Absolutely no hardware or Operating system lock. Combine data from different sources; model them together or separately. Use your preferred measurement hardware and operating system.

A QUICK START-UP GUIDE

I. Introduction.

This document is intended for the first-time users of TFCompanion and gives a brief overview of capabilities and basic functionality of the software.
Other resources: UserGuide (Online/UserGuide from TFCompanion the main menu), Tutorials (Online/Tutorials from TFCompanion the main menu)

TFCompanion™ *is a powerful and user-friendly software application for thin film analysis. It is a fusion of optical metrology, material science, and process development experience with the latest computer technology.*

- **Calculate filmstack parameters based on measurement results**
- **Simulate measurement sensitivity and optical response from the filmstack**
- **Estimate measurements repeatability and optimize measurement recipe**
- Measurements data can be imported from the text (ASCII) file in direct data acquisition and network data transfer (TCP IP) are also supported.
- Extensive library of material's optical properties is included. New materials can be added by user manually or imported from the text file.
- Wide range of parameterized materials is supported (Cauchy, Sellmeier, EMA, Lorentz oscillator, Lorentz-Drude, Tauc-Lorentz, etc.)
- Results can be presented in a tabular form; 2D or 3D plot
- Multiple spectra and different types of data (ellipsometry, reflectance, transmittance) can be used together
- Multiple sample analysis and linked layers/materials are supported
- Parameters offsets (instruments matching), angle-of-incidence & spectral resolution effects are supported

SOFTWARE FOR THIN FILM DATA ANALYSIS

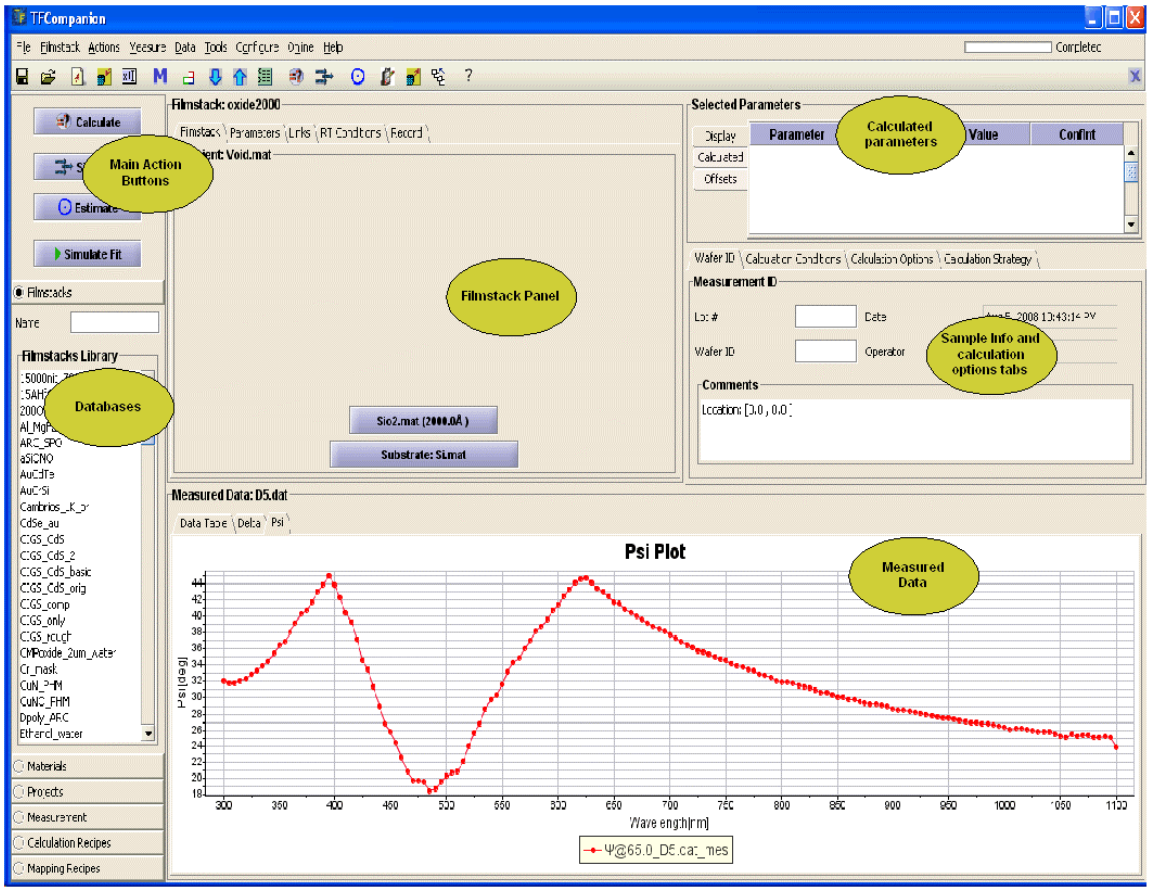

Fig. 1 **TFCompanion main screen includes several panels:**

Databases(filmstack, materials, etc) - left sidebar
Action buttons – sidebar (above databases)
Measured data – bottom panel/chart
Filmstack – central panel
Calculation parameters – top right-corner panel
Sample info and Calculation options – below calculation parameters

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II. Calculation of filmstack parameters

You just measured the sample, how to determine the physical parameters of this sample (like thickness of the layers)?

Optical measurements are indirect - they are measuring optical response of the sample not the properties themselves. One needs to solve an "inverse problem" in order to find the value of actual physical properties of interest. The "inverse problem" is solved numerically by finding the best fit between the measured and calculated data and physical properties are inferred from the model that gives the best fit.

In order to determine properties of the sample based on measured data, one needs to do the following:

1. Create an optical model (filmstack) of sample.
2. Select calculated parameters i.e. parameters you would like to determine
3. Import measured data
4. Calculate

a). Creating filmstack.

TFCompanion allows easily create a filmstack: one can add/remove layers directly in the main screen. **Note.** Large a complex filmstacks can be edited/created in the Filmstack dialog (Filmstack/Edit Filmstack from the main menu).

One can use following icons in the toolbar to quickly add ( ) of remove ( ) the layer. We can also select material in the database and add it as a layer (Fig. 2,3)

We will start with a Si substrate and add SiON layer (250nm).
Fig. 2 and Fig. 3 illustrate the process of adding a layer.

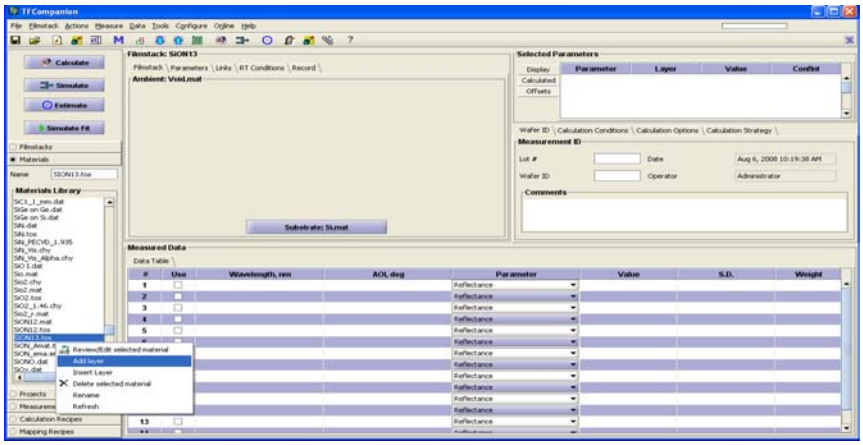

Fig. 2 Adding layer to filmstack

Fig. 3 This dialog appears after action (Fig. 2) and prompts to enter thickness of the layer.

Now we need to select calculated parameters.

b). Selecting calculated parameters

We would like to determine the SiON layer thickness and n,k values at 248nm.
First we select thickness (Fig. 4). Next we select n,k at 248nm (Fig.4,5). The SiON material we are using represents optical dispersion using Tauc-Lorentz approximation (TLA) – it is a parameterized materials. This mean that we calculate TLA parameters and "display" n, k values. On Fig. 4 we selected n,k and 248nm wavelength but nothing happened yet – we need to check Solve checkbox and select TL parameters (Fig. 5).

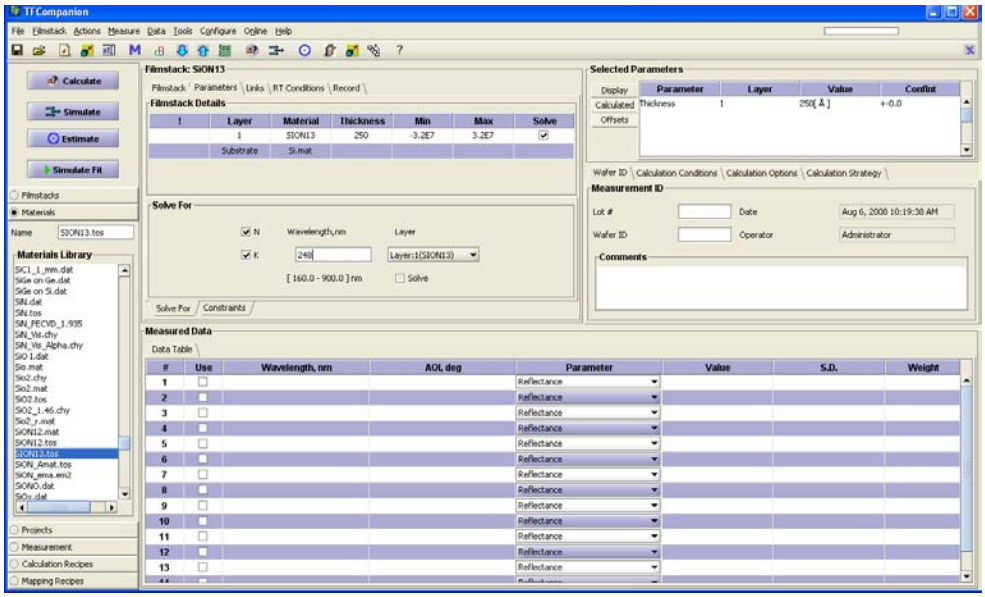

Fig. 4 Selecting calculated parameters. Thickness is selected and the current values is displayed in calculated parameters table.

