cw-Terahertz Data Analysis Software

1) Introduction

The software package “TOPTICA Continuous-Wave Terahertz Analysis“ enables postprocessing of data acquired with TOPTICA’s TeraScan systems.

The software does not need to be installed. To start it, just open the executable file (cwthz-dataanalysis.exe).

The user interface consists of four windows (Fig. 1): two Plot Windows, a Settings + Analysis Window, and a Data Selection Window.

The data set to be analyzed *always* has to be chosen in the Data Selection Window.

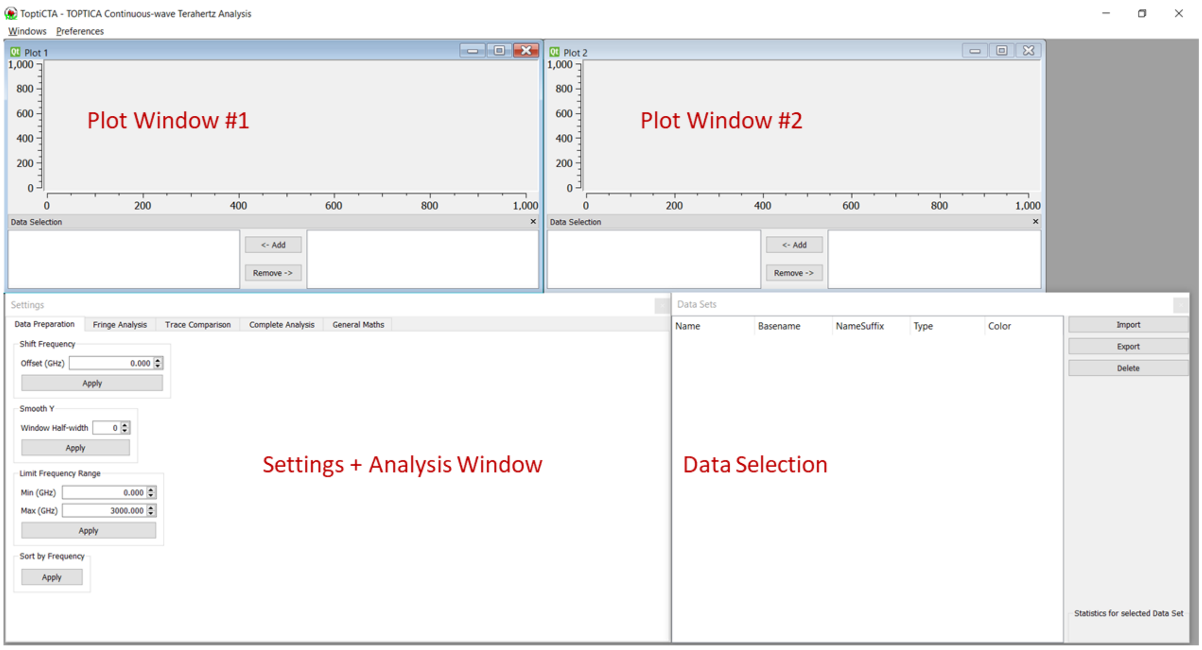


Fig. 1: User interface of the cw-Terahertz Data Analysis Software.

Datasets are identified both by their filename and their type. Measurements performed with fixed optical path lengths (“fringe scans”) produce datasets of type “Fringe”. Measurements carried out with the help of fiber stretchers produce datasets of type “Amplitude” and “Phase”. If needed, you can change the type manually: a double-click on the type of a dataset (and then on the arrow on the right-hand side) opens a pull-down menu.

Each analysis step generates a new dataset, which is added to the Data Selection Window. Some operations change the type of the dataset, e.g “Fringe to Amplitude”, where the input is of type “Fringe” and the output is of type “Amplitude”. For other operations, e.g. offset correction or frequency sorting, input and output datasets are of the same type. You can export and save any dataset to file by highlighting it and clicking **Export** in the Data Selection Window.

