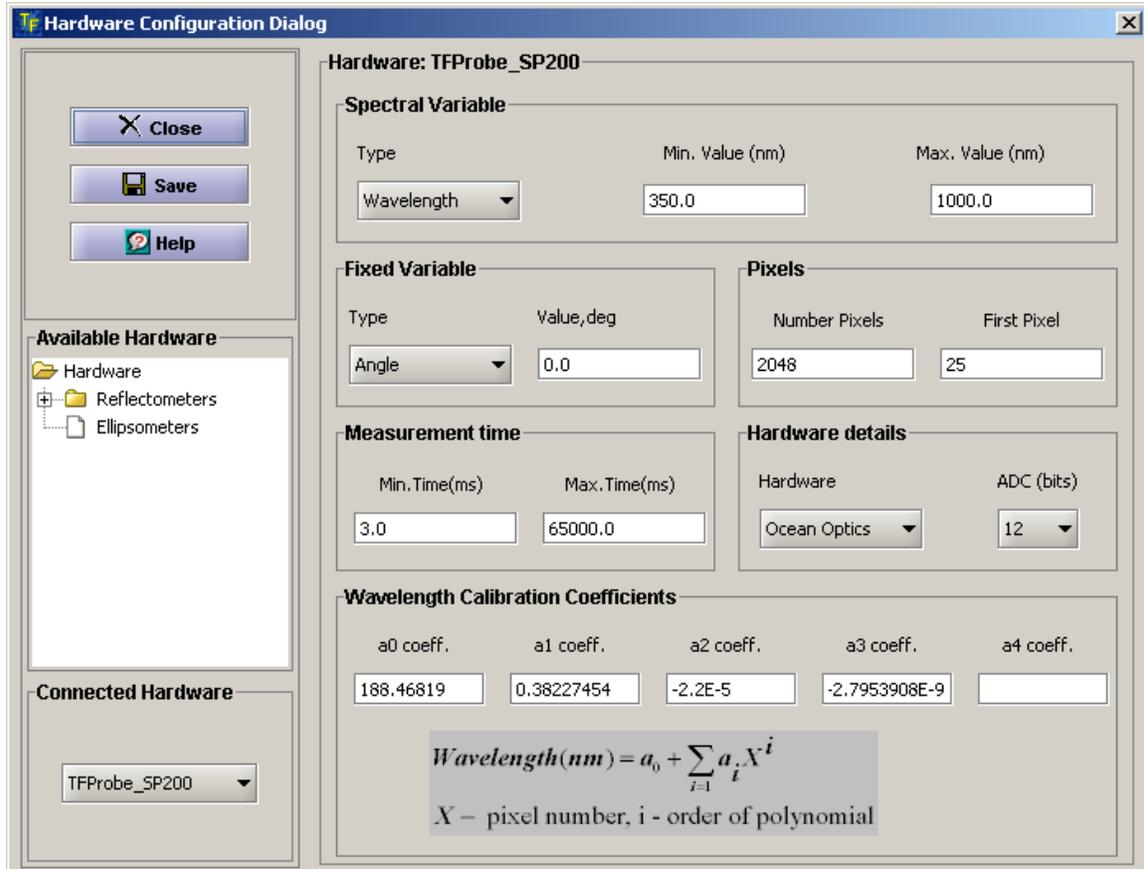


Fig. 3.9.3.1 Hardware configuration dialog

3.10 Calculation and Measurement Recipes.

3.10.1 Introduction

Calculation and measurement recipes are used to encapsulate relevant information and are saved in the database. Measurement recipe is used only with integrated version of the software. Calculation recipe can be used both with the standalone and integrated version of the software.

3.10.2 Calculation recipes

It is common both in R&D and production to repeatedly analyze the same or slightly different type of the sample. Calculation recipes provide a convenient way of saving relevant calculation information; it allows to encapsulate information about filmstack, calculated parameters and offsets used in the calculations. Calculation recipes can be

saved to database and used repeatedly to streamline calculation setting and provide consistency.

3.10.2.1 Preparing calculation recipe

Calculation recipe does not really require special preparation – it allows to save the conditions set for the current calculation. One needs to prepare conditions for regular calculation: load filmstack, select calculation and display parameters, select offsets (optional). To save calculation recipe – select **File/Save Calculation recipe** from the main menu.

3.10.2.2 Using calculation recipe

The records of all available calculation recipes in the database are displayed in the side panel (main dialog) under **Calculation recipes** tab. To load recipe select the record, right-click mouse and select **Load recipe** from the popup menu – recipe will be loaded and all the calculation conditions setup (filmstack, calculation & displayed parameters, offsets). Now one needs only to load measured data and start calculations.

3.10.2.3 Using offsets

Parameters offset is a convenience methods to correct calculation results – offset values are subtracted from the calculated values of respective parameters before displaying the results. Offsets are typically used to correct calibration or to enable instruments matching.

To set/edit offsets – select **Offsets** tab in **Selected Parameters** tab and edit value next available displayed parameters.

3.10.3 Measurement recipes

Measurement recipe encapsulates information about measurement conditions, filmstack model and calculated parameters. Measurement recipe can be created using measurement Recipes dialog and saved to the database.

There are three types of the measurement recipes:

- *Calibration recipe.* This recipe has a special attribute (**Calibration** checkbox in Attributes panel must be checked). Calibration recipe is used with the selected check sample (or no sample in the case of transmittance). The results of the measurement performed with the Calibration recipe are saved in the special file. This file is automatically referenced during regular measurements of the same type (e.g. reflectance -reflectance reference calibration, transmission – transmittance calibration).
- *No-filmstack recipe.* **No Filmstack** checkbox must be checked in the **Attributes** panel. This recipe enables measurement without the use of the filmstack model (to filmstack parameters calculation). The measured data can be collected and saved to database. User can later analyze it using different filmstack models.
- *Full recipe.* This recipe includes measurement conditions, filmstack and calculated parameters of the filmstack. Application of the full recipe combines

the measurement itself (data collection) and fitting of the measured data to the calculated data (in order to determine the values of filmstack parameters). When measurement is done the value of calculated filmstack parameters and the fit of the measured vs. calculated data are displayed

3.10.3.1 *Preparing measurement recipe.*

To prepare measurement recipe user need define the measurement properties and condition:

- Selecting the parameters of the measured spectrum in **Spectrum definition** panel (Select spectral variable, measurement range and measured parameter). After spectrum is defined use **Add** button in the **List of Measurement** panel to add this spectrum
- Define measurement conditions (use **Measurement conditions** panel)
- Select attribute in **Attribute** panel depending on the type of the recipe (no attribute need to be selected for the full recipe) and select the target hardware (optional)
- If recipe includes filmstack – select filmstack (load from the database), select calculation and displayed parameters (the interface is the same as ion main menu and has the same functionality)
- Use Save button to save measurement recipe to the database

3.10.3.2 *Using measurement recipe*

A list of available measurement recipes is displayed in the side panel in main dialog (Measurement recipes tab). Select a record, right-click the mouse and select Load Recipe from the popup menu. Measurement recipe should be loaded before any measurement can be started.

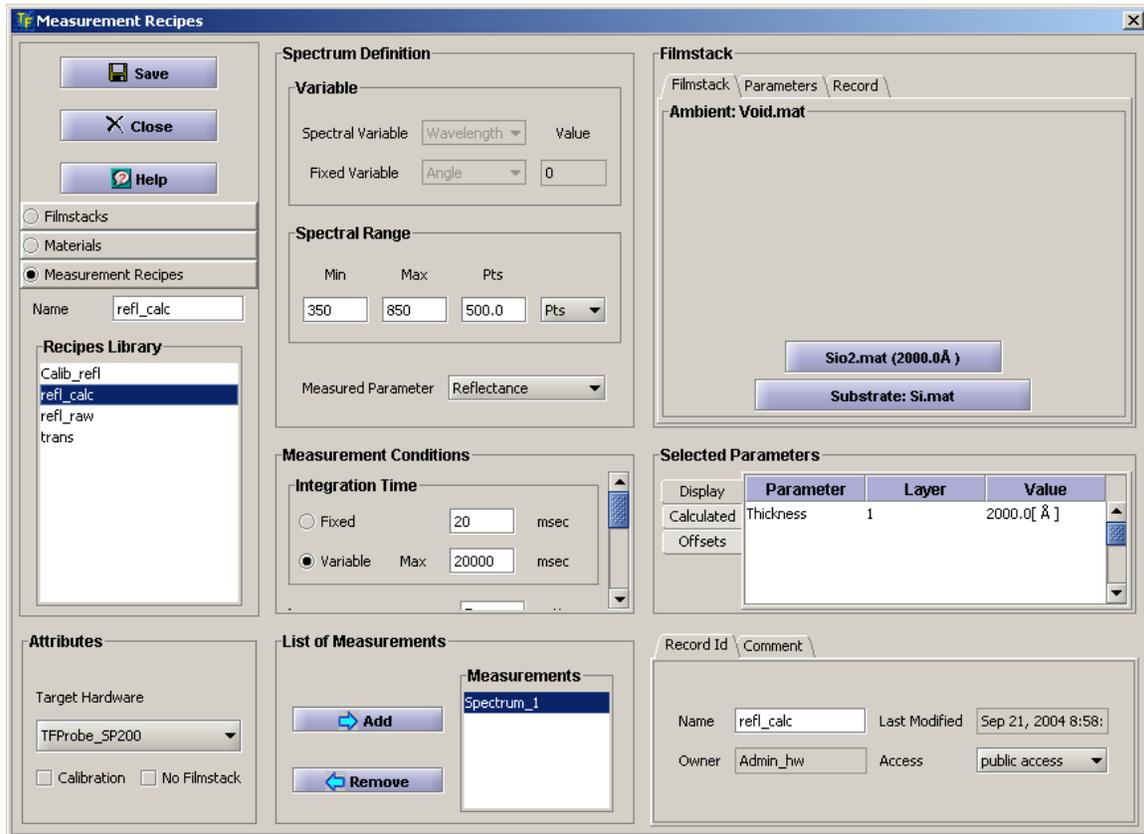


Fig. 3.10.3.1 Measurement recipe dialog (Creating and editing measurement recipes)

3.11 Batch Processing (Calculation) of the Measurements

i This feature is available in the Advanced version of TFC Companion

3.11.1 Introduction

Batch processing allows calculation of the filmstack parameters using selected set of independent measurements. Each measurement can be matched, independently, with the specific filmstack or the same filmstack can be matched to all the measurements. It is also possible to “instrument” the filmstacks i.e. use the results of the independent measurements (SEM, etc.) to modify certain filmstack parameter(s) using a script file.