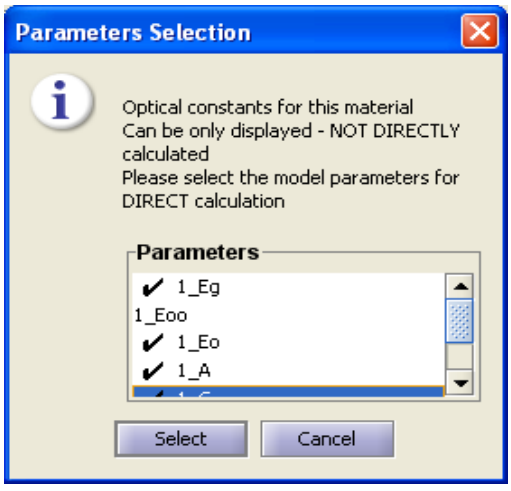

Fig. 5 User is prompted to select TLA calculated parameters (this dialog appears after selecting Solve checkbox in Fig. 4)

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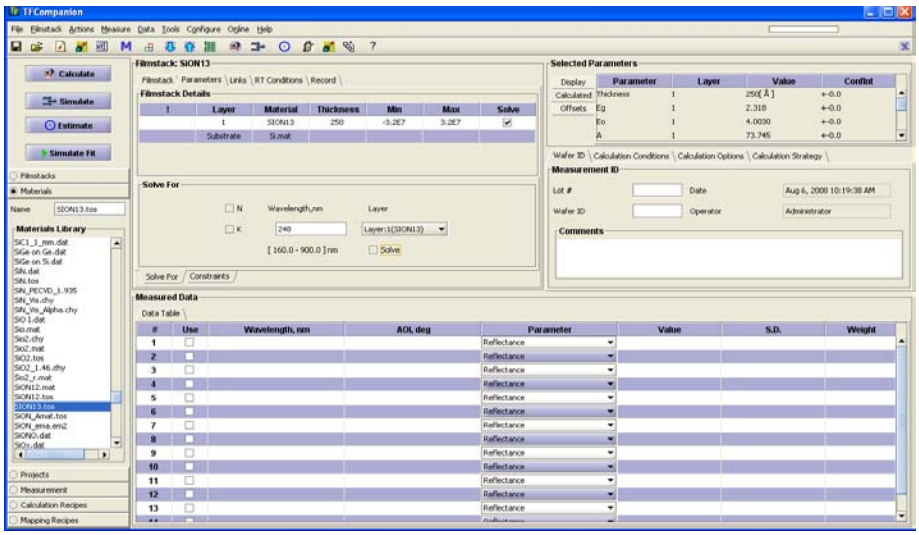

Fig. 6 Now calculated parameters are selected (they are displayed in the Parameters table)

c). Importing measured data

We will import measured data from the text file. Use File/Import Measured data from the main menu or **M** icon in the toolbar. We will import two spectra Reflectance and ellipsometry data.

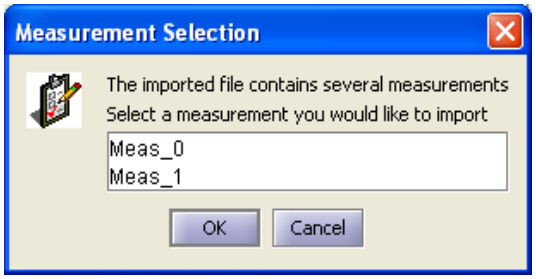

Fig. 7 User is prompted to select measured data. This dialog appears because file included two spectra

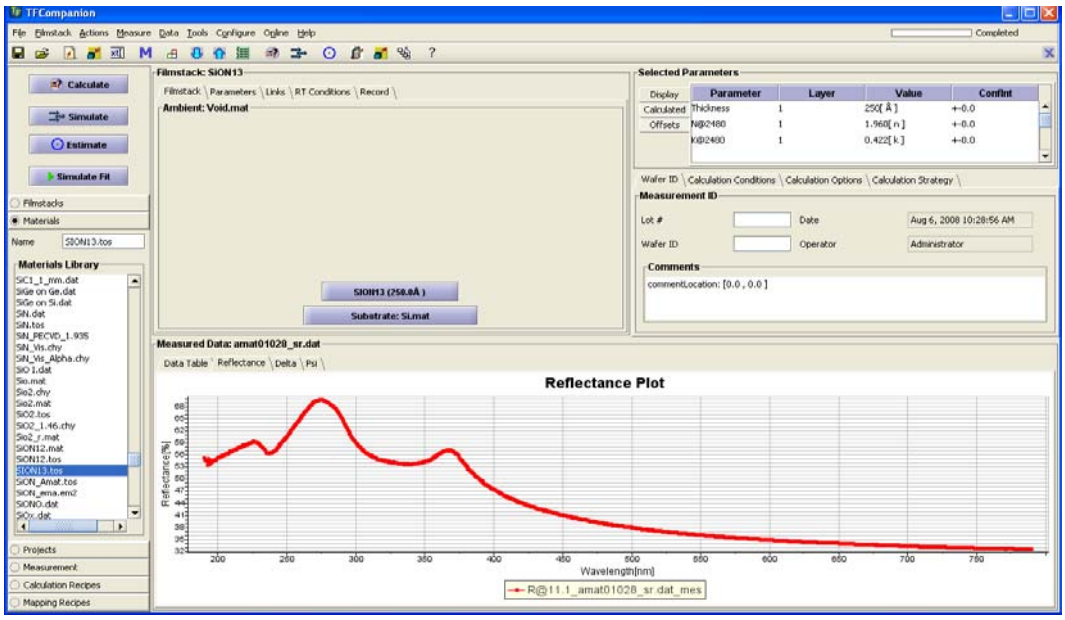

Fig. 8 Measurement data is imported and displayed

d). Calculation

Now we have measured data and filmstack model – time to calculate.

Select Calculate button and 1-2 s results appears (Fig. 9). We can export the results of calculation using File/Export Calculation results.

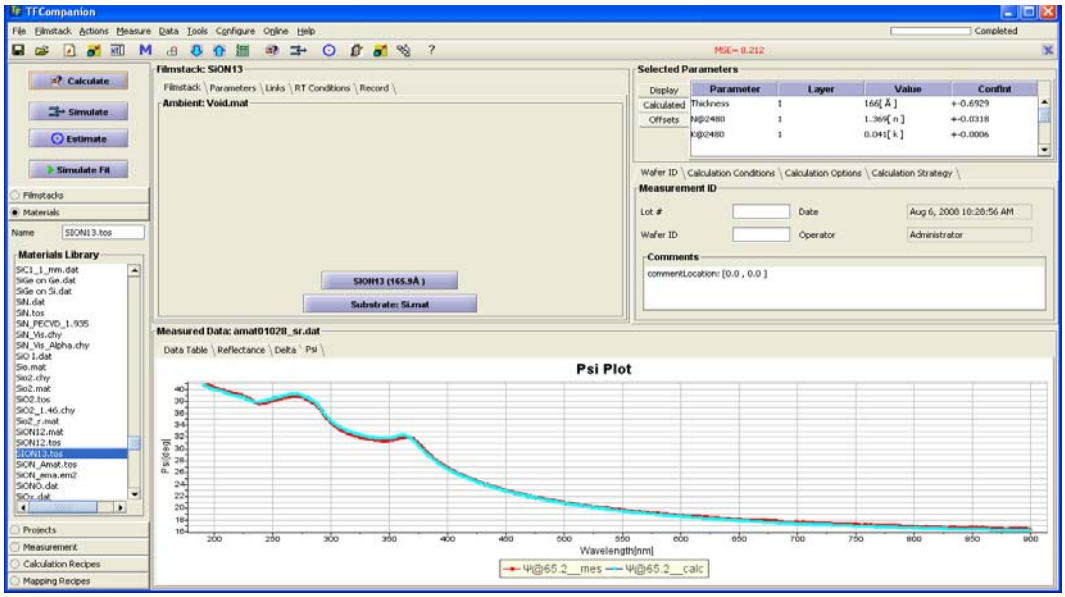

Fig. 9 Calculation results. The values of calculated/displayed parameters are in Parameters table. Measured vs. Calculated data fit is displayed in the plot. The MSE (mean-square estimate), indicating the goodness of fit is displayed in the toolbar (in red).

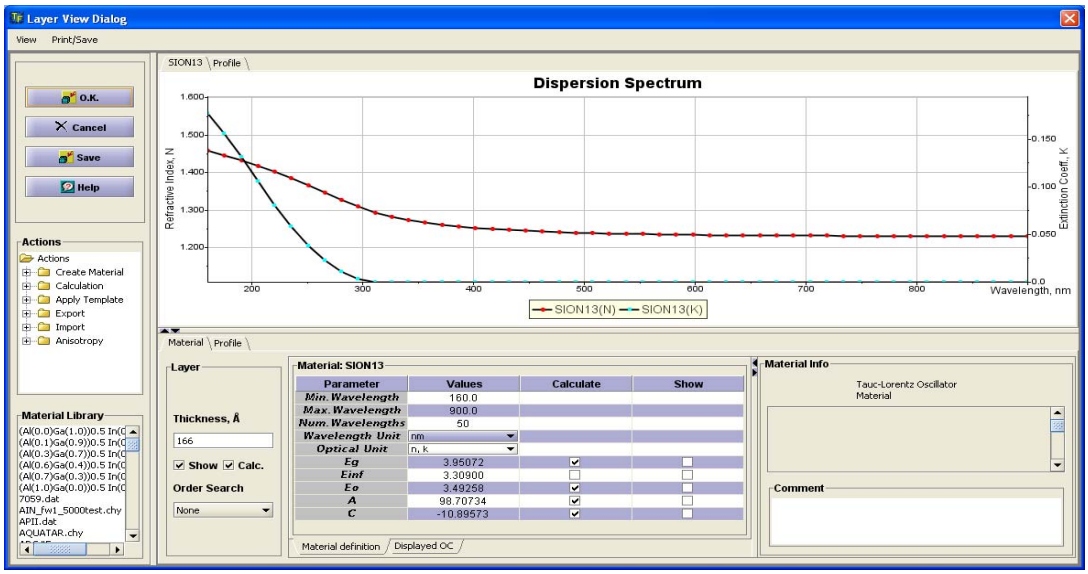

Fig. 10. Layer dialog show the details of the SiON dispersion. This dialog appears after user click on the layer in the main screen.

Sometimes, one needs to adjust the model and repeat calculation until a good fit is achieved.

If after several attempts you still cannot achieve reasonable fit or calculation results do not make sense, it maybe because of one of the following reasons:

- ✓ Filmstack does not accurately represent the real sample
  Try to start with most simple filmstack and add complexity gradually. You can experiment with changing filmstack parameters and use **SimulateFit** button to see the effect of the changes (**SimulateFit** does not perform the fit – just compares measured data with the selected filmstack model).
- ✓ Nominal values of the parameters are too far off
  If your nominal thickness is far off algorithm may not be able to find the solution. Try the **grid/order search**, it allows to perform calculation with different starting values – the best-fit result is selected as a solution. See Advanced topic below

- ✓ Calculated parameters are strongly correlated (too many calculated parameters or not enough measured data)
  Use Calculation Dialog (Actions/Calculate from the main menu) to determine parameters correlation and other details see Advanced topics below

Advanced topics:

1. Grid/Order search
2. Parameter correlation/Calculation dialog

1. Grid Search

Grid/Order search allows selecting a set of starting thickness values in a specified range. It instructs the software to perform calculation using each of the values and selects the best result.
There are two order search option: Standard and Custom
Standard option automatically selects the range and points. Custom option allows more flexibility in selecting specified range and number of points.