In the default settings, each of the original datasets imported is automatically assigned a different color. This color is kept for all of the datasets that subsequent analysis steps may produce. You can change the color by double-clicking on the color field and then on the grey square that appears on its right-hand-side end, which opens a “Select Color” window (Fig. 2). You can also change the overall color settings in the “Preferences” menu in the top-left corner (the default settings are: “Default curve color – Inherit from parent data set”).

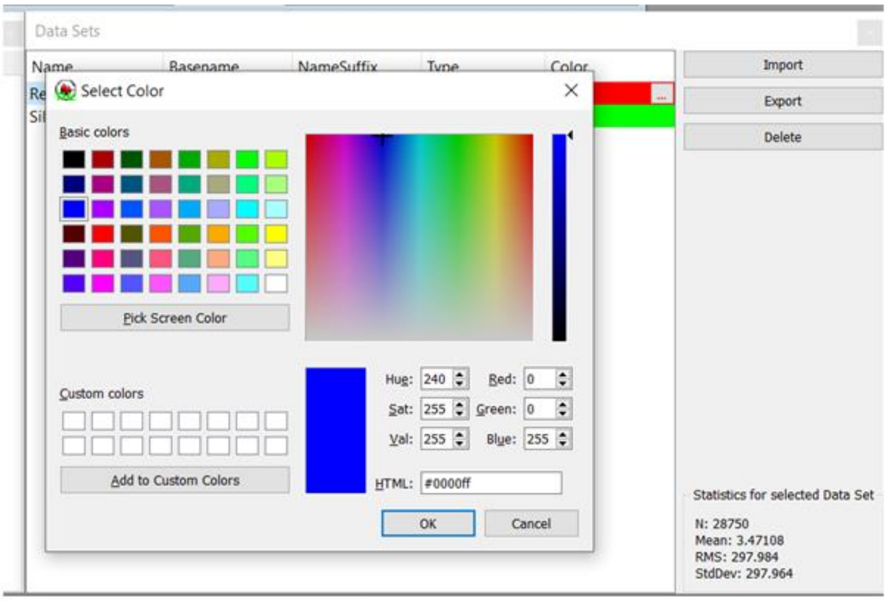


Fig. 2: Color selection.

At any stage, you can also display datasets in either of the Plot Windows. Simply select the dataset and click **Add** in the respective Plot Window.

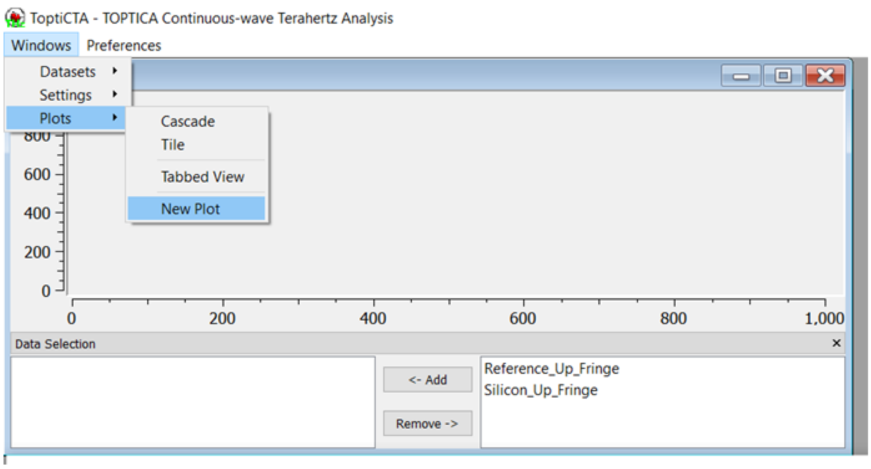


Fig. 3: Creating new plots.

You can close any plot window at any stage, and open new ones via the menu in the top-left corner (**Windows → Plots → New Plot**), as shown in Fig. 3.