Some of the applications are:

- processing the results of a gauge study;
- processing mapping results e.g. uniformity of the parameters across a wafer or production load.
- processing the results of kinetic measurements e.g. in-situ measurements

- processing the set of totally independent measurements

3.11.2 Prepare Batch calculations.

To start batch processing, select **Actions /Production Batch** option from the Main menu. This will bring up BatchPrepareDialog (Fig. 3.11.1). This dialog allows creating a set of matched Filmstack- Measurement pairs, select measurement parameters and display options.

Current batch file directory (last used location) is used to populate the Measurements list. To select another directory -use the **LoadMeas** button. All files from the selected directory will be listed, but they are not read and parsed at this time. Measurement files are read and parsed only when they are copied to the Process Table or reviewed (double clicked). Batch processing is NOT limited to batch measurement files (files that contain several measurements) - all measurement files formats supported by TFCompanion can be used.

i One can double click on any record either in the Lists or in the Table to drill down and review/ modify data as needed.

All filmstacks available in the current database are automatically loaded and listed in the Filmstack List. To select other database one can use the **LoadFilmstacks** button to navigate to the location of desired database.

i One can double click on the filmstack record to review the details and/or select calculated parameters

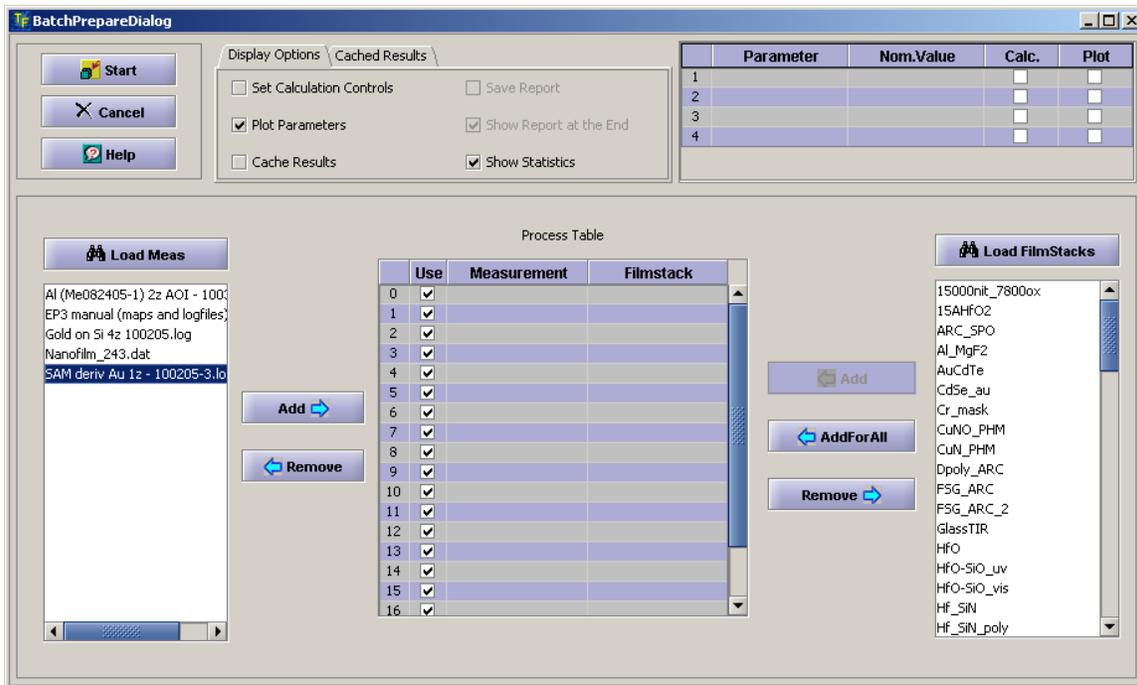


Fig. 3.11.1 BatchPrepareDialog allows creating a set filmstack-measurement pairs for batch processing

3.11.2.1 Reviewing Measurements.

Measurement data can be reviewed in the LoadMeas list or in the **ProcessTable**. In either case, Data Selection Dialog will be displayed to show the content of the measured data on a spectra level with ability to drill down to the actual measured data in each of the spectra. There is a slight difference between reviewing measured data in the **LoadMeas** List and in a **ProcessTable**.

a). *Reviewing Measurements in Load Measurements List.*

When user double-clicks on a record in the List (or select a record and use review option in the pop-up menu), measurement file is read and parsed (if it is a first time) or taken from the cache during subsequent calls. If it is a batch measurement file, separate measurements are created with the following names: `<n>_<mesfile>`, where `<n>` stands for a sequence number of the measurement and `<mesfile>` is a name of the measurement file.

In the case of the batch measurement file, a list of the measurements is displayed (*Fig. 3.11.2*) prompting user to select a measurement for review.

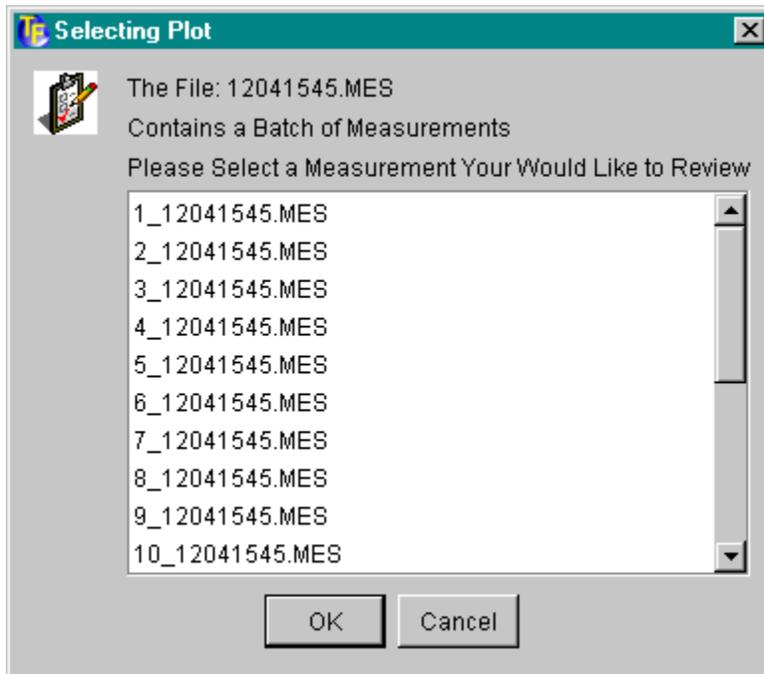


Fig. 3.11.2 Selecting a measurement for review from the batch measurement file.

Selection of the measurement brings Data Selection Dialog. User can deactivate some of the Spectra in the measurement or some measurement Points. All the measurements will be cached in memory (no data in File is affected).

b). *Reviewing Measurements in Process Table.*

When user double-clicks on a measurement record in the Process Table-Data Selection Dialog is displayed. Any selecting/deselecting of the measurement point or spectra is saved in memory.

3.11.2.2 Copying Measurement Data from List to Process Table.

There are two ways to copy files from the **Load Measurements List**:

1. Select one or several records and click **Add** button. Measured data will be added to the Process table, starting from the first available row.
2. Select one or several records and click the right-click mouse and select copy from the pop-up menu. Click mouse at the Table's row where the record should be copied and select Paste from the pop-up menu.

3.11.2.3 Loading Filmstacks.

Available filmstacks are loaded from the default database (normally db/flm.db) automatically. Use the **Load Filmstacks** button to select and load other available databases.

3.11.2.4 Reviewing/Modifying Filmstacks.

Filmstacks can be reviewed/modified either in the **Load Filmstacks List** or in the **Process Table**. Double click on a Filmstack record (or select review from the pop-up menu) and a Filmstack dialog will appear. To drill down to a layer level double click on a layer record. User can select parameters to calculate and, if needed, modify the filmstack.

After filmstack is added to the **Process Table**, selected calculated parameters are displayed in the **Parameter Table** (in the top right corner of the screen).