Grid Search can be set in the Layer Dialog – select and click on the layer to open the dialog

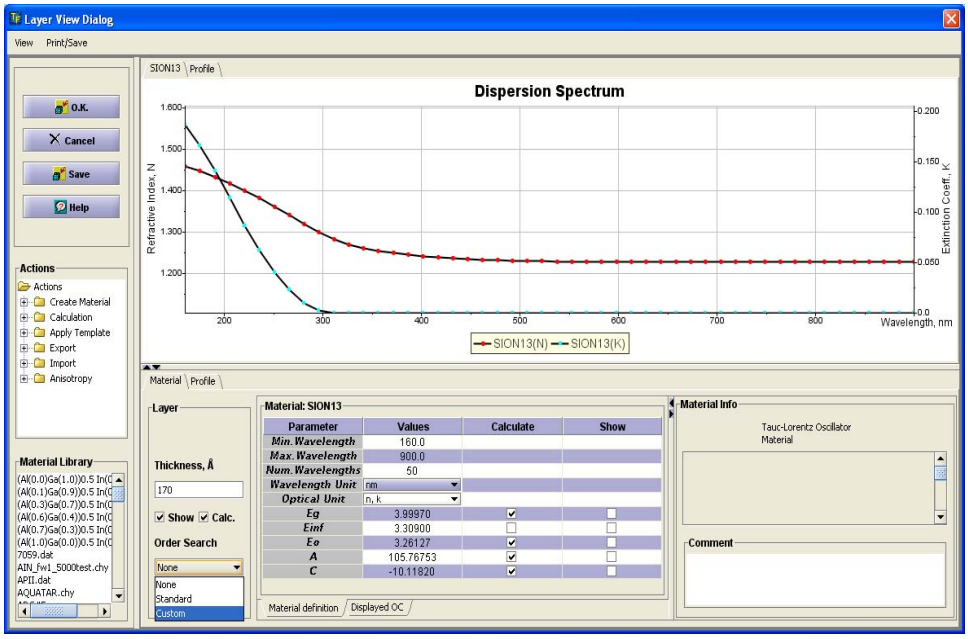

Fig. 11. Select Grid Search type in the Layer dialog

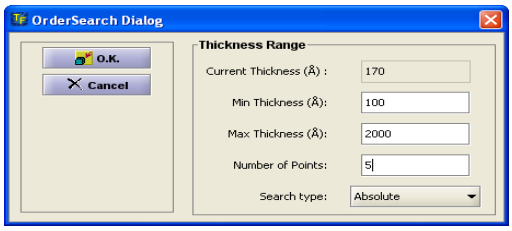

Fig. 12 Custom Grid search dialog appears (after user action in Fig. 11) Enter the range of thickness and number of points here

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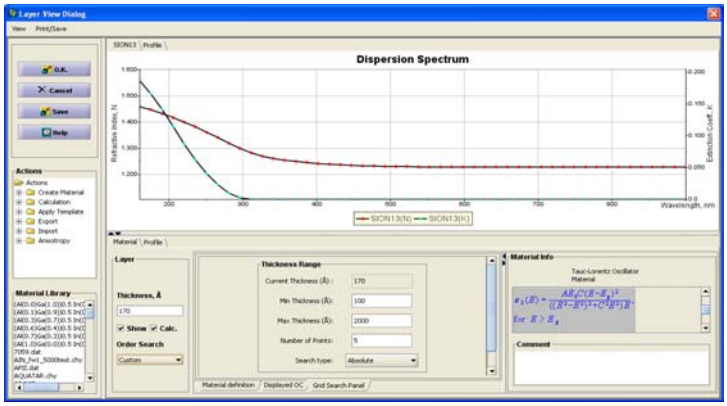


Fig. 13 Layer Dialog is updated and showing grid data (now click OK to return to the main screen)

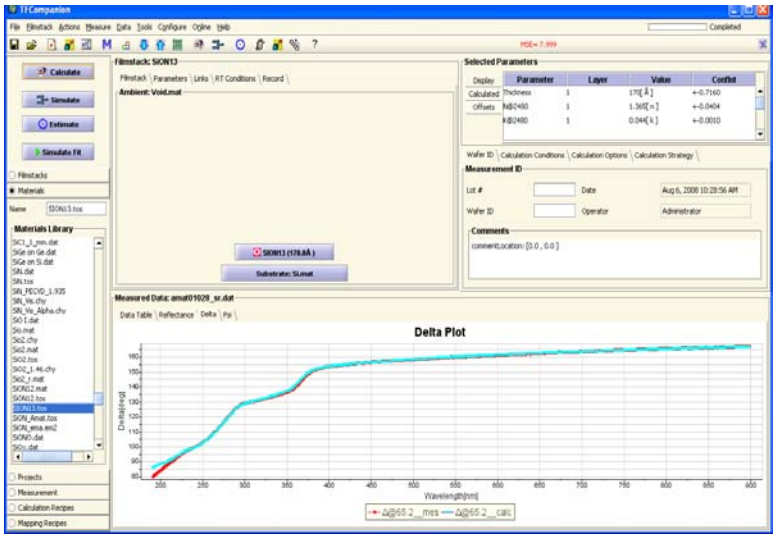


Fig. 14 Order search is now set - icon indicates the layer that was set

2. Parameter correlation/Calculation dialog

Calculation Dialog allows more controls and detailed analysis of the calculation results. Use **Actions/Calculate** from the main menu to start Calculation dialog

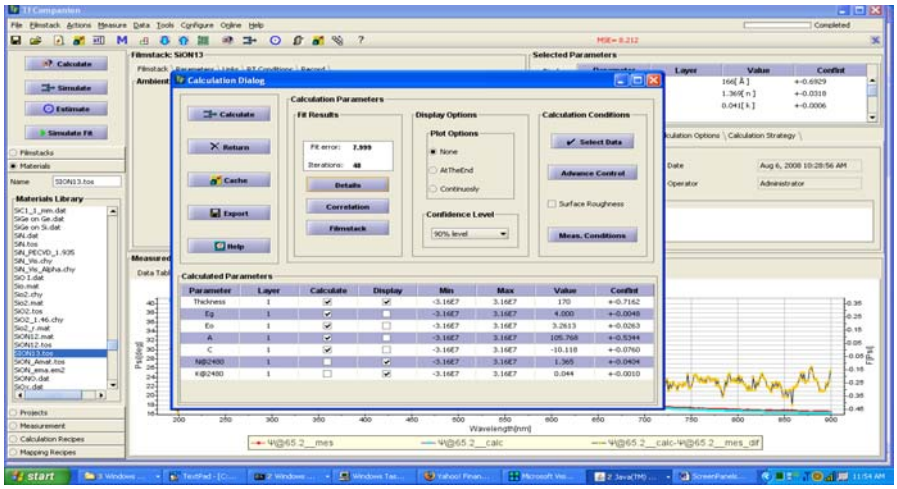
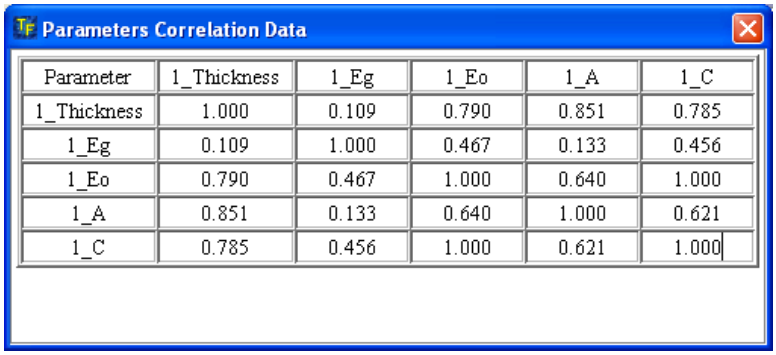


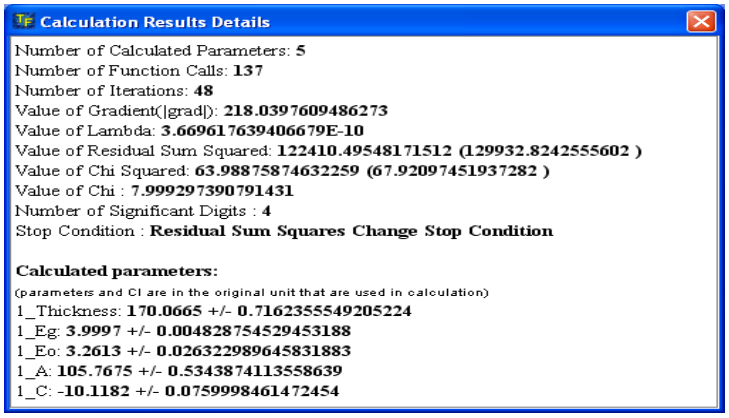
Fig. 15 **Calculation dialog displays the results of calculation**



Parameters Correlation Data

Parameter	1_Thickness	1_Eg	1_Eo	1_A	1_C
1_Thickness	1.000	0.109	0.790	0.851	0.785
1_Eg	0.109	1.000	0.467	0.133	0.456
1_Eo	0.790	0.467	1.000	0.640	1.000
1_A	0.851	0.133	0.640	1.000	0.621
1_C	0.785	0.456	1.000	0.621	1.000

Fig. 16 **Parameter correlation matrix is displayed from Calculation dialog (Correlation button)**



Calculation Results Details

Number of Calculated Parameters: **5**
Number of Function Calls: **137**
Number of Iterations: **48**
Value of Gradient(|grad|): **218.0397609486273**
Value of Lambda: **3.669617639406679E-10**
Value of Residual Sum Squared: **122410.49548171512 (129932.8242555602)**
Value of Chi Squared: **63.98875874632259 (67.92097451937282)**
Value of Chi : **7.999297390791431**
Number of Significant Digits : **4**
Stop Condition : **Residual Sum Squares Change Stop Condition**

Calculated parameters:
(parameters and CI are in the original unit that are used in calculation)
1_Thickness: **170.0665 +/- 0.7162355549205224**
1_Eg: **3.9997 +/- 0.004828754529453188**
1_Eo: **3.2613 +/- 0.026322989645831883**
1_A: **105.7675 +/- 0.5343874113558639**
1_C: **-10.1182 +/- 0.0759998461472454**

Fig. 17. **More calculation details (user selected Detail button in Calculation Dialog)**

IV. Materials

TFCompanion includes an extensive library of materials. User can import additional materials from text file or create using manual input.
There are two basic types of the materials:

- ✓ Tabular, i.e. material's dispersion is represented as a table of optical constants vs. wavelengths.
- ✓ Parameterized materials i.e. dispersion is represented using a formulae with finite number of parameters.

Tabular material representation is working well for very stable materials e.g. Si or SiO2. For many materials, optical properties depend on growth, manufacturing or deposition conditions and may vary significantly.

Parameterized materials allow adjusting optical dispersion depending on specific properties of the material. These materials also allow better utilize spectroscopic measurements information since number of parameters is always less then a number of measurement wavelengths. Additional flexibility can also lead to calculation problems – one can get unphysical results if approximation is used incorrectly or too many parameters are calculated.

TFCompanion supports a large range of parameterized materials from Effective-medium approximation (EMA) and Cauchy to Classical, Tauc-Lorentz and Drude-Lorentz oscillators approximations.

1. Creating new parameterized material.

When creating new parameterized material, one typically desire to have it match the optical dispersion of the corresponding tabular material (is available). This is done for at least two reasons:

- ✓ To verify that selected dispersion approximation is adequate
- ✓ Have reasonable starting values of the parameters

For example, Al2O3 properties can vary significantly and we would like to represent its dispersion using parameterized material.
To accomplish this, one can follow these steps:

1. Start Material Dialog (Fig. 18)
2. Select material to display (Fig. 19)
3. Al2O3 is a dielectric material with a smooth dispersion – Cauchy approximation should represent this dispersion well. We will create a new Cauchy material (Fig. 21-23) and name it Alumina.chy
4. Now we can fit this material to a 'target' – our tabular Al2O3 material (Fig. 24-28). Cauchy coefficients are adjusted to represent accurately Al2O3 dispersion. Now we can save Alumina.chy to a database as a new material.