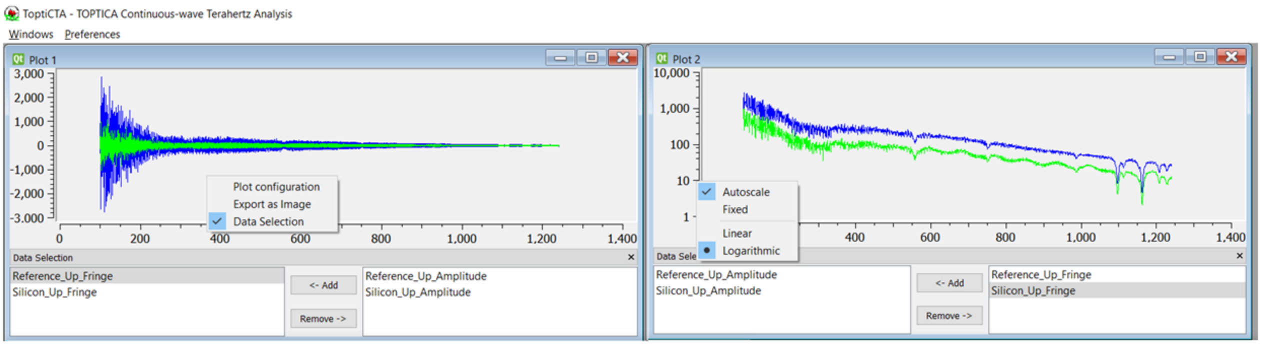


Fig. 4: Plot Windows with configuration settings.

A right-mouse click *in the graph* opens a dialog that enables you to change the properties of the plot, e.g. the colors of individual graphs (Fig. 4). You can choose to have a plot exported as a graphics file (**Export as Image**). The **Data Selection** option hides and displays the Data Selection menu as well as the "Add" / "Remove" buttons for this specific graph.

A right-mouse click *on the vertical or horizontal axis* allows you to change the scale, e.g. from a linear to a logarithmic display. You can also disable autoscaling and define fixed borders for the displayed parameter range.

Selecting a data file and clicking **Remove** deletes the graph from the plot.

2) Application Examples

<u>2.1 Calculation of Transmittance and Refractive Index of a Sample from a "Fringe" Spectrum</u>

1. Select the reference measurement: Click **Import** in the Data Selection Window to open an import dialogue. Navigate to the correct folder, pick the raw-data file and confirm with **OK** (Fig. 5). The name of the dataset and its type ("Fringe") will be displayed in the Data Selection Window.

2. Select the sample measurement via the same procedure.

NOTE! If the data files represent "down" scans, you need to click **Sort by Frequency** in the Data Preparation tab of the Settings + Analysis Window (Fig. 6). This will rearrange the data files as "up" scans, i.e. with frequencies in rising order, and produce a dataset with the same name and the extension "(2)". You may delete the original dataset(s) thereafter.

3. Click on the *reference* measurement in the Data Selection Window. Select the Fringe Analysis tab in the Settings + Analysis Window. Enter the (approximate) number of data points in a fringe halfwave (i.e., number of frequency steps between a phase minimum and maximum) in the input field **# of Points Compared**. Clicking **Apply** then generates a dataset that contains the envelope spectrum of the reference measurement. The new dataset is of type "Amplitude" (Fig. 7).