 *Selected parameters from only the first filmstack in the Table are displayed in the Parameter Table. This is a limitation of the current version.*

 *Once calculated parameter is selected, corresponding filmstack records in the ProcessTable have a following icon . Select Show (in addition) to Calculate option for the parameters that need to be displayed during the batch calculation.*

3.11.2.5 Adding Filmstacks from a List to a Process Table.

There are two ways to copy filmstacks from the **Load Filmstacks List**:

1. Select one or several records and click **Add** button. Measured data will be added to the Process table, starting from the first available row.
2. Select one or several records, click right-click mouse and select copy from the pop-up menu. Click mouse at the Table's row

where the record should be copied and select Paste from the pop-up menu.

3. Select ONE filmstack record in the List and click **AddToAll** button. Selected filmstack will be added to match all available measurement records in the Table.

i If calculated parameters were selected in the filmstack in the List – iteration icon **i** will appear in front of corresponding record when the filmstack is added to the Process Table.

3.11.2.6 Selecting Display Options

Display Options tab panel is located on the top of the dialog and has several options (checkboxes):

- a). **Set Calculation Control** – selection of this checkbox displays **Advanced Control Dialog** that enables selection of calculation condition (Marquardt minimization). In most cases, default values are adequate and no adjustments are necessary.
- b). **Plot Parameters** – enable plotting of the calculated parameters (trend plot) during the batch calculation run.
- c). **Cache Results** – enables caching of the full data for each measurement for post-mortem analysis (e.g. plotting calculated vs. modeled data etc.). The cached data can be reviewed at **Review Compare Center (Data/Review Data)** from the main menu and select Calculations tab)

i This automatic Caching is different from the explicit Caching selected in the Batch Run Dialog. Explicit Caching saves the data necessary for reviewing and comparing trend charts for different runs.

- d). **Show Statistics** – shows statistics (min/max. s.d.) during the calculation run.

3.11.2.7 Review Cached data

To review cached data – select **Cached Results** tabbed panel on the top of the dialog. All Cached records are displayed in the list (these are records of *explicitly cached* data in the Batch Run Dialog - not automatic caching results). To display the results of the calculations – select the record, right-click the mouse and select Display Plot from the popup menu. The plot will be displayed in the separate window. Several records can be compared on one plot. Use Hide Plot option in the pop-up menu to remove the plot of selected record.

3.11.2.8 Using script to “instrument” filmstack

This option allows to modify filmstacks parameters using the script file (*.fmf). The *.fmf file format is described in

<http://www.semiconsoft.com/html/download/docs/FilmstackModificationFormat.pdf>

Select any filmstack in the Process Table, right-click mouse and select “Modify Filmstack” option from the popup menu. The user is prompted to select the *.fmf file that is loaded and modifications are applied to the filmstacks in the Process Table.

3.11.2.8 Link measured data.

This option allows modifying all the measured spectra in the **Process Table** using selected spectra as a template. Select the measurement in the **Process Table** (user can double click to modify it), right-click mouse and select **Link Spectra** for the popup menu. Typical use of this option will be when all the measured data is collected in the same fashion e.g. map or gauge study. In this case, user can modify one spectra (measurement) e.g. selecting different weights for some points or deactivating some parts of the measurement. After this- select this measurement as a template to modify all other measurements.

3.11.3 Running Batch Calculations

Select **Start** button in **BatchPrepareDialog** to start processing. Measurements are processed sequentially and the results are continuously displayed in the **BatchRunDialog**. This dialog has four areas:

- TextArea. Results of the calculations for each measurement are displayed here. Results are displayed continuously and the area can be scrolled to review all the records.
- TrendCharts Area displays calculated parameters for each measurement and 90% confidence interval (red bar) for each value.
 -  X-axis has a “zoom-box” to change the scale dynamically. To Zoom OUT -- Hold **Ctrl** key and click left-hand mouse button on X-Axis. To Zoom-IN—Hold **Ctrl** key, press the left-hand mouse button and move the mouse to select the X-axis region to Zoom. When you release the button, selected area will be zoomed.
 -  To view the plot in a separate, full screen window right click mouse on the plot tab or above and select zoom from the popup menu
- Results Statistics Table continuously display Average, S.D. and Min/Max. Values of the parameters are updated after each calculation.
- Current Status panel display calculation progress.

Use the **Stop** button to stop calculation. You will have an option to

- **Restart** calculation. This will start calculation from the beginning (First measurement);
- **Continue** calculation. This will continue calculation from the point where they were stopped;
- **Cancel**. This will return control to the BatchPrepareDialog.
- **Cache**. Allows explicitly cache the results of calculation for review and comparison with other runs.
- **Export**. Allows export the results to a text file (csv or tab spaced format).

3.12 Performance Specification Estimator (PSE).

i *This feature is available in Enterprise edition of TFC Companion*

PSE is an extension of an Error Estimator (section 3.7) that allows greater control over simulation process and is more flexible. In particular, it allows setting of several variable parameters in the filmstack (vs. only one in Error Estimator), creation of full performance recipes (saved in the XML file), running batch calculations of selected performance recipes, calculate metrics to compare simulated performance to required specification. PSE allows exploring system performance on the full range of possible parameter variation. For example, if one is interested in performance on three-layer filmstack (e.g. ONO). The user can set the range of the thickness for all three layers and explore all the possible combination of these thicknesses (selecting 10 points for each thickness will give total 1000 different filmstacks). Each such parameter combination (filmstack) is referred to as a "measurement point". PSE defines several performance metrics:

- *Global metrics*: Percent of the measurement points with parameters measured within the specification
- *Parameter metrics*: Percent of the measurement points with selected parameter measured within the specification

PSE includes **PerformanceWizard** and **PerformanceBatch**.

PerformanceWizard allows creating manually, or loading from the XML file, a performance recipe and running it – one recipe in a time. Manually created or edited performance recipe can be saved to the XML file.

PerformanceBatch allows loading performance recipes from selected XML file and running them unattended – in the batch. The results of the calculations are saved to a file and can be reviewed by the operator after calculations are completed.

3.12.1 PerformanceWizard

Performance recipe contains three different pieces of information:

- Measurement recipe (measured spectra signature and noise)
- Variable and calculated filmstack parameters and spec on calculated parameters
- Calculation conditions (number of trials, confidence level, etc.)

Performance Wizard contains four changing panels: three data input panels screens and one final Calculation Panel. These panels can be browsed/toggled using **Next** and/or **Previous** buttons at the right bottom of the screen. Each panel allows manually input to a separate section of the Performance recipe or load it from XML file. Full recipe can be loaded at the final **Calculation Panel**.

Left side of the Performance Wizard is common - not changing with the switching of panels. It contains control buttons (**Cancel**, **Save** and **Help**) and two lists - **Current Filmstack** and **Calculated Parameters**.

Calculated Parameters list is displaying filmstack parameters that are calculated. Check mark next to parameter name indicates that spec repeatability is set for this parameter.

Current Filmstack list displays the Filmstack. It can be used to set calculated parameters- double-click on the layer/substrate invokes a detailed **Layer View**.

Bottom panel contains drop-down box and **Measured Spectra** list. Drop-down box lists records from the XML file with Performance recipes. Displayed records are context sensitive and are changing depending on the panel displayed, e.g. Measurement recipes records are displayed while Measurement Panel is active. User can load different portions of the Performance recipe while corresponding Panel is active. It is recommended to load full Performance recipe that is displayed when Calculation Panel (last panel) is active.

i Special care needs to be taken when combining portions from the different recipes - they can be inconsistent, e.g. parameters not matching filmstack etc. Loading of the full recipe is recommended instead.

3.12.1.1 Adding Measurement Recipes.

The measurement Recipe panel allows input of the measured data details such as type of the spectrum, range, number of points, measurements errors, etc. Unlimited number of measurement spectra can be added. The data can be input manually or loaded from the XML file.

Measurement recipe consist of measurement spectra definitions. Recipe can include unlimited number of spectra. Each spectra is defined by the type and range of spectral variable (Wavelength or Angle), number of points, one or more measured parameters (Delta, Psi, etc.) and measurement s.d. of the parameters at each point.

Following are the steps to manually create and add measurement spectra definitions to the recipe:

- Select spectral *Variable type* (Wavelength or Angle) from drop-down box. *Minimum* and *Maximum* values text boxes are populated automatically with default values. Set the maximum, minimum values, number of points and select the unit.
i Default wavelength range is defined by the filmstack. To expand beyond this range requires editing modification of the filmstack.
- Select *Fixed Variable* (Wavelength, Angle) and set its value.
- Select measured parameters from the list of the *Available Parameters* and use the *Add* button to add them to the *Measured Parameters* list.
- Add measurement s.d. and weight to each spectral point. To do this select a parameter from the *Measured Parameters* list and press the *Error* button. Use the displayed table to set s.d. and weight.

Spectrum definition is now completed, use *Add* button to add it to the measurement recipe. The Spectrum Definition is added to Measured Spectra list. To remove definition, highlight spectrum in Measured Spectra list and use Delete option of the Popup menu (right hand mouse button activates the popup menu).