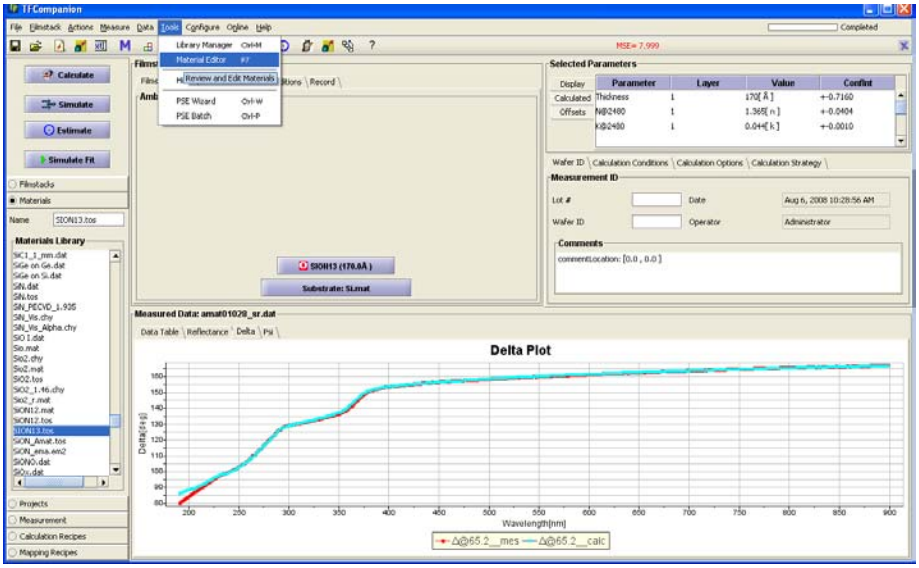


Fig. 18 **Select Tools/Materials Editor to start Materials Dialog**

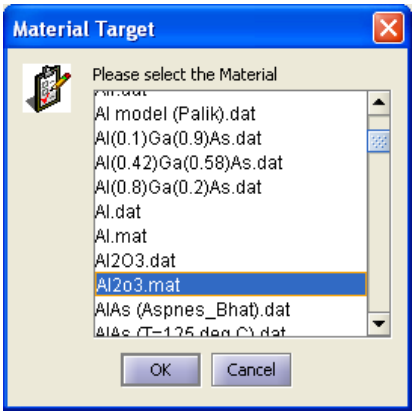
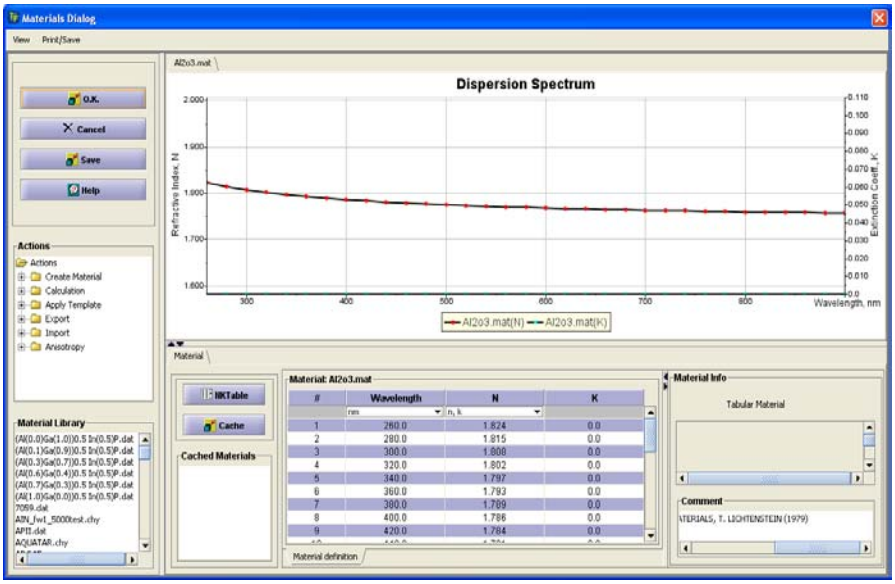


Fig. 19 **Select material to display in the Materials Dialog**



Fig, 20 **Selected material (Al2O3) is displayed in the dialog**

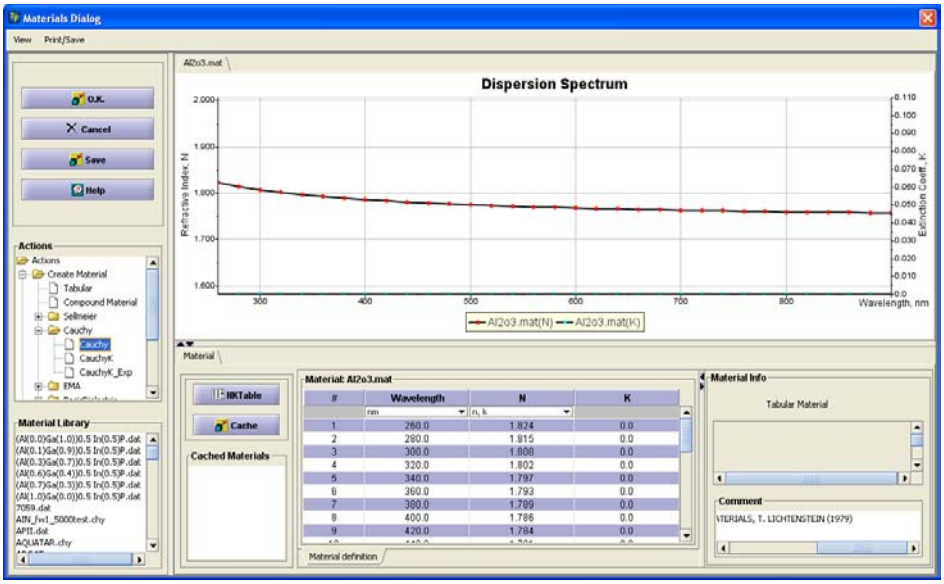


Fig. 21 **Select Create Material/Cauchy/Cauchy from the Action tree (left sidebar)**

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Fig. 22 **Give new material a name**

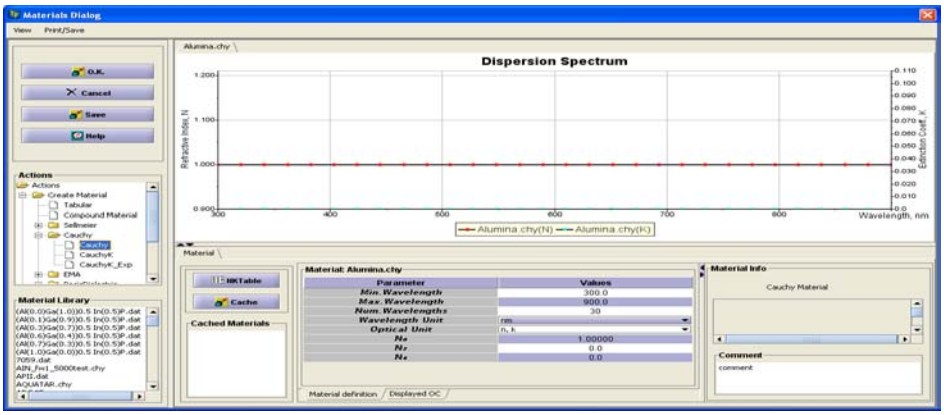

Fig. 23 **New Cauchy material is created with default values of the parameters**

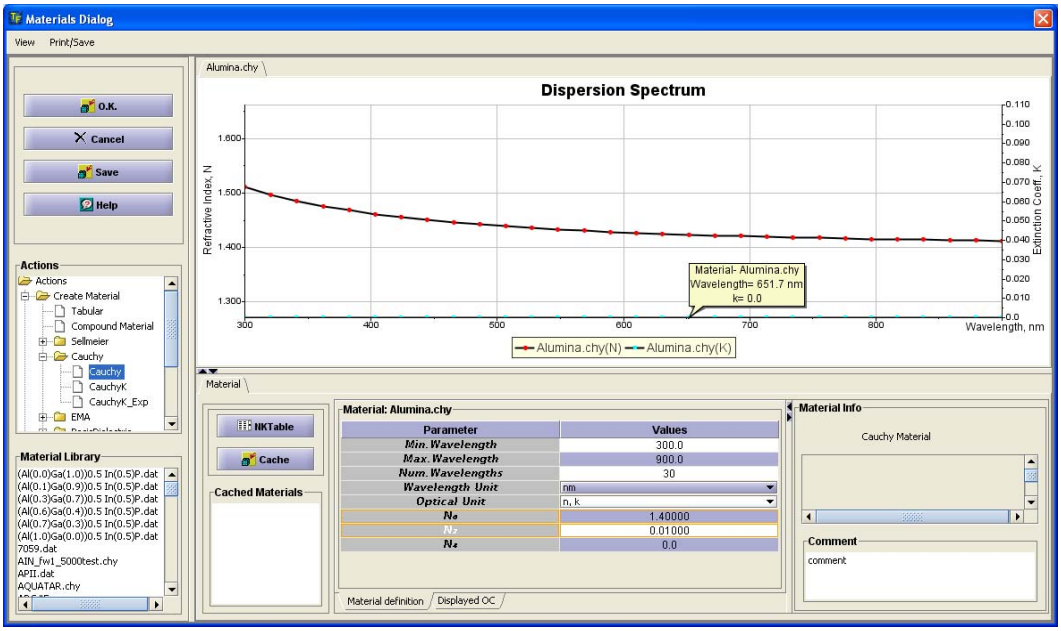

Fig. 24 **Change default values to some reasonable values (we will need only N0 and N2 coefficients)**

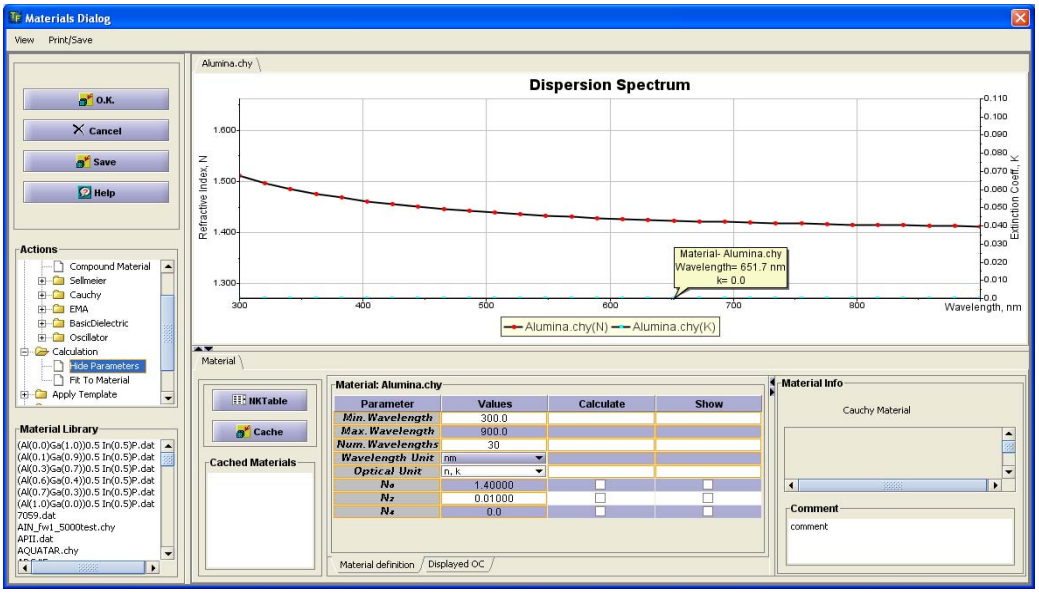

Fig. 25 **Select Calculation/Show Parameters from Action tree (this shows checkboxes next to parameters)**