4. Repeat Step 3 for the *sample* measurement, to generate the envelope spectrum of the sample.

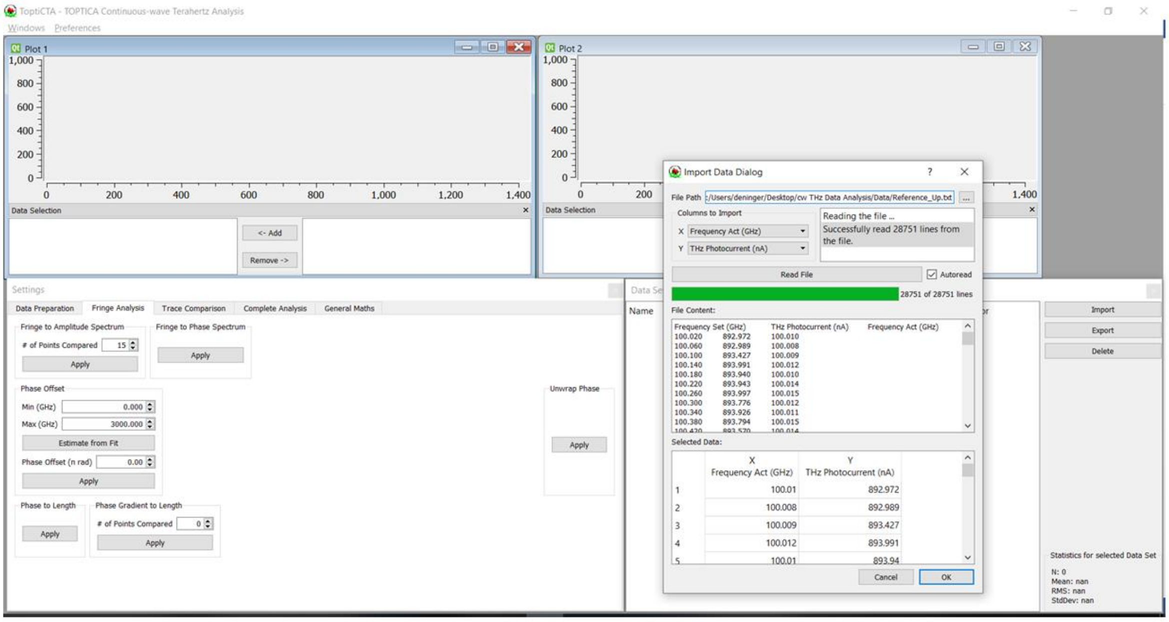


Fig. 5: Selecting the reference file.

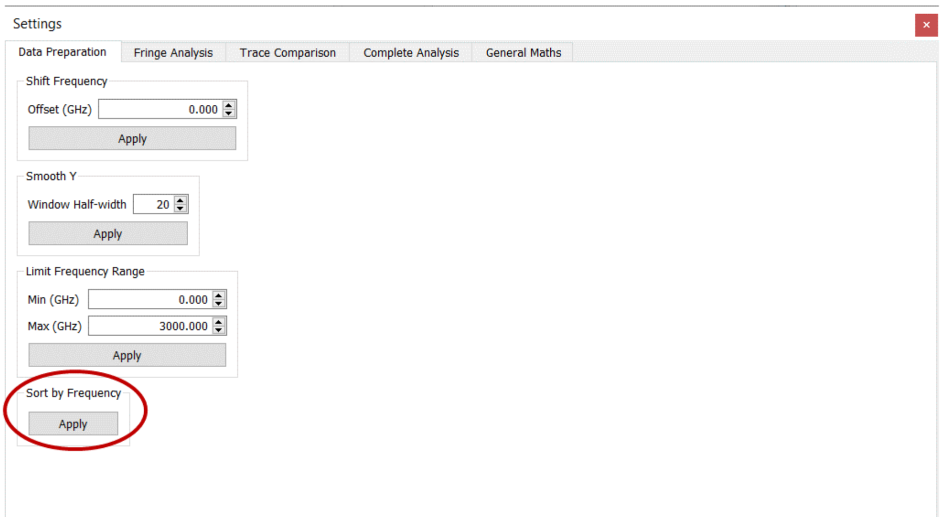


Fig. 6: Sorting data by frequency (only relevant for “down” scans).