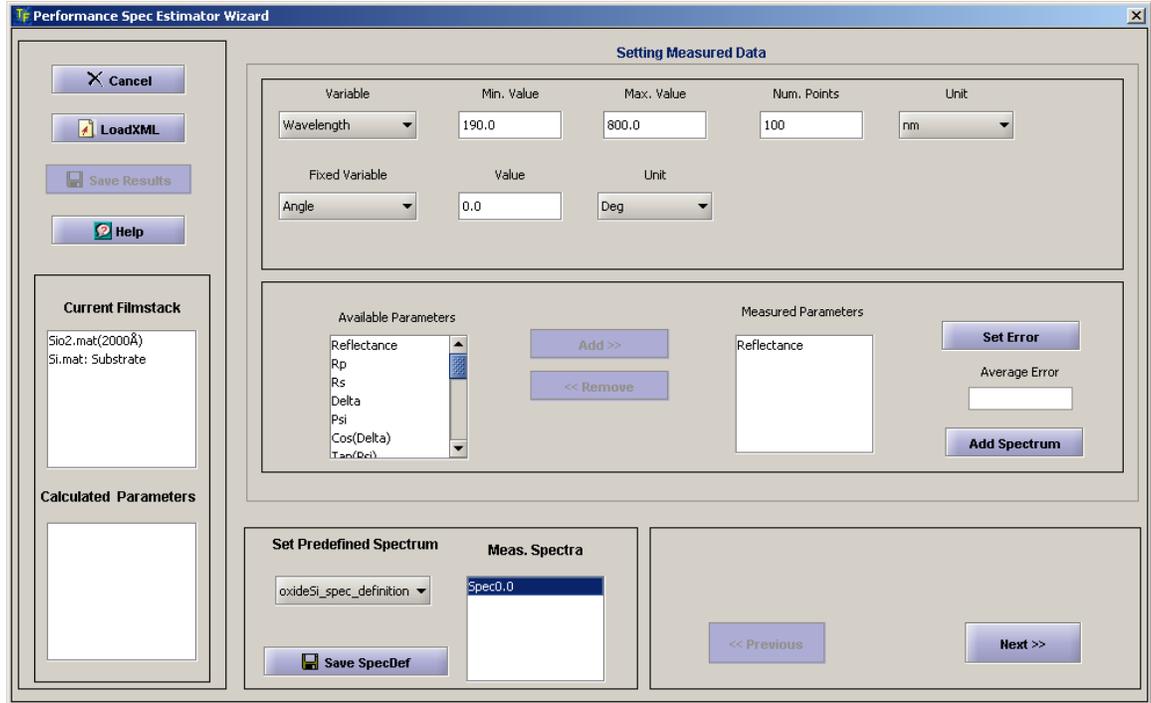


Fig. 3.12.1 Performance Wizard - Measurement Recipes panel.

a) Adding s.d. (measurement error) and weights to spectral points.

Selection of the Error button during building of spectra invokes the Error Input Table. This Table allows to input error (s.d.) of selected measured parameters (Delta, Psi, Reflectance, etc.) and relative weight coefficients for each spectral point.

Error and weight columns of the Table are editable (you may need to double click the a cell to use editing mode). To set the same value for all the cells in the row, the user can invoke popup dialog and use *Set All Errors* or *Set All Weights* menu item, respectively. The meaning of the *Error* is different depending on the type selected in the *Error Type* drop-down. *Standard* type refers to measurement s.d.; in the case of *Value Dependent* type the meaning of the errors in this table changes to Relative Coefficients (the actual s.d. are input in a separate table that is invoked when Error Value button is pressed). These *Relative Coefficients* (coeff) are adding spectral dependence to *Value Dependent* errors (s.d.) and final error=coeff*s.d.

PDF type of the error can be selected from the Error Distribution drop-down list. The default distribution in Normal (gaussian).

b) Value dependent errors.

In some cases, measurement s.d. depends on the value of the measured parameter. One example is Reflectance measurement. *Value Dependent Error Table* allows breaking down the range of measured value on several regions and defining s.d. for each of them. User can either assign constant s.d. (relative or

absolute value) to each region or assign s.d. as a function (polynomial approximation) of value (relative or absolute) for a region or whole range; Definitions of s.d. for different regions can be different but all need to be either in relative or absolute values. User is prompted to select Absolute or Relative type after clicking the *Set Ranges* button.

- Defining and setting errors.

Breakdowns the total range on regions, unless you want to assign one error to all range. Ranges need to be contiguous - the max of previous range equals the min of the next range.

 Reflectance range needs to be defined in fractions (0-1.0)

For each range, input s.d. as a single number or a set of polynomial coefficients (of the s.d. approximation) in Coeff. Values row. Polynomial coefficients are coma separated, e.g. 1.0,2.0,2.5 means $s.d.=1.0+2.0x+2.5x^2$, where x is a Value. Consequently, in the simplest case, a single number will set a fixed value for this range. User can input either absolute or relative value of the s.d.

 Absolute values are in % (not fractions).

Click *Set Ranges* button. The ranges are check for consistency, sorted and set. If the setting was successful the values are plotted on the chart.

 Chart always displays relative values of s.d.

- Plotting errors.

After errors are defined and set they are automatically plotted. Plot displays relative s.d. by default even if they are defined as Absolute in the table. User can change this default display and scale using Popup menu. Popup menu is invoked by right-hand mouse button (mouse pointer should be over chart area). The following options are available in the Popup menu:

Relative - displays relative s.d. values;

Relative_log - displays relative s.d. values in logarithmic scale;

Absolute - displays absolute s.d. values;

Absolute_log - displays absolute s.d. values in logarithmic scale.

 Sometimes plot does not scale properly after conversion- use interactive scale change (below) to correct this.

Chart is interactive and users can select/magnify range. To select region, press and hold shift key and use mouse pointer to draw selected area on the plot. After you release the shift key the area will be magnified. To scale back, press and hold shift key and click right- hand mouse button.

3.12.1.2 Setting Variable Parameters

Variable filmstack parameters ranges can be set the second panel (use the Next button to switch to this panel from the first panel). User can define unlimited number of the variable parameters. For example, if filmstack has three layers, the user may decide to select all three thicknesses as variable parameters and define the range and number of points for each of these parameters. The result will be that repeatability is calculated for all the different combinations of layer thicknesses that are defined.

Following are the step to select and set *Variable* parameters in the Filmstack:

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- Select the layer record in the *Current Filmstack* list (Upper panel- *Parameters Selection*) and click *Add* button or just double-click the record. **Layer Creator** dialog will appear showing detailed layer view. Select the *Show* checkbox next to a layer parameter you would like to make a *Variable*.
 If you would like a *Variable* parameter also to be calculated, select a *Calculate* checkbox in addition to a *Show* checkbox.
 All selected parameters will appear in the *Variable Parameters* list. If you would like to select other parameters - repeat the selection.
- In order to set a *Variable* select a record in the *Variable Parameters* list, input the *Minimum*, the *Maximum* values, the *Number of Points* and click the *Set Parameter* button. Repeat this operation to all the parameters in the *Variable Parameters* list. Once parameter is "set" a check mark appears next to the record in the *Variable Parameters* list.

3.12.1.3 Setting calculation conditions and specs

Calculation Conditions panel (panel #3) allows to select calculation options and set specification for the calculated parameters.

a) Setting Specification for calculated parameters.

Specification has to be set for each calculated parameters. Its meaning and value is defined by the selected Options: *Confidence Limit* and *Repeatability type*. These options can be selected from the respective dropdowns and are set for All the parameters at the same time. Repeatability type can be either "Relative" or "Absolute". "Relative" type indicates that Repeatability spec is set in %% of calculated value, "Absolute" type indicates that the spec is set in absolute values (the default units are Angstroms for thickness and n, k for Optical constants). The *confidence limit* can be selected from the 1σ to 3σ range. If the confidence limit option is set to 1σ , *Repeatability spec* values are interpreted as 1σ specs.

 Change from an *Absolute* to a *Relative* repeatability type will automatically update specification that was set before the change. However, the change of the *Confidence limit* options is NOT automatically propagated and need to be reset manually.

b) Setting of Calculation Conditions.

There are three Calculation conditions options that can be selected from the dropdown boxes: *Number of Trials*, *Parameter Type* and *Estimate Type*.

Number of Trials defines the number of repeated calculations. Each trial is performed with the new synthetic data set. It is important to have a statistically meaningful number of trials. In most cases, 50 trials prove to be adequate. However, in the case of direct Monte-Carlo option selection more trials may be needed in some cases (several hundred). Number can be selected from the dropdown box or input manually.

Parameter type can be *Direct* or *Aggregate*. The *Direct type* defines only directly measured parameters (e.g. thickness). The *Aggregate type* allows defining parameters that are not directly measured but calculated from the measured parameters. In particular, n, k values of the parametrically defined material (e.g. Cauchy) are *Aggregated* parameters; - parametric coefficients are measured directly but n, k values are calculated from these measured

parameters values. Selection of the *Aggregate type* invokes detailed *LayerView* for available layers (sequentially) that allow direct selection of aggregated parameters. Conversion to Direct type is handled automatically.

3.7.1.4 Calculation results display.

Calculation panel (4th panel) allows starting calculation, reviewing calculation results and saving the results.

Calculation panel has *Synopsis* window that displays the summary information about current *Performance recipe* – the *Measurement recipe*, *Calculation conditions* and parameters that were set (manually or loaded) to Performance Wizard.

To start calculations select the *Start Calculations* button. *Performance Wizard* will check if all the conditions are consistent and all the needed data is available and start the calculations. The progress of calculations can be monitored using progress bars. The results of the calculation are displayed continuously in the *Results Table* as they become available. The *Performance Metrics* are calculated only after calculations are completed.

To stop calculation use the *Stop* button.

i Calculation will not abort immediately; it may take few seconds to complete calculations already in progress

To start new calculation - use the *Reset Results* button to clear the results of current calculation before modifying/editing conditions to run new calculation.

To load full recipe from the current XML file use *Select Full Recipe* drop-down. All recipes available in current XML file are listed in the *Select Full Recipe* drop-down. Selecting the record from the drop-down will load the recipe.

i Any recipe data previously set in *Performance Wizard* will be overwritten with this recipe.