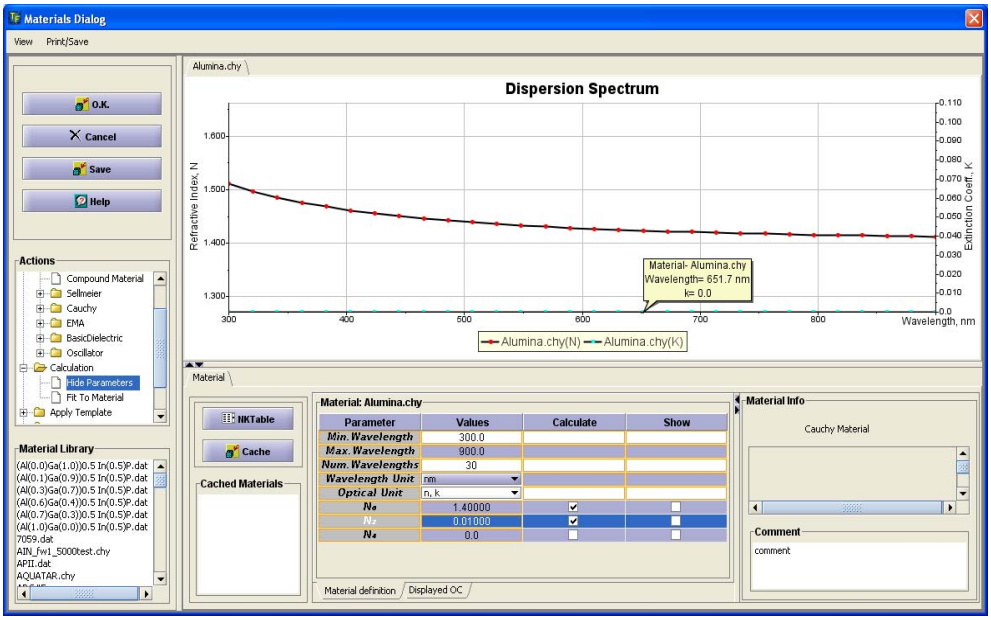

Fig. 26**. Select parameters we want to adjust (N0,N2) and check boxes next to them**

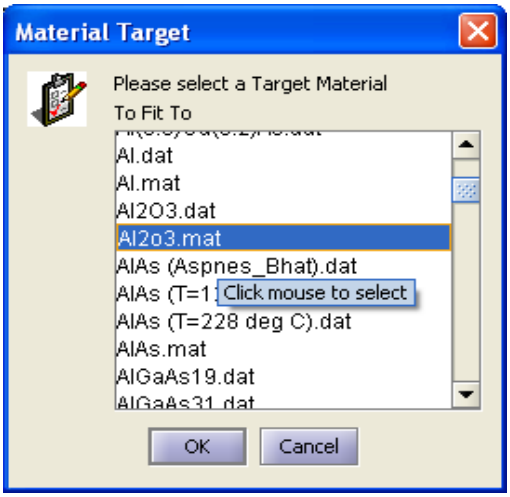

Fig. 27 **This dialog appears after we select "Fit to Material" in the action tree. We select Al2O3.mat as a target here.**

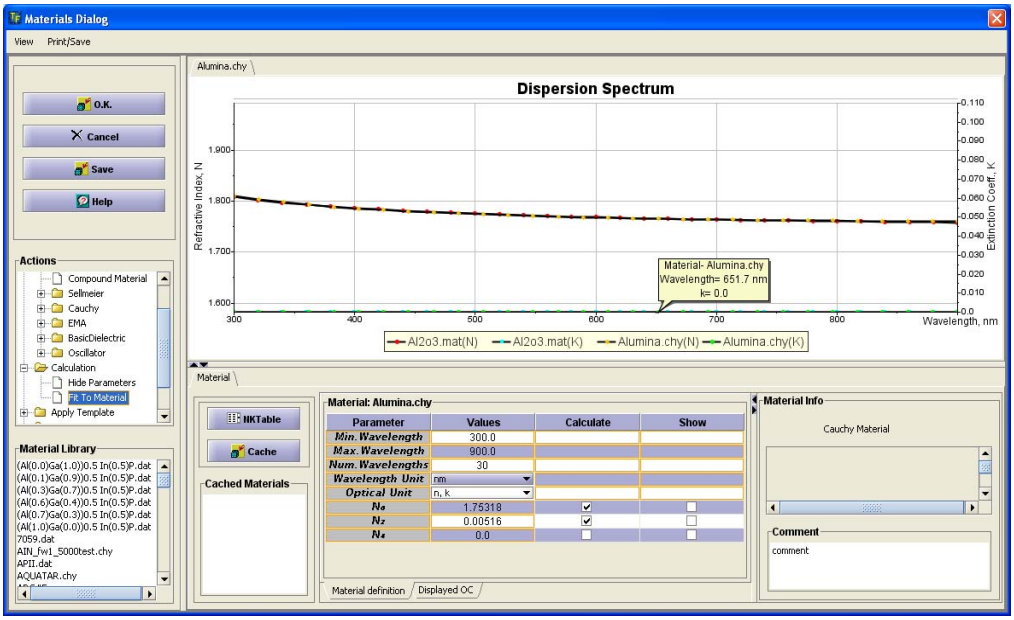

Fig. 28 **Calculation is completed. Now our new material (alumina.chy) matches exactly the dispersion of the target tabular material (Al2O3.mat)**

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V. Batch and mapping data support in TFCompanion.

TFCompanion supports batch processing of the measured data using Production Batch option. The batch is a sequence of measurements e.g. kinetic measurements (in-situ or in-line monitoring) or XY mapping measurements.

Following is an example of processing mapping measurements.

1. XY mapping measured data: format and data importing.

Measured mapping data as other batch measurements can be imported from file as a concatenation of the measured spectra. Each spectrum corresponds to one XY point. Standard TFCompanion format supports measurement point position that is defined in the header of the file ("Location" flag identifies the x,y coordinates of the point).
Below is an example of mapped data format that shows two measured points [27,39] and [30,39]

```
TFC_DATA
#comment
#Date:May 28, 2008 12:42:05 PM
#Location:27.00,39.00
#WaferId:ID
#WaferLot:
#User:Admin_hw
Wavelength:Angle:Reflectance
nm
600.0   0.0   0.2372
600.2   0.0   0.2381
600.4   0.0   0.2376
****** skip********
899.8   0.0   0.3291
900.0   0.0   0.3331
TFC_DATA
#comment
#Date:May 28, 2008 12:42:11 PM
#Location:30.00,39.00
#WaferId:ID
#WaferLot:
#User:Admin_hw
Wavelength:Angle:Reflectance
nm
600.0   0.0   0.2271
600.2   0.0   0.2296
```

```
600.4   0.0   0.2290
600.6   0.0   0.2347
600.8   0.0   0.2394
  ******* skip********
899.0   0.0   0.4041
899.2   0.0   0.4025
899.4   0.0   0.4035
899.6   0.0   0.4087
899.8   0.0   0.4156
900.0   0.0   0.4190
```

2. Testing model.

Before batch processing, one needs to build a filmstack and it is advisable to test the calculation using one point. To do this one can import a single measurement from the batch file from the main menu.