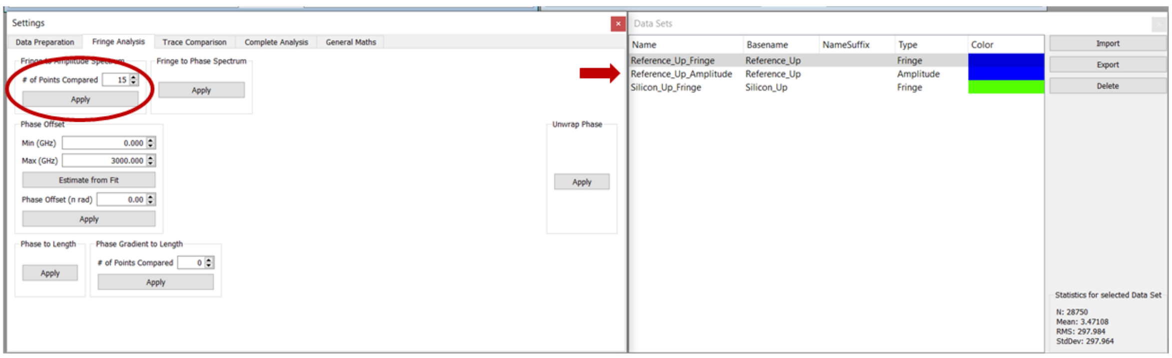


Fig. 7: Generating an amplitude spectrum from “fringe” data.

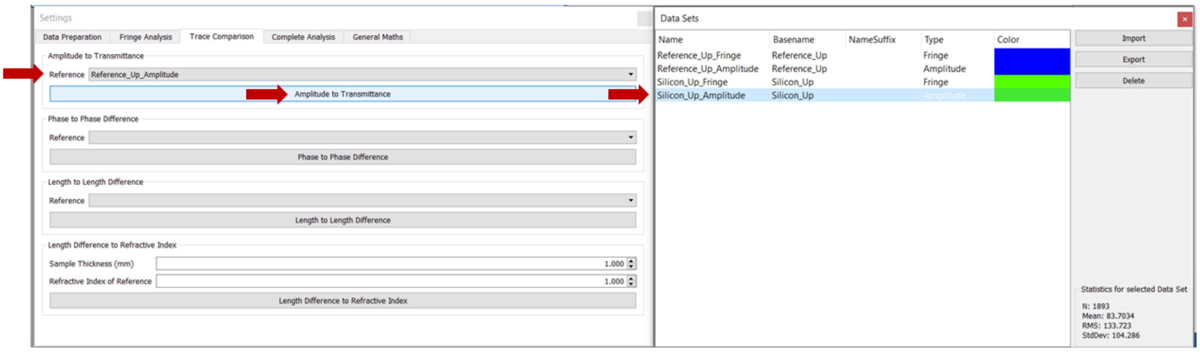


Fig. 8: Transmittance calculation.

5. In order to calculate the transmittance, select the Trace Comparison tab in the Settings + Analysis Window. Make sure that in section Amplitude to Transmittance, the proper reference spectrum is chosen. In the Data Selection Window, highlight the dataset that you wish to analyze (Fig. 8) and click the **Amplitude to Transmittance** button. You may want to plot the result.