3.12.2 Performance Batch

Performance Batch allows loading performance recipes from an XML file and running them in a "batch" - unattended. For manual creation of the recipes and their sequential execution - use **PerformanceWizard**.

Performance Batch results are displayed continuously for each recipe as calculation progresses. Calculation results of each recipe are saved in a separate file in the <TFCompanion_installation>/simulation/batch directory; the name of the file is "*recipe name*"_batch.csv. Performance Metrics calculation results are saved in the file-*BatchMetricsResult.csv* in the <TFCompanion_installation>/simulation/batch directory. Performance metrics results from all recipes in the batch are saved in this one file.

Preparing and running Batch calculations.

Available Recipes list is displaying all the recipes available in the current XML file. User can load another XML file using the *Load* button. To add a recipe to the batch, select the name in **Available Recipes** list and use the **Add** button - the recipe is added to the batch and displayed in **Selected Recipes** list. To remove a recipe from the batch, select the name in the **Selected Recipes** list and click the **Remove** button. After all the desired recipes are added to the batch (as displayed in the **Selected Recipes** list)- click the **Start** button.

Performance Recipes are loaded and processed sequentially in the order they are displayed in **Selected Recipes** list. The detailed synopsis of the currently processed recipe is displayed in **Current Recipe** text panel. The progress and details of the current recipe calculation are displayed in the separate, **Calculation** Tab. The **Calculation** Tab offers the same detailed view of the calculation as **Performance Wizard**. User can switch between the **BatchRun** and **Calculation** tabs. **Performance Metrics** results for individual recipes are continuously displayed in the **Calculation Log** text panel; at the same time they are added to a *BatchMetricsResult.csv* file. Calculations continue until all the recipes are processed and results are saved, unless the batch run is stopped before completion.

The **Stop** button can be used to stop the batch run. The run will stop after calculation of the current recipe is completed. To stop the current recipe calculation immediately user can toggle the **Calculation** tab and use **Stop Calculations** button there.

i This immediate termination of the current recipe calculation is not recommended-Performance Metrics results for the terminated recipe that are not correct, may be added to *BatchMetricsResult.csv* file.

Batch Calculation Progress bar is showing the % of the recipes that are currently processed.

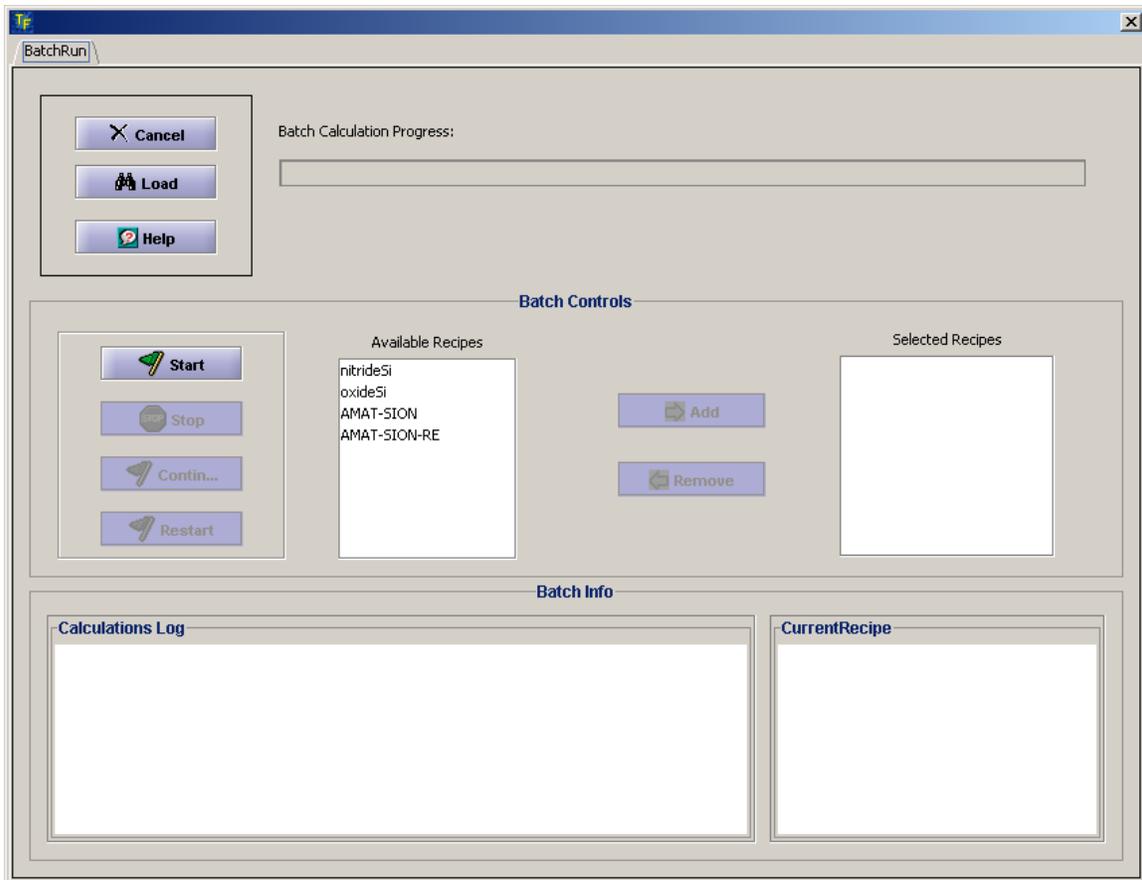


Fig. 3.12.2 Performance batch dialog

4. Database and Users administration.

TFCompanion uses embedded object database to maintain following records:

- Filmstacks
- Materials
- Projects
- Calculation recipes
- Measurement recipes
- Measurement data
- Users (separate database)

Management of the Users database (adding, removing users, changing privileges, passwords) can be done in **User Administration** dialog. Use **Configure/User Administration** from the main menu. Access to users database is available only through **User Administration** dialog.

Management of all other databases can be done in **Library Dialog (Tools/Library Manager)** from the main menu). At the same time, one can also add, remove or rename database records in various places in TFCompanion:

- 4 Main dialog sidebar displays a list of database record and allow to perform some the operations (remove or rename record)
- 5 Materials, Layer and Filmstack dialogs sidebars displays relevant database records User can remove or rename selected records.

4.1. User Administration

Management of the Users database (adding, removing users, changing privileges, passwords) can be done in **User Administration** dialog. Use **Configure/User Administration** from the main menu. Access to users database is available only through **User Administration** dialog.

The user *Administrator* is a super-user and it has the highest privilege level. Administrator can create any other user with the same or lower level of privileges. Administrator account cannot be removed but default password (psw) can be changed. All user belong to the group **All**. Administrator can create subgroups for organizing the users.

Each user has several attributes:

- **Access level** (Administrator, Engineer, Operator)
- **Capability Level**. This defines TFCompanion capabilities user is allowed to use. Administrator always has the capability corresponding to purchase edition but can assign low capability for other users. E.g. if TFCompanion –RE Advanced is purchased. All users will have Advanced capabilities but Administrator can assign –R (only reflectance data analysis) or –E (only ellipsometry data analysis) for some users.
- **Operation type** (Standalone or integrated). Administrator has a *Standalone* operation type but can create another user that has Integrated operation type. It is convenient to have separate users for standalone and Integrated operations because user interface is changing depending on operation type (it also prevent unnecessary attempts to communicate with the hardware that is not connected).

- Password, hint, answer. These are assigned by administrator and can be changed by the user later on.

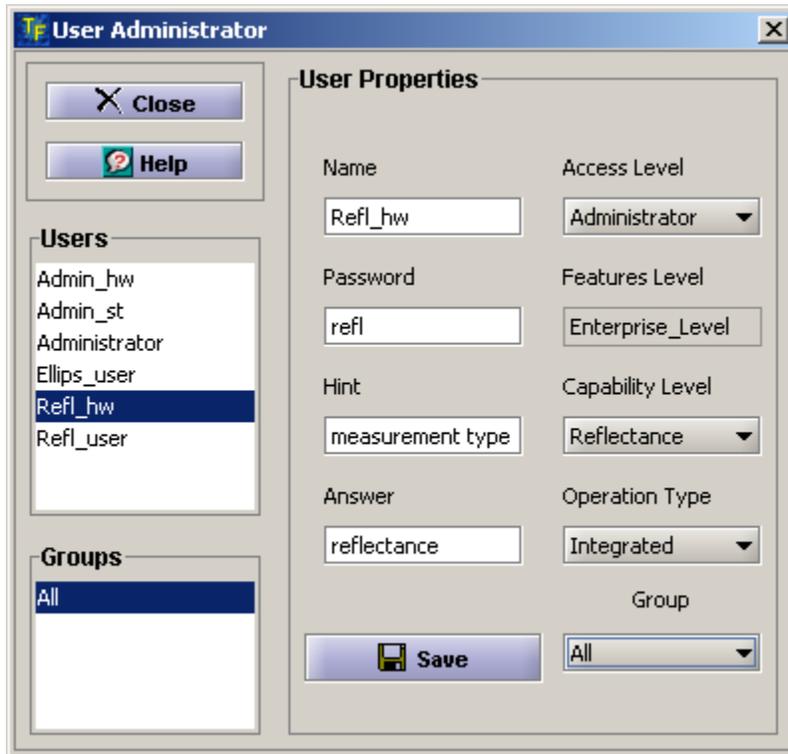


Fig. 4.1 User Administration dialog

4.2 Database Administration

TFC Companion uses embedded object database to maintain following records:

- Filmstacks
- Materials
- Projects
- Calculation recipes
- Measurement recipes
- Measurement data

Library Dialog (Tools/Library Manager from the main menu) allows to manage these databases:

- Import text file data (separate files or zipped)
- Import data from other TFC Companion databases or from previous database version used with TFC Companion version 2.6 and earlier (*.zip)
- Export data to XML file
- Rename database records
- Remove database records

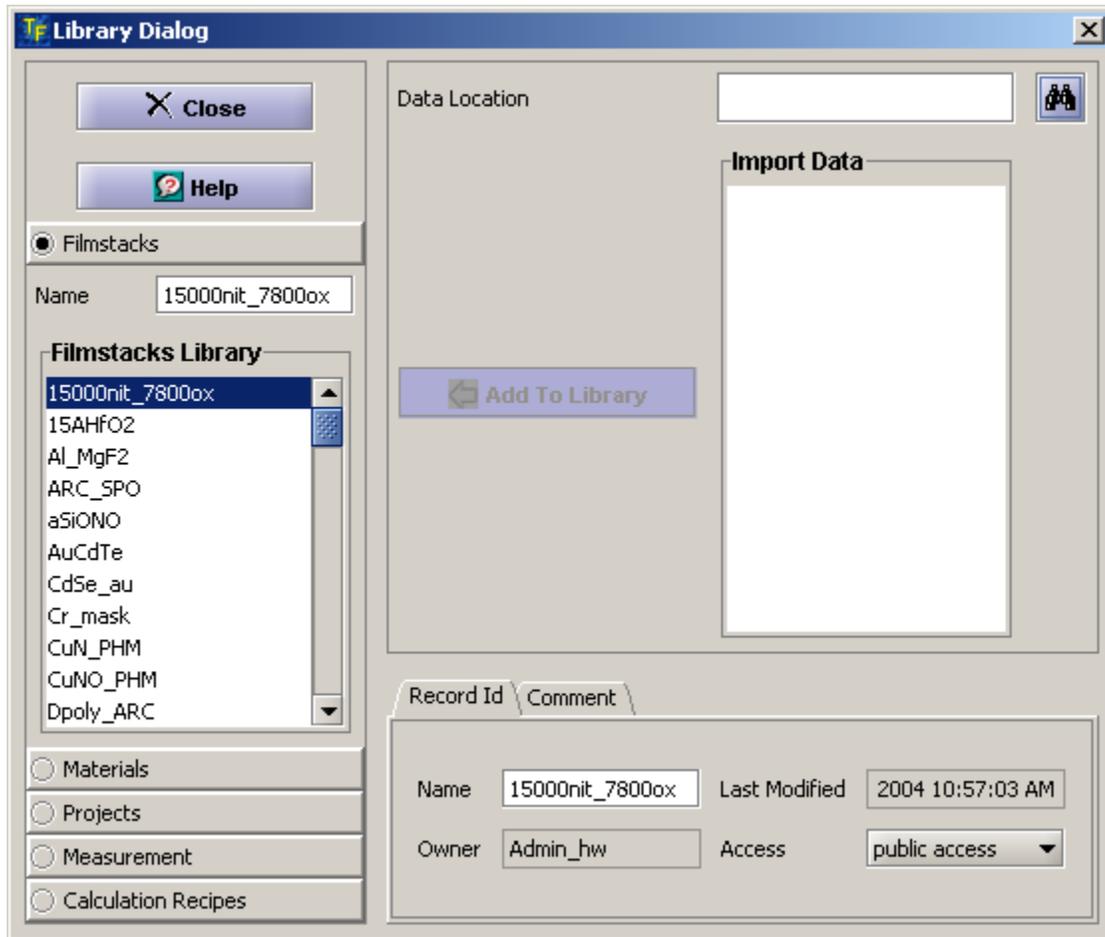


Fig 4.2.1 Library dialog

5. Imaging data analysis

TFC Companion support data analysis of the image data: Imaging Ellipsometry, Reflectometry and Transmittance are fully supported. Import and analysis of the standard imaging file is supported.

Appendix I TFC Companion features matrix

Technical Feature	Description	Standard Version			Advanced version	Enterprise version
		-R	-E	-RE		
Measured/Simulated data¹						
Δ (Delta)	ellipsometry	-	✓	✓	✓	✓
Ψ (Psi)	ellipsometry	-	✓	✓	✓	✓
Cos Δ	ellipsometry	-	✓	✓	✓	✓
Tan Ψ	ellipsometry	-	✓	✓	✓	✓
X	ellipsometry	-	✓	✓	✓	✓
Y	ellipsometry	-	✓	✓	✓	✓
Reflectance	normal,p,s	✓	-	✓	✓	✓
Transmittance	normal,p,s	✓	-	✓	✓	✓
Absorbance	normal,p,s	✓	-	✓	✓	✓
<i>Spectral variable</i>						
Wavelength	Å,nm,µm, cm ⁻¹ ,eV	✓	✓	✓	✓	✓
Angle	deg,rad	✓	✓	✓		
<i>Data Acquisition(DA)</i>						
Manual input		✓	✓	✓	✓	✓
Text File Import	SOPRA, Woollam, Nanometrics, Rudolph, BIL, TFC Companion, JY- Horiba formats	✓	✓	✓	✓	✓
Direct data acquisition and control*	TFProbe series (reflectometers & ellipsometers)	✓	✓	✓	✓	✓
Custom integration acquisition and control	Any hardware				✓	✓
Build-it-yourself Instrument integration	Spectrometer +CCD w/DAC support (UV, Vis,	✓	✓	✓	✓	✓

	IR)					
Sensitivity Analysis						
Parameters						
$\Delta, \Psi, \text{Cos}\Delta, \text{Tan}\Psi, X, Y$		-	✓	✓	✓	
Reflectance, Transmittance, Absorbance	Normal, p,s	✓	-	✓	✓	
Technical Feature	Description	Standard Version			Advanced version	Enterprise version
		-R	-E	-RE		
Wavelength	Å,nm,µm, cm ⁻¹ ,eV	✓	✓	✓	✓	✓
Angle	deg,rad	✓	✓	✓	✓	✓
<i>Sensitivity variable</i>						
Wavelength, Angle, any of the filmstack parameters (thickness, etc.)		✓	✓	✓	✓	✓
Calculation	Calculation of filmstack parameters from the fit to measured data					
Modified Marquardt- Levenberg (global) method		✓	✓	✓	✓	✓
Confidence intervals and correlation coefficients		✓	✓	✓	✓	✓
Modified Genetic method		-	-	-	✓	✓
Batch measurements		-	-	-	✓	✓
Mapped measurements		-	-	-	-	✓
Wavelength/Angle resolution correction		-	-	-	-	✓
Error estimation	Estimation of filmstack parameters measurement precision					
Error estimator	One parameter variation	-	-	-	✓	✓
PSE Wizard	Unlimited parameters and ranges	-	-	-	-	✓
PSE Batch	proccession of pse recipes	-	-	-	-	✓
Materials						
Tabular (NK Table)		✓	✓	✓	✓	✓
Cauchy		✓	✓	✓	✓	✓
CauchyK		✓	✓	✓	✓	✓
Cauchy Exponential		✓	✓	✓	✓	✓
Sellmeier		✓	✓	✓	✓	✓

Sellmeier2		✓	✓	✓	✓	✓
EMA (2 and 3 component)	Bruggeman	✓	✓	✓	✓	✓
Harmonic oscillator	Lorentz oscillator	✓	✓	✓	✓	✓
Tauc-Lorentz Oscillator		✓	✓	✓	✓	✓
Drude-Lorentz oscillator		✓	✓	✓	✓	✓
Cody- Lorentz	Improvement of Tauc-Lorentz	✓	✓	✓	✓	✓
Cody-Lorentz-Urbach	Extension of Cody- Lorentz	✓	✓	✓	✓	✓
Form Birefringence approximation	Low-frequency spatial gratings	✓	✓	✓	✓	✓
Binary Compound approximation	Composition interpolation	✓	✓	✓	✓	✓
Import/Export materials From/to text file	SOPRA, TFCompanion formats	✓	✓	✓	✓	✓
Conversion from parameterized models to a Tabular (NK table)		✓	✓	✓	✓	✓
Conversion from Tabular material to parameterized model	Fitting parameterized model to a tabular data	✓	✓	✓	✓	✓
Anisotropic materials (uniaxial, biaxial) ²⁾	Tabular and all parameterized models	-	-	-	✓	✓
Materials database	included in distribution	✓	✓	✓	✓	✓
Filmstacks						
Inhomogeneous layer	Linear and Gaussian profiles	-	-	-	✓	✓
Surface roughness correction		✓	✓	✓	✓	✓
Incoherent layers		-	-	-	✓	✓
Linked layers & materials		-	-	-	✓	✓
<i>Presentation Graphics</i>						
2D interactive	plots (dispersion, results of simulation/calculati on, etc.)	✓	✓	✓	✓	✓
3D interactive plots (surface, contour and 3D line)	Simulation, sensitivity results	✓	✓	✓	✓	✓
Printing and exporting plots		✓	✓	✓	✓	✓
Productivity features						

Project/workspace environment		✓ ✓ ✓	✓	✓
Templating mechanism	One click operation	✓ ✓ ✓	✓	✓
Customization (individual for each user)	Units, resolution, appearance, etc.	Only for one user	for one user	✓ ³⁾

¹⁾ Complete list of supported parameters see Appendix III

²⁾ Partially implemented

³⁾ Customized on request

Appendix II TFCompanion import data format

Updated May 12, 2005

Revision 1.5. Original format specification: This format is fully supported from build 04182005. (April 14, 2005)

Revision 1.6. Added new parameters: Delta_T, Psi_T, Phase_Rp, Phase_Rs, Phase_Tp, Phase_Ts. Supported in build 05122005 (May 12, 2005)

Introduction

This document defines the data format, herein after TFC_format, for importing measured data (ellipsometry, reflectance, transmittance) in TFCompanion software. TFC_format is introduced for the convenience of the users; TFCompanion software also supports import of the data in other widely used formats -Sopra, Woollam, Nanometrics, Beaglehole Instruments, Rudolph, Jobin-Yvon (support for other formats can be added on request - free of charge). The purpose of TFC_format is to give a flexible and convenient way to import measured data into TFCompanion. This format is also used to export simulated data from TFCompanion.