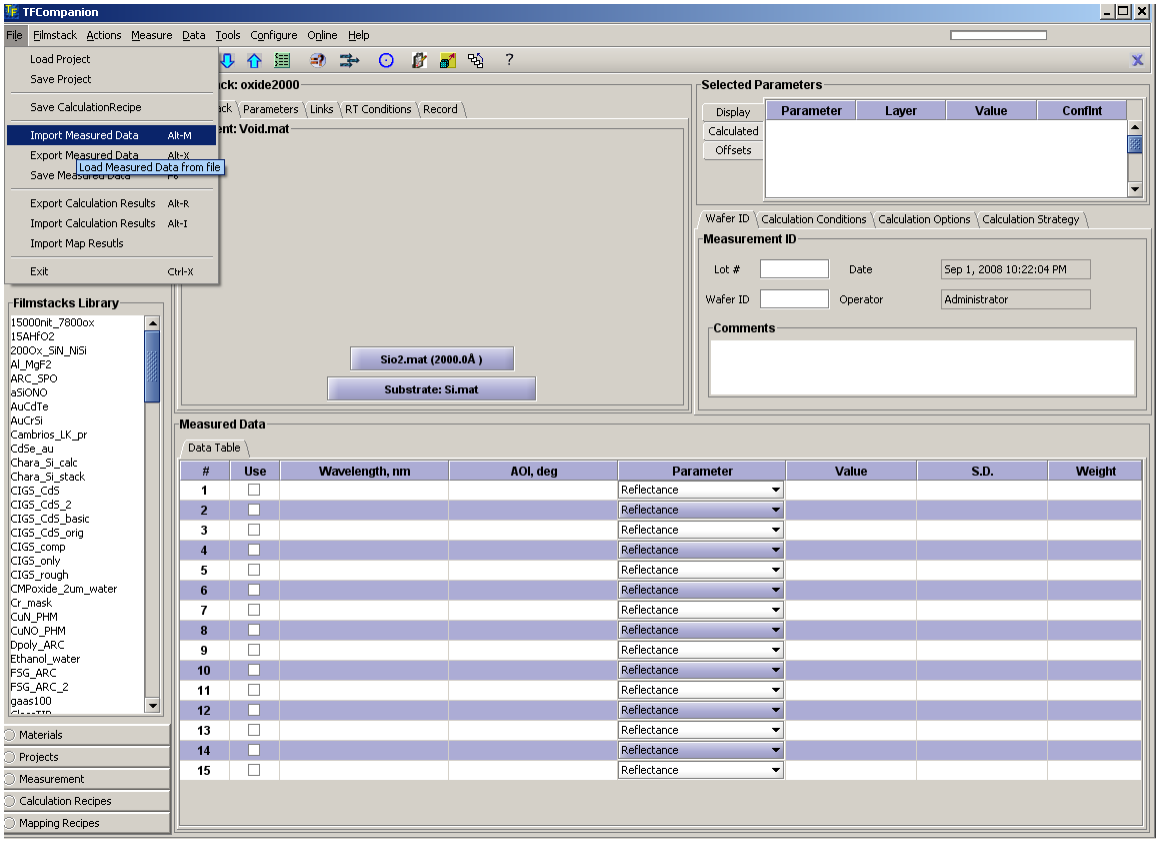


Fig. 29 **Importing measured data (testing calculation on one measured point).**

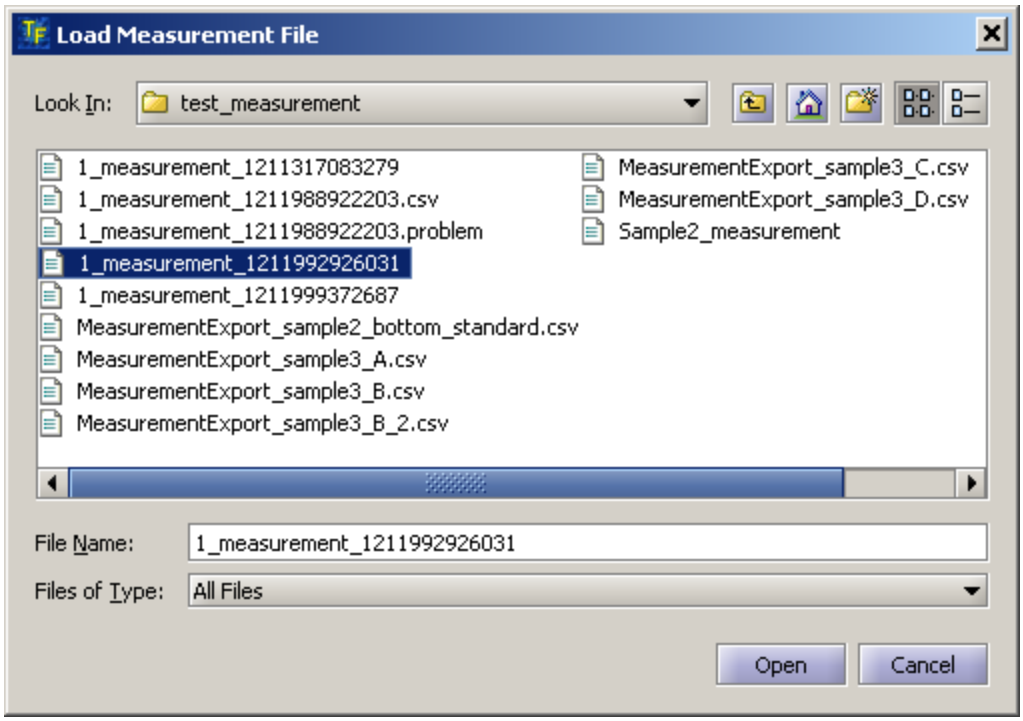


Fig. 30 **Select measured data file**

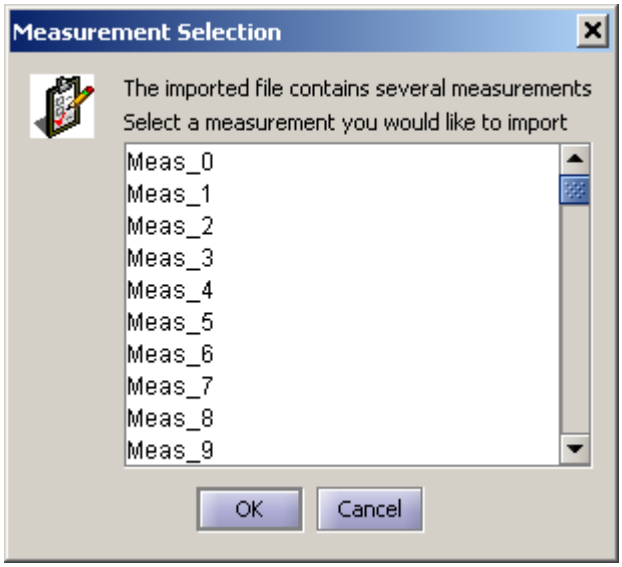


Fig. 31 **Select measurement spectrum (point) from the batch file**

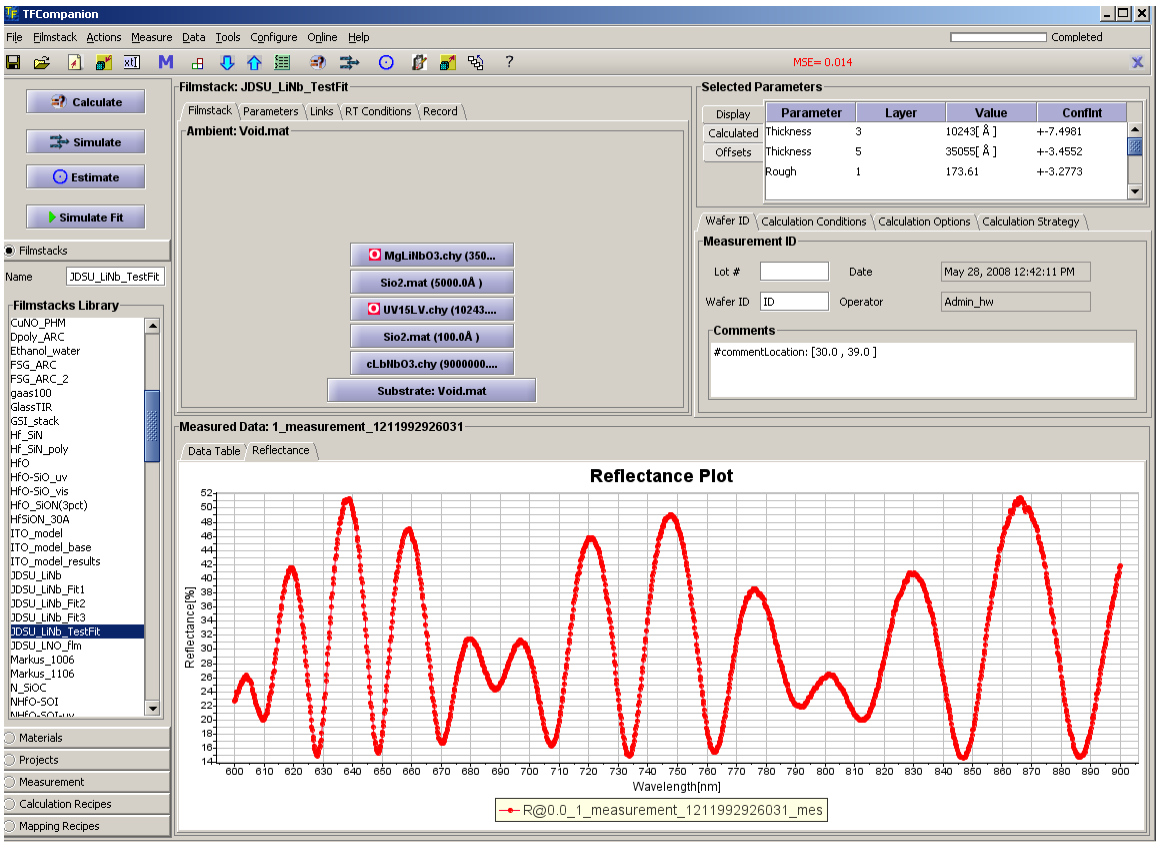


Fig. 32 **Measured point (spectrum) is imported as standard measurement**

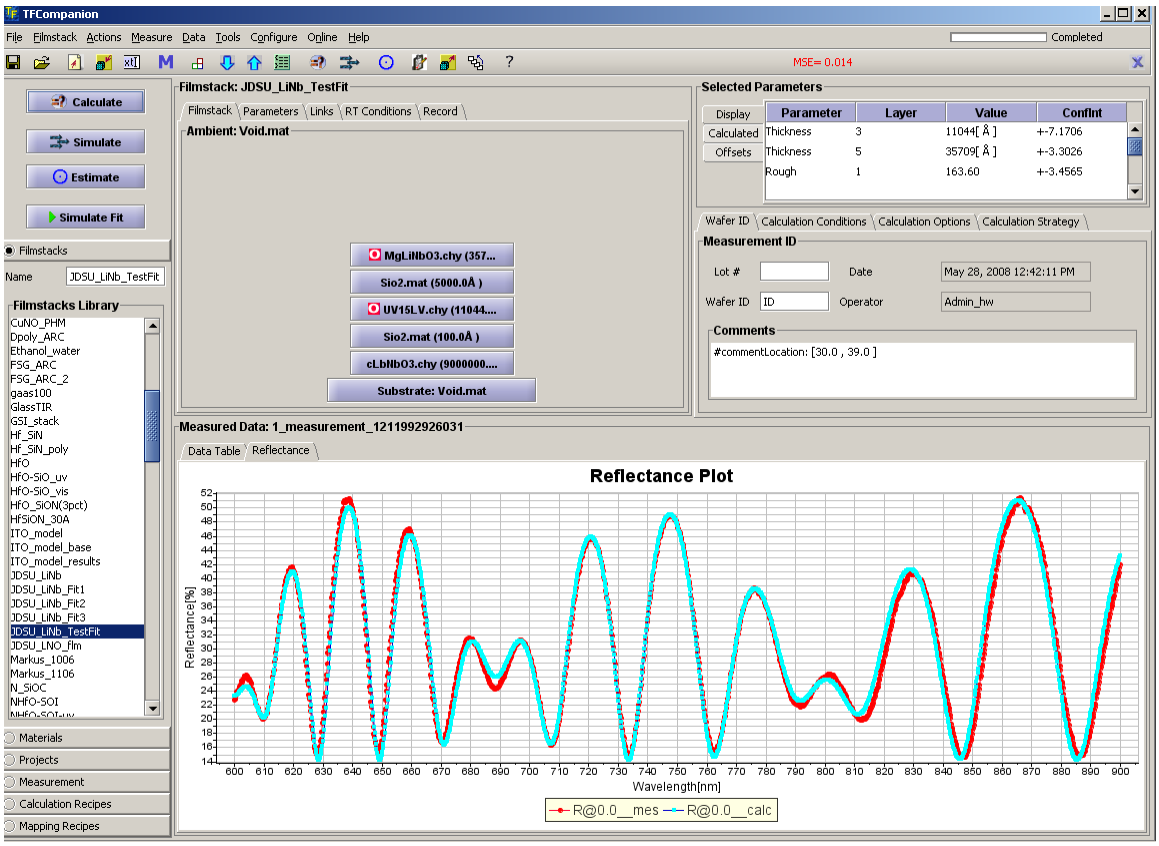


Fig. 33 **Filmstack is selected and calculation is tested on imported spectrum**

If this is a new filmstack – we need to save it in the database (to use later in the batch processing). Now we a ready to do batch processing of the full data set.

3. Using batch dialog to process mapping data

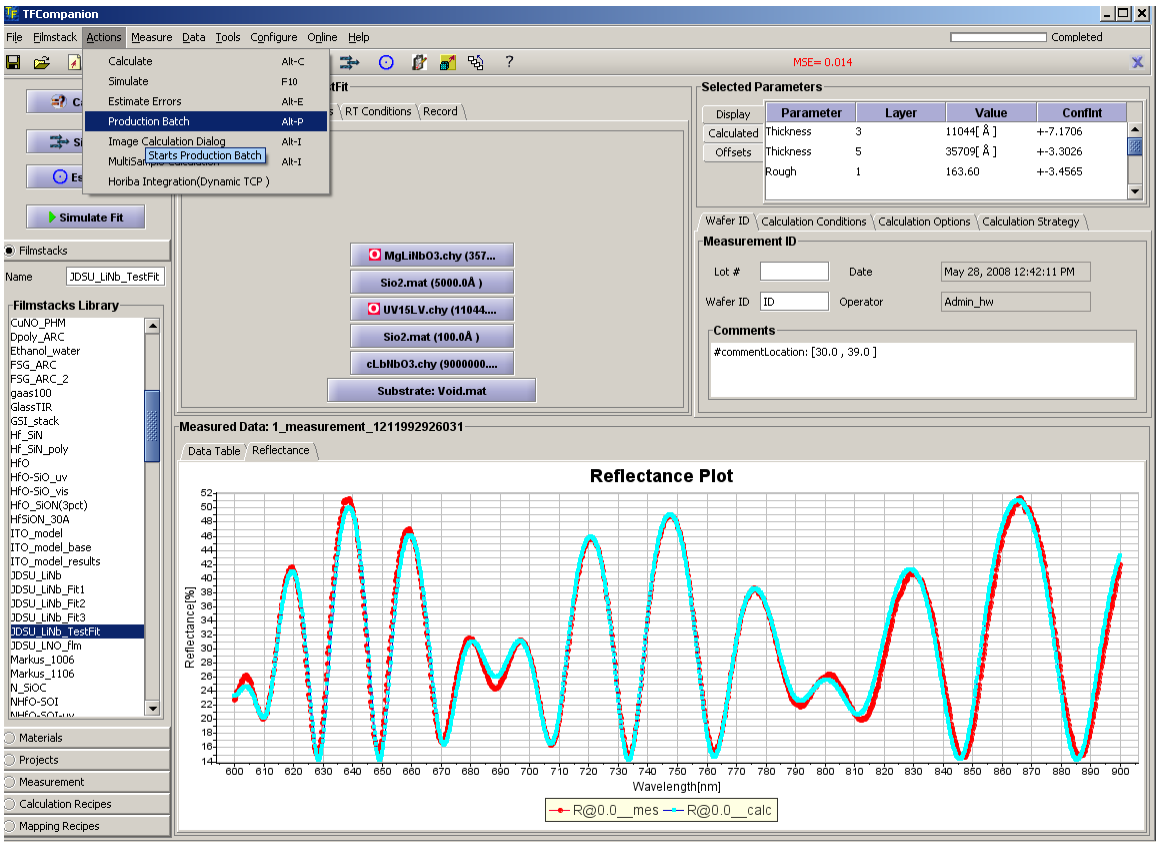


Fig. 34. **Select "Production Batch" from the Action menu to start the Batch dialog.**