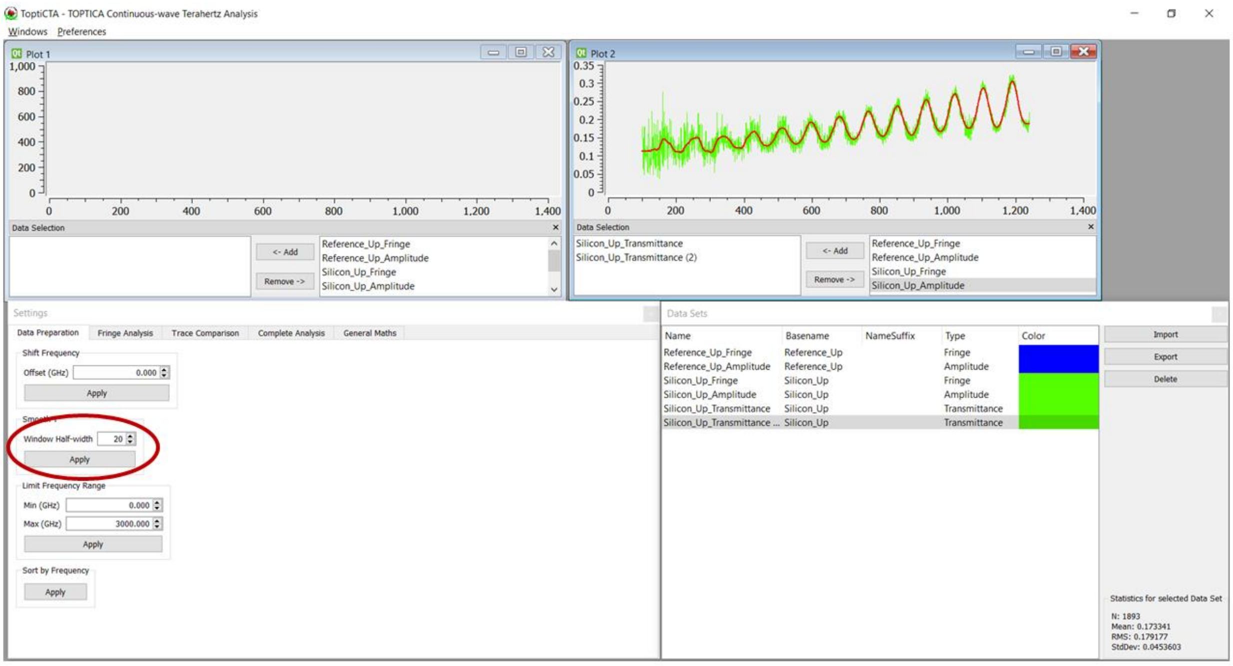


Fig. 9: Smoothing. Plot 2 shows the transmittance spectrum of a piece of silicon, without (green line) and with smoothing (red).

6. In case you want to smooth the transmittance spectrum, click on the respective dataset in the Data Selection Window. Return to the Data Preparation tab in the Settings + Analysis Window. Define the Window Half-Width (i.e., halfwidth of a moving average filter) and click **Apply**, as shown in Fig. 9.

NOTE! Any dataset can be smoothed, at any stage in the analysis.

7. In order to compute a phase spectrum, click on the original *reference* measurement in the Data Selection Window. This is the dataset of type “Fringe”. Then click **Apply** in the “Fringe to Phase” section of the Settings + Analysis Window. The resulting phase spectrum should show a straight line with a positive slope. The offset will most likely differ from zero (Fig. 10).

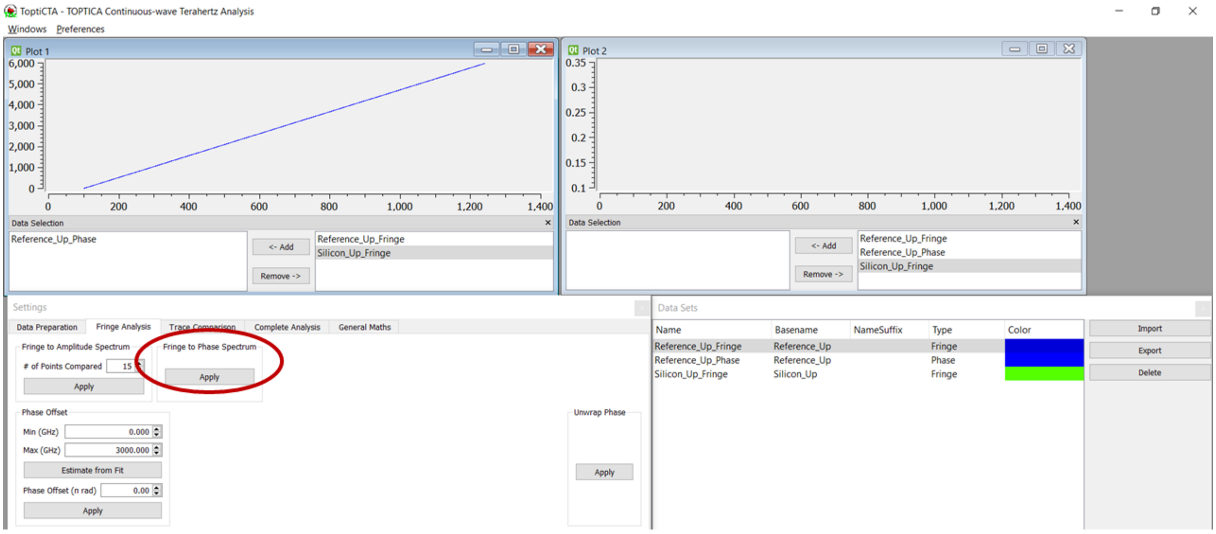


Fig. 10: Phase spectrum with incorrect offset (evident from the graph in Plot 1: when extrapolated to zero, the y-intercept is negative).