File Encoding

Encoding does not need to be limited to ASCII (8-bit signed characters) except for reserved words as described in the next section. Comments can use Unicode encoding for formula, symbols etc. The data itself can use standard formatting or scientific notation. E.g. 0.36234E2 or 36.234 are both legal and represent the same value.

Note. *European convention of decimal comma instead of decimal point is not supported in this version because of the conflict with the csv (comma-separated values) format for Excel. (Data columns can be separated by either space or comma)*

File Header

The header has the following format:

```
TFC_DATA
# This is a comment for testing
# Date: <measurement date>
# Location:<x,y coordinates>
# WaferId:<wafer name>
# WaferLot:<lot number>
```

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```
# User: <user name>
# polarizer:<azimuth>
# analyzer:<azimuth>
#compensator:<azimuth>
<spec_variable>:<spec fixed parameter>:<parameter_1>:<parameter_2>:sd_<parameter1>:sd_<parameter2>
<spec_variable unit>-<spec_fixed_variable unit>
```

Description:

1.TFC_DATA is a reserved word. It should always be present and indicates the beginning of the header

2. The lines starting with # (pound) are comments but these are structured comments with the reserved words: Date:, Location:, WaferId:, WaferLot:, User:. If no reserved words are present – the text is considered a unstructured comment and saved as a regular text. The comments are optional – any or all comment lines can be skipped. When the data is imported -the header information is displayed in the WaferID panel in the main screen of TFCompanion.

3. Following line “# **This is a comment for testing**” has no reserved words and considered a regular text comment. This comment is read without parsing and displayed in the Comment text box (WaferID panel on the main screen)

4. In following line “# **Date: <measurement date>**” ‘Date:’ is a reserved word. Value <measurement date> is not currently parsed and may have free format. However it is recommended that format be consistent with ANSI-C strftime () function with the format specifier “%d %B %Y %H:%M:%S”(e.g. 14 April 2005 17:01:03).

5. Following line “# **Location:<x,y coordinates>**” indicate measurement location. ‘Location:’ is a reserved word. <x,y coordinates> has two values (doubles) separated by comma, these values correspond to x, y coordinates of the measurement point

6. Following line : “# **WaferId:<wafer name>**” indicate the wafer name. **WaferId:** is a reserved word, <wafer name> can be any string.

7. Following line : “# **WaferLot:<lot number>**” indicate wafer lot. **WaferLot:** is a reserved word, :<lot number> can contain any string.

8. Following line : “# **User: <user name>**” indicate operator who took the measurement. **User:** is a reserved word, <user name> can be any string.

9. Following line “ polarizer:<azimuth>” indicates polarizer azimuth in deg.

10. Following line “analyzer:<azimuth>” indicates analyzer azimuth in deg.

11. Following line “compensator:<azimuth>” indicates compensator azimuth in deg.

Note. Items 9,10,11 are used only in the cases when some of the measured or simulated parameters are system dependent (e.g. alpha,beta in case of RAE or RPE system)

Parameters markers.

Following line give parameters markers, each marker correspond to a data column:

```
<spec_variable>:<spec fixed parameter>:<parameter_1>:<parameter_2>:sd_<parameter_1>:sd_<parameter2>
```

1. <spec_variable> is a variable of the measured spectrum. It can be either **Wavelength** or **Angle**.

2. <spec fixed parameter> is a fixed parameters of the measured spectrum It can be either **Wavelength** or **Angle** (obviously <spec_variable> and <spec fixed parameter> are complimentary – can not be the same parameter)

- 6 <parameter_1>:<parameter_2>:.....:<parameter_n> are column separated markers for measured parameters. Number of parameters is unlimited. Following are reserved words for valid parameters: **Delta, Psi, CosDelta, TanPsi, X, Y, Reflectance, Normal Reflectance, Rp, Rs, Transmittance, Normal Transmittance, Ts,Phase_Rp,Phase_Rs,Phase_Tp,Phase_Ts,Delta_T,Psi_T** (see Appendix III on details of supported parameters)

Almost all combinations of parameters are allowed the only limitation is that parameters represent "unique values"- different representation of the same value is not allowed. E.g. Delta and CosDelta are illegal in the same spectra, but Delta and Psi, or Delta and TanPsi are legal.

4. sd_<parameter_1>:sd_<parameter_2>:....: sd_<parameter_n> are optional marker for standard deviations (s.d.) of measured parameters. No particular order is required – the attribution is in the name, e.g. sd_Delta is s.d. of Delta

5.<spec_variable unit>-<spec_fixed_variable unit> is the unit of the spectral variable and fixed variable (unit are separated by dash). If units are missing or invalid – the default units are used.

For wavelength following units are supported: A, nm, um, eV, inv_cm that correspond to (Angstrom, nanometer, micrometer, electron-volt, cm^{-1}); for Angle – Rad, Deg that correspond to (radian, degree). If the unit is missing the default unit is assumed (nm for wavelength, deg. for angle).

Example1: nm-deg Example2: nm The result of parsing is the same for Examples1 and Spectral variable is assumed in nm and fixed variable in deg

Data

The data should be either space or comma separated. The number of columns should correspond the number of markers. Each line corresponds to one data point. Following units are used for date: Delta, Psi, Delta_T, Psi_T, Phase_Rp, Phase_Rs, Phase_Tp, Phase_Ts (**degrees**), Reflectance, Transmittance, Rp, Rs, Normal Reflectance, Normal Transmittance, Tp, Ts are **fractions**.

General

All markers are case sensitive reserved words and should be reproduced exactly. Empty lines are allowed anywhere – they are skipped during parsing. Lines that contain '[' (open square bracket) are ignored like empty lines – they can be placed anywhere to keep personal comments

Multiple spectra.

Multiple spectra can be concatenated in one file. There is no limitation on the number of spectra and each spectra can have different parameters. Each spectrum has it own header, markers and data. **It is expected that all spectra are having the same spectral variable (either wavelength or angle).**

Following is an example of the data file with one spectrum:

```
TFC_DATA
# This is a comment for testing
# Date: April 12,2005
```

Location:10,5

WaferId:TestWafer

WaferLot:1

User: Leo

[This line is ignored by the parser because it has '[' symbol. You can insert these lines anywhere

Wavelength:Angle:Delta:Psi:sd_Delta:sd_Psi

[unit line below can be ignored because nm is a default unit, but it is a good practice to have it anyway

[full unit string would be 'nm-deg'

nm

240.1 70.00 93.931937 21.774168 0.2 0.1
242.3 70.00 143.497753 31.700100 0.2 0.1
277.9 70.00 88.559312 40.880459 0.2 0.1
313.5 70.00 62.057384 47.162740 0.2 0.1
349.1 70.00 92.054787 31.639227 0.2 0.1
384.8 70.00 146.911641 23.414678 0.2 0.1
420.4 70.00 165.730292 17.913739 0.2 0.1
456.0 70.00 127.284931 17.942006 0.2 0.1
491.6 70.00 100.333732 20.165835 0.2 0.1
527.3 70.00 82.527480 22.826088 0.2 0.1
562.9 70.00 69.307711 25.692062 0.2 0.1
598.5 70.00 58.367353 28.778249 0.2 0.1
634.2 70.00 48.110483 32.008534 0.2 0.1
669.8 70.00 37.562377 35.072711 0.2 0.1
705.4 70.00 26.145824 37.700070 0.2 0.1
741.0 70.00 14.035120 39.409103 0.2 0.1
776.7 70.00 2.050270 39.907003 0.2 0.1
812.3 70.00 8.818438 39.262259 0.2 0.1
847.9 70.00 17.941343 38.000471 0.2 0.1
883.5 70.00 25.405193 36.433384 0.2 0.1
919.2 70.00 31.510164 34.776733 0.2 0.1
954.8 70.00 36.538703 33.171257 0.2 0.1
990.4 70.00 40.745241 31.678275 0.2 0.1
1026.0 70.00 44.329460 30.315294 0.2 0.1
1061.7 70.00 47.439311 29.078936 0.2 0.1
1097.3 70.00 50.182053 27.957401 0.2 0.1
1132.9 70.00 52.635146 26.936578 0.2 0.1
1168.5 70.00 54.854846 26.002771 0.2 0.1
1204.2 70.00 56.899952 25.153131 0.2 0.1

Appendix III Parameters and conventions used in TFCompanion

TFCompanion follows common naming convention using subscripts _s and _p (e.g. R_s , R_p) indicating p-polarization (in the plane of incidence) and s-polarization (perpendicular to plane of incidence). TFCompanion support several different representations of Ellipsometry parameters that are described in this document. Both reflectance and transmittance Ellipsometry parameters are supported; _T is added to the name of the parameter to indicate that it is related to Transmission Ellipsometry. Two different sign conventions (Azzam and Beaglehole) of Ellipsometry parameters are supported as well as Delta convention and can be selected in configuration defaults setup.

I. Reflectance, Transmittance and Absorption parameters.

Measured parameters (intensity) indicated by capital characters, amplitudes indicated by small characters.

a). Reflectance parameters

R_p - reflectance of the p-polarized light; $R_p = |r_p|^2$

R_s - reflectance of the s-polarized light; $R_s = |r_s|^2$

Reflectance – unpolarized reflectance; $\text{Reflectance} = \frac{R_p + R_s}{2}$

Normal Reflectance – reflectance at 0 angle of incidence (from the normal to the surface). The presence of Normal Reflectance as a separate parameter allows to calculate it simultaneously with other angle dependent parameters.

b). Transmittance parameters

Note. Transmittance is calculated from ambient to substrate (substrate is infinite). Substrate should be set as void.mat (and any finite thickness material as a first layer).

T_p - transmittance of the p-polarized light; $T_p = |t_p|^2$

T_s - transmittance of the s-polarized light; $T_s = |t_s|^2$

Transmittance – unpolarized transmittance $\frac{T_p+T_s}{2}$

Normal Transmittance – transmittance at 0 angle of incidence (from the normal to the surface).

c). Absorption parameters

Note. Absorption is calculated indirectly as a complimentary parameter using equation $R+T+A=1$ (R-reflectance, T – transmittance, A- absorption) for each type of the absorption units.

A_p- absorption of the p-polarized light; $A_p=1-T_p-R_p$

A_s- absorption of the s-polarized light; $A_s=1-T_s-R_s$

Absorption – unpolarized absorption $\frac{A_p+A_s}{2}$

Normal Absorption – absorption at 0 angle of incidence (from the normal to the surface).

II. Ellipsometry parameters

TFCompanion supports conventional system independent Ellipsometry parameters and system dependent Ellipsometry parameters (as of build 06282005). All parameters are supported for reflectance and transmittance Ellipsometry.

a). System independent Ellipsometry parameters

Conventional ellipsometry parameters (Δ, Ψ) for isotropic system are defined using following equation:

$$\rho = \frac{r_p}{r_s} = \text{Re}(\rho) + i \text{Im}(\rho) = \tan \Psi e^{i\Delta} \text{ for reflectance ellipsometry}$$

$$\text{where } \tan \Psi = \frac{|r_p|}{|r_s|};$$

$$\Delta = \text{Phase}_{Rp} - \text{Phase}_{Rs}$$

$$\text{alternative representation: } X = \frac{2\text{Re}(\rho)}{(1 + \tan^2 \Psi^2)}; Y = \frac{2\text{Im}(\rho)}{(1 + \tan^2 \Psi^2)}$$

and

$$\tau = \frac{t_p}{t_s} = \text{Re}(\tau) + i \text{Im}(\tau) = \tan \Psi e^{i\Delta} \text{ for transmittance ellipsometry}$$

$$\text{where } \tan \Psi = \frac{|t_p|}{|t_s|}$$

$$\Delta = \text{Phase}_{Tp} - \text{Phase}_{Ts}$$

$$\text{alternative representation: } X_{-T} = \frac{2\text{Re}(\tau)}{(1 + \tan^2 \Psi^2)}; Y_{-T} = \frac{2\text{Im}(\tau)}{(1 + \tan^2 \Psi^2)}$$

Delta – ellipsometry Δ parameter.

Psi - ellipsometry Ψ parameter.

CosDelta – ellipsometry $\cos\Delta$ parameter

TanPsi – ellipsometry $\tan\Psi$ parameter

Phase_Rp –absolute phase (θ_p) of R_p

Phase_Rs –absolute phase (θ_s) of R_s

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Delta_T – ellipsometry Δ parameter for transmission.
 Psi_T - ellipsometry Ψ parameter for transmission.
 CosDelta_T – ellipsometry $\cos\Delta$ parameter for transmission
 TanPsi_T – ellipsometry $\tan\Psi$ parameter for transmission
 Phase_Tp –absolute phase (θ_{p_T}) of T_p
 Phase_Ts –absolute phase (θ_{s_T}) of T_s
 X, Y parameters provide alternative of Δ, Ψ representation
 X_T, Y_T parameters provide alternative of Δ_T, Ψ_T representation.

The interesting property of X, Y parameters is that they are also directly measured quantity in PME (Photoelastic modulator ellipsometry). Assuming $A=P=45\text{deg}$ (Analyzer/Polarizer azimuth angle).

The following expression shows the connection:

$$X = \frac{I_{2f}}{I_{dc}} = \frac{4J_2(\delta_0)\text{Re}(\rho)}{1+\tan^2\Psi^2+2J_0(\delta_0)\text{Re}(\rho)} = \frac{2\cos\Delta}{1+\tan^2\Psi^2}$$

$$Y = \frac{I_f}{I_{dc}} = -\frac{4J_1(\delta_0)\text{Im}(\rho)}{1+\tan^2\Psi^2+2J_0(\delta_0)\text{Im}(\rho)} = \frac{2\sin\Delta}{1+\tan^2\Psi^2}$$

where I_f is the signal at PM oscillation frequency;

I_{2f} is the signal at double PM frequency;

I_{dc} is the DC component of the signal;

J_n is a Bessel function on n^{th} order

b). System dependent ellipsometry parameters

Measurement system does not, normally, measure conventional ellipsometry parameters directly, instead the system specific parameters are measured and conventional ellipsometry parameters are calculated by taking into account system configuration.

1. Rotating analyzer ellipsometer (RAE) or Rotating polarizer ellipsometer (RPE).

RAE or RPE are some of the most simple and widely used ellipsometry measurement systems.

The time –dependent signal collected from the detector can be expressed in the following form:

$$I(t) = I_0 \{1 + \alpha \cos(2ft) + \beta \sin(2ft)\},$$

where f is the frequency of rotating element.

α, β parameters are directly measured values in RAE or RPE system and, in the case of isotropic system, they can be related to the $\tan\Psi$ and $\cos\Delta$ values using following equations:

$$\tan \Psi = \tan P \left(\frac{1+\alpha}{1-\alpha} \right)^{1/2};$$

$$\cos \Delta = \frac{\beta}{(1-\alpha^2)^{1/2}};$$

where P is polarizer azimuth in RAE or analyzer azimuth in RPE

Alpha is α parameter for reflectance ellipsometry

Beta is β parameter for reflectance ellipsometry

Alpha_T is α parameter for transmission ellipsometry

Beta_T is β parameter for transmission ellipsometry

2. Rotating Compensator ellipsometry (RCE)

The time –dependent signal collected from the detector can be expressed in the following form:

$$I(t) = I_0 \{1 + a_2 \cos(2ft) + b_2 \sin(2ft) + a_4 \cos(4ft) + b_4 \sin(4ft)\};$$

where f is the frequency of compensator rotation.

For the case of isotropic system parameters a_2 , b_2 , a_4 , b_4 can be easily expressed as a function of azimuth angle of Polarizer (P), Analyzer (A), retardation of compensator (δ) and Δ , Ψ parameters. For a simple case of $P=45$, $A=0$ equations are as follows:

$$a_0 = 1 - 0.5(1 + \cos \delta) \cos \Psi$$

$$a_2 = 0;$$

$$b_2 = \sin \delta \sin 2\Psi \sin \Delta / a_0$$

$$a_4 = -0.5(1 - \cos \delta) \cos 2\Psi / a_0$$

$$b_4 = 0.5(1 - \cos \delta) \sin 2\Psi \cos \Delta / a_0$$

A2 – a_2 parameter for reflectance ellipsometry

B2 – a_4 parameter for reflectance ellipsometry

A4- a_2 parameter for reflectance ellipsometry

B4- b_4 parameter for reflectance ellipsometry

A2_T – a_2 parameter for transmission ellipsometry

B2_T – a_4 parameter for transmission ellipsometry

A4_T- a_2 parameter for transmission ellipsometry

B4_T- b_4 parameter for transmission ellipsometry

Conventions

1. Delta convention

Some measurement systems (e.g. RAE) can distinguish between 0-180deg and 180-360 deg Delta bidrants. In this case Delta is only defined in 0-180 deg. range TFCpanion supports both 0-180deg and 0-360 deg. Convention.

2. Sign convention

There are several conventions in Delta calculation that depends on whether optical constant are represented in $n+ik$ or $n-ik$ form and the sign of reflectance used for substrate.

TFCompanion follows Azzam convention by using internally dielectric constant in the form $\varepsilon_1 - i\varepsilon_2$. The consequence of using this convention is that $\Delta_{\text{Azzam}} = 180\text{deg}$ for reflection from bare substrate.

Beaglehole convention set $\Delta_{\text{bil}} = 0\text{deg}$ for reflection from bare substrate.

$$\Delta_{\text{bil}} = 180 - \Delta_{\text{Azzam}}$$

TFCompanion supports both Azzam and Beaglehole conventions that can be selected in configuration defaults setup.

Note. Aspnes convention uses $\varepsilon_1 + i\varepsilon_2$ convention and $\Delta_{\text{bil}} = -\Delta_{\text{Aspnes}}$; Aspnes convention is currently not supported