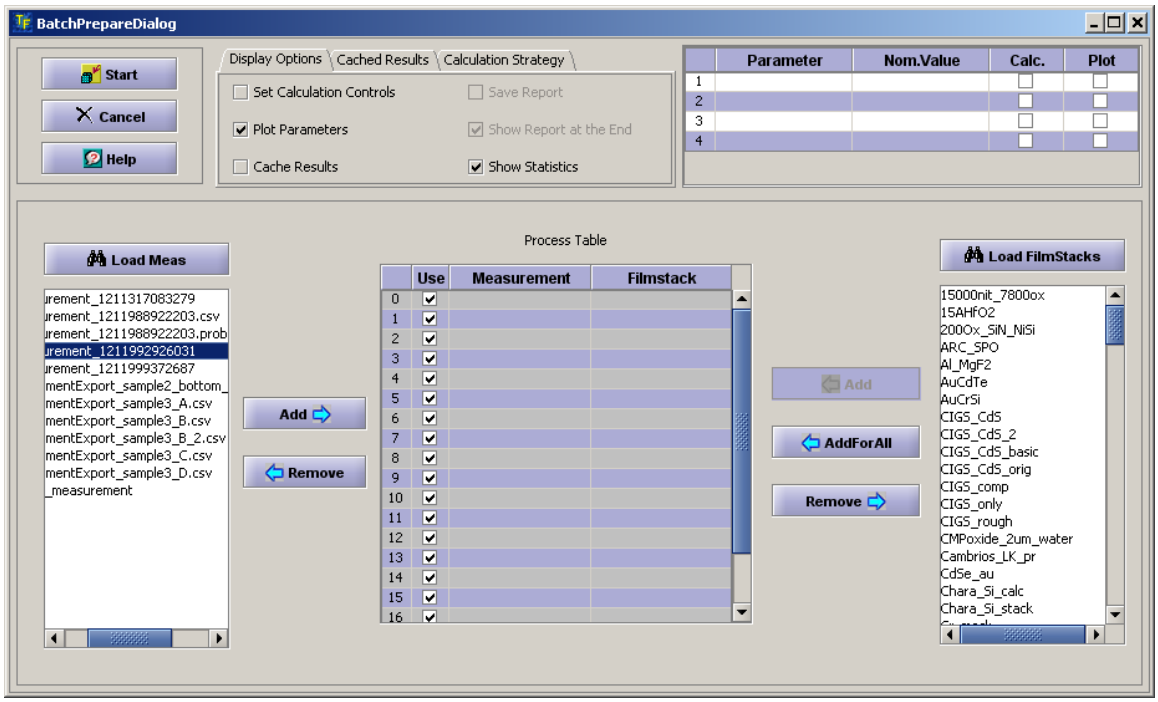


Fig. 35 **Batch Dialog allows top select measured data and matching filmstack(s).**

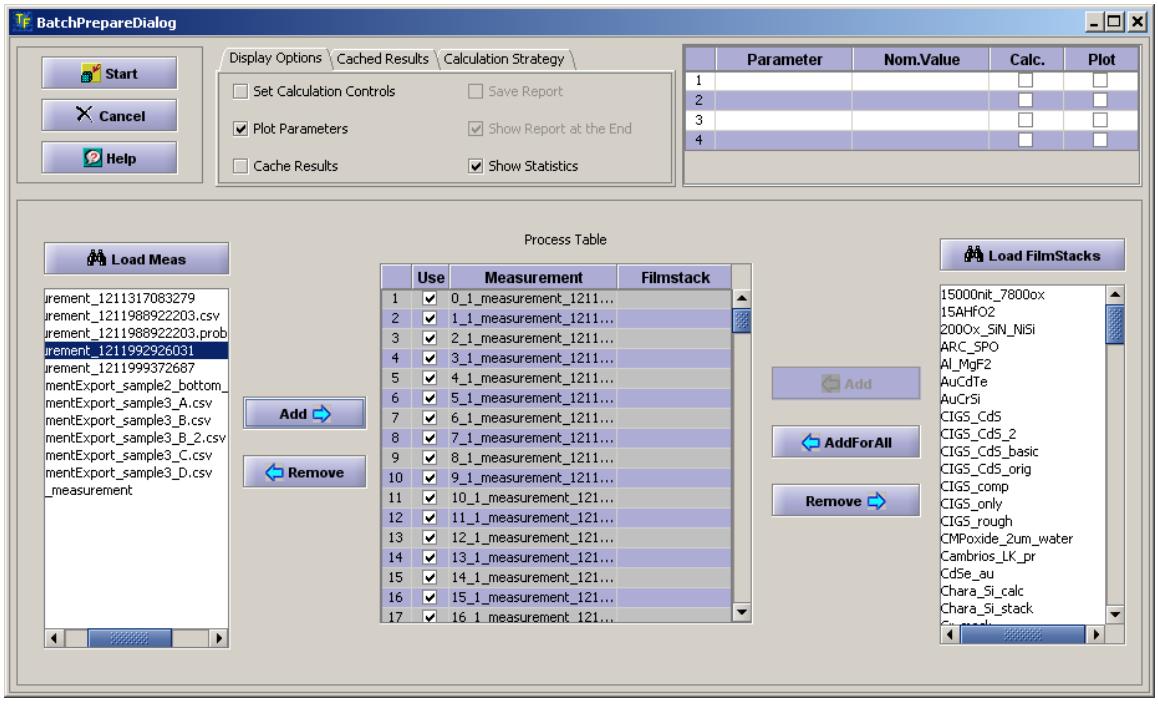
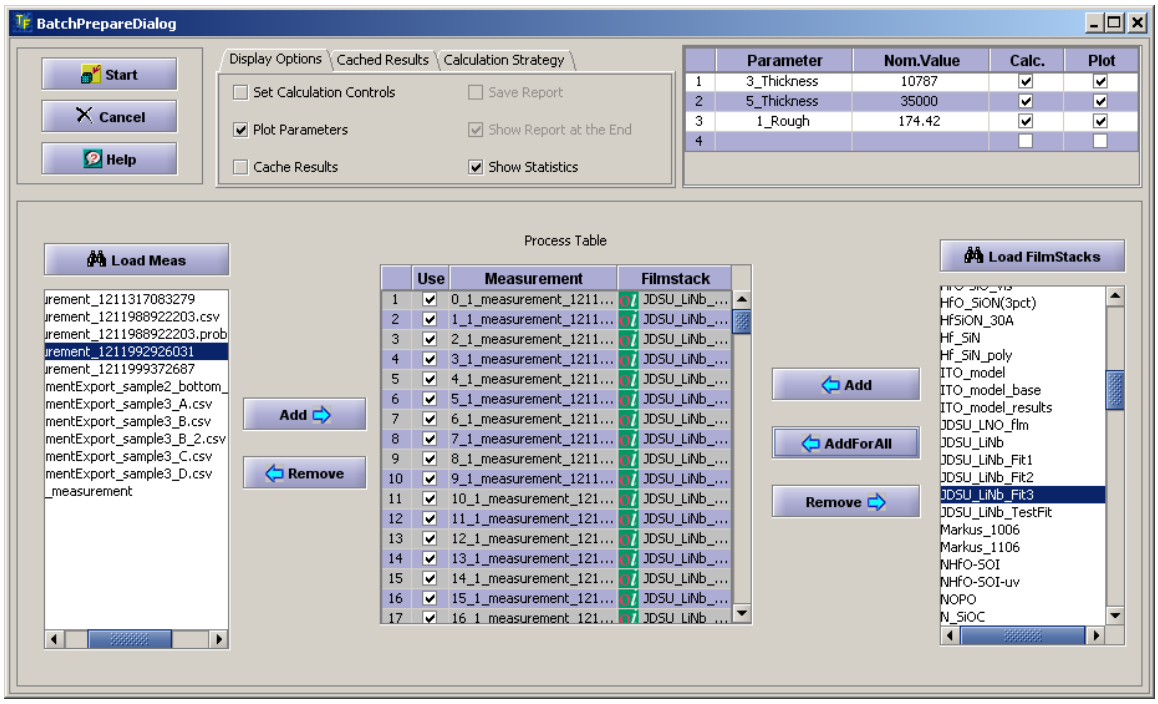


Fig. 36 **Select and Add a batch file with the measured mapping data**



Fig, 37 **Select and Add a filmstack (this filmstack was previously testing on one point measurment). Now we can select Start – to start calculation**

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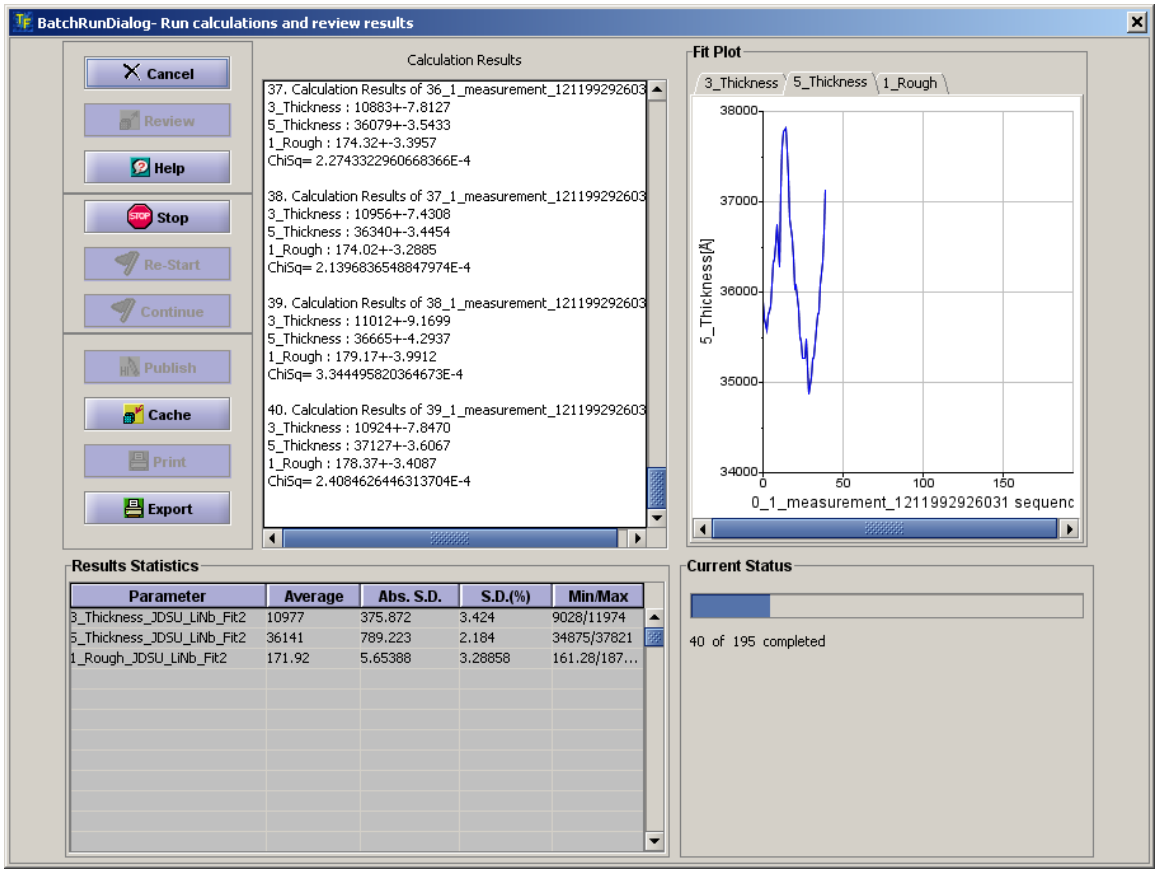
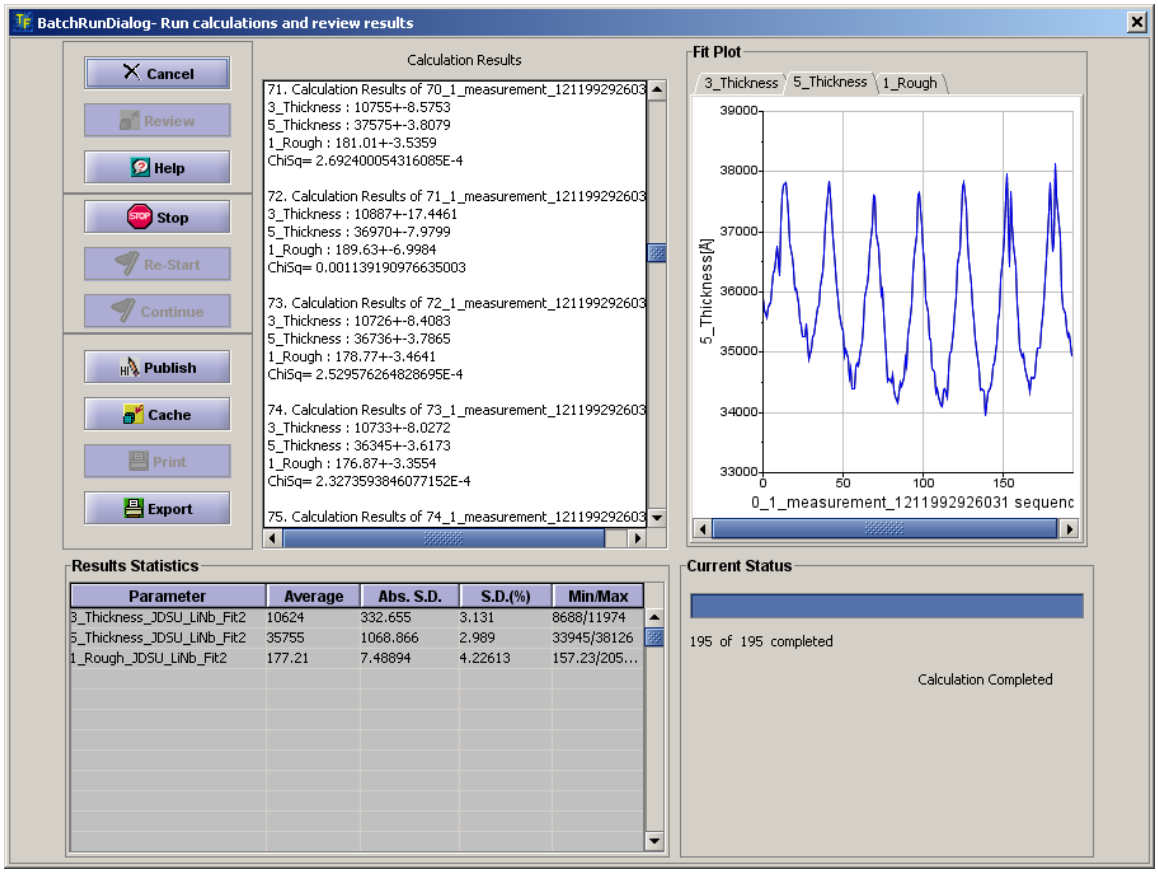


Fig, 38**. Calculation is started: results of the calculation is displayed on the chart and detailed data for each point is displayed in the text window. The results summary and statistics is displayed in the table.**



Fig, 39 **Calculations are completed an we select "Publish" to display the results as a 3D chart.**

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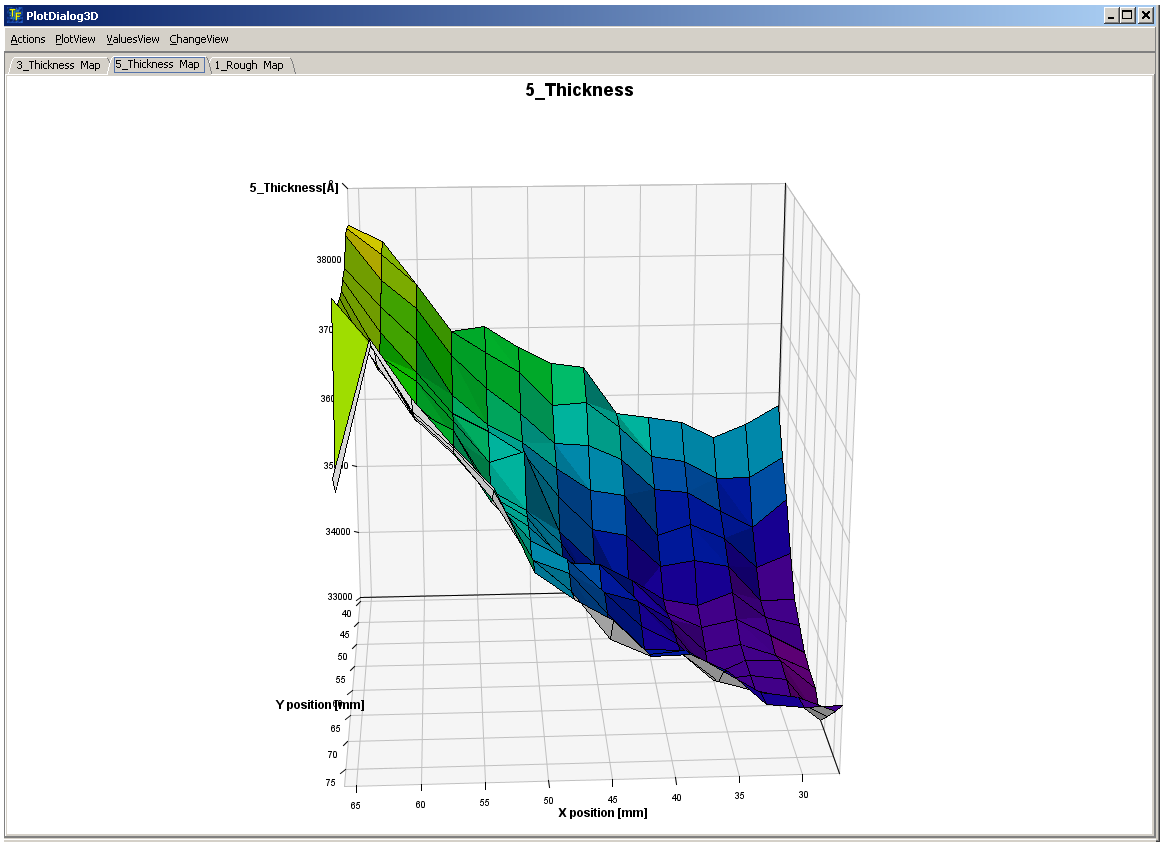

Fig. 40 **Displaying results of calculation as a 3D chart: XY coordinates correspond to X,Y mapping coordinates and Z axis corresponds to the measured parameter (thickness in the chart).**

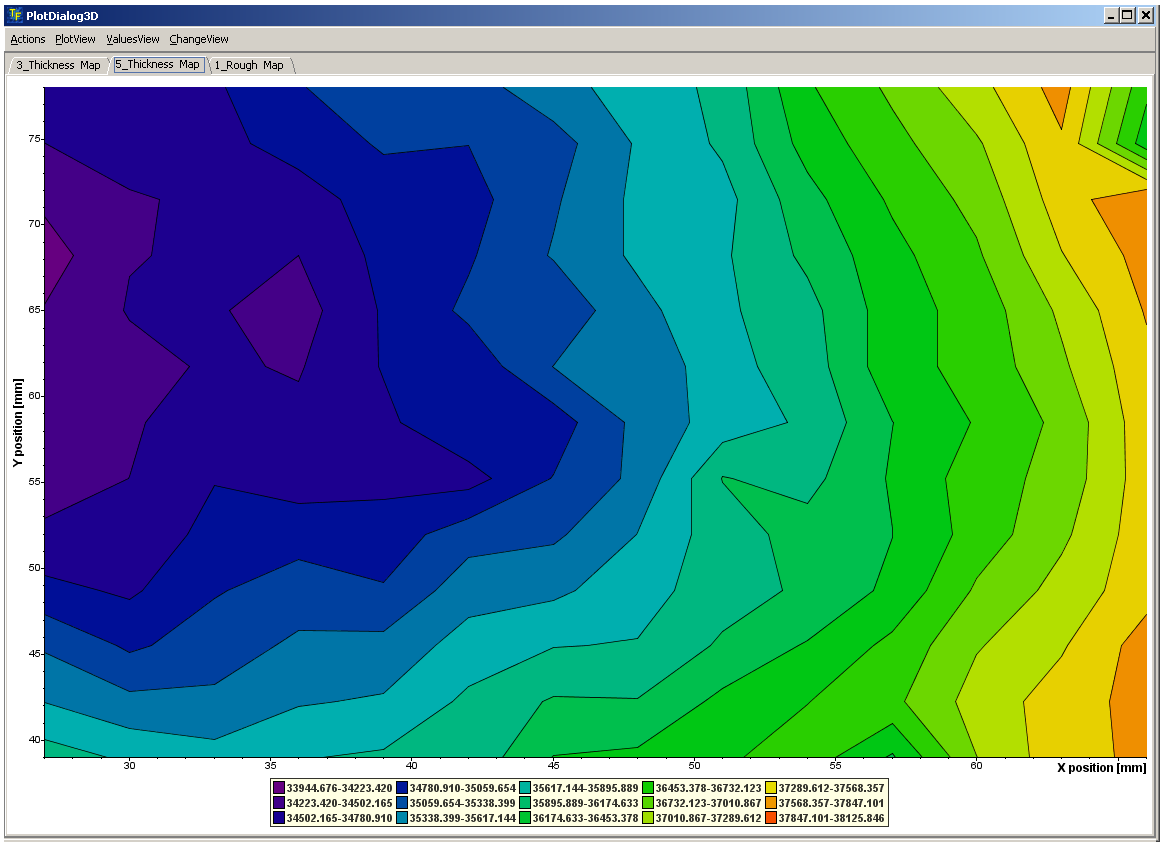

Fig. 41 **The Fig. 12 3D chart is displayed as contour map (thickness values are color coded).**

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