8. To correct the phase offset,

   a. Click on the resulting dataset (type "Phase") in the Data Selection Window.
   b. Click **Estimate from Fit** in the "Phase Offset" section of the Settings + Analysis Window. The software performs a linear fit of the phase spectrum. The resulting offset is displayed in the "Phase Offset" field.

NOTE! If sections of the spectrum are dominated by noise, you can restrict the frequency range used for the fit via the settings **Min (GHz)** and **Max (GHz)**.

   c. Confirm the phase offset by clicking **Apply**, as shown in Fig. 11. This generates a new dataset, the name of which ends with "Phase (2)".

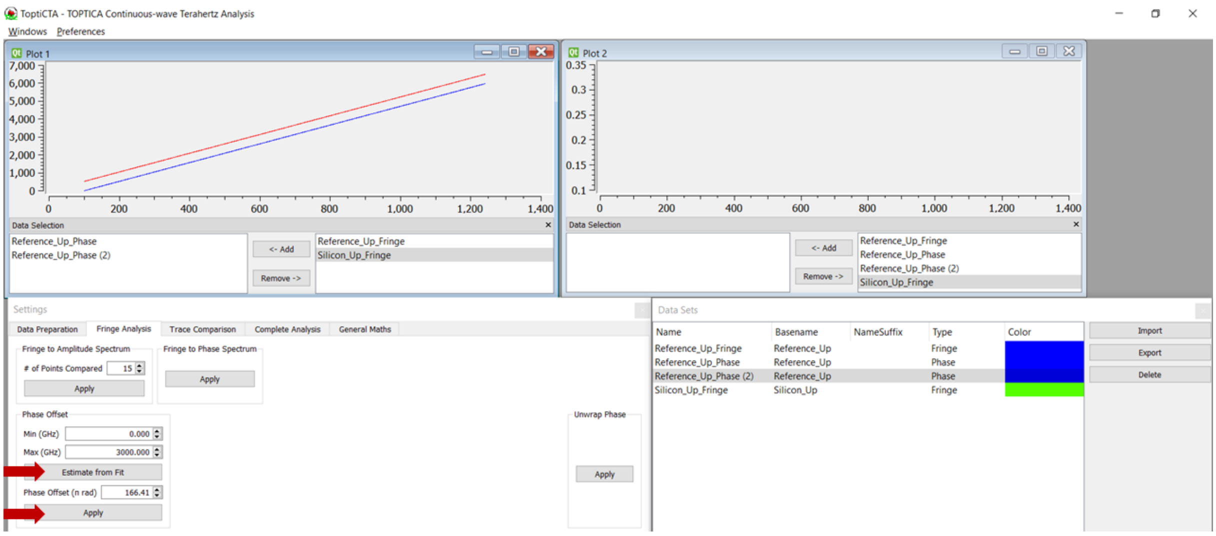


Fig. 11: Phase offset correction. In Plot 1, the blue curve shows a phase spectrum with incorrect offset (same data as in Fig. 10) and the red curve shows the offset-corrected spectrum.

d. In order to verify if the offset correction worked, click on the new “Phase (2)” dataset in the Data Selection Window. Click **Phase to Length** in the Settings + Analysis Window. Plot the resulting Length graph. The Length graph should be as smooth as possible. In particular, it should not exhibit an upwards or downwards bend towards low frequencies (Fig. 12).

NOTE! Phase spectra are displayed in [rad] as multiples of π. Length spectra have units of [mm]. The Length graph displays the deviation from zero path difference ΔL (see TeraScan manual, section 1.1.2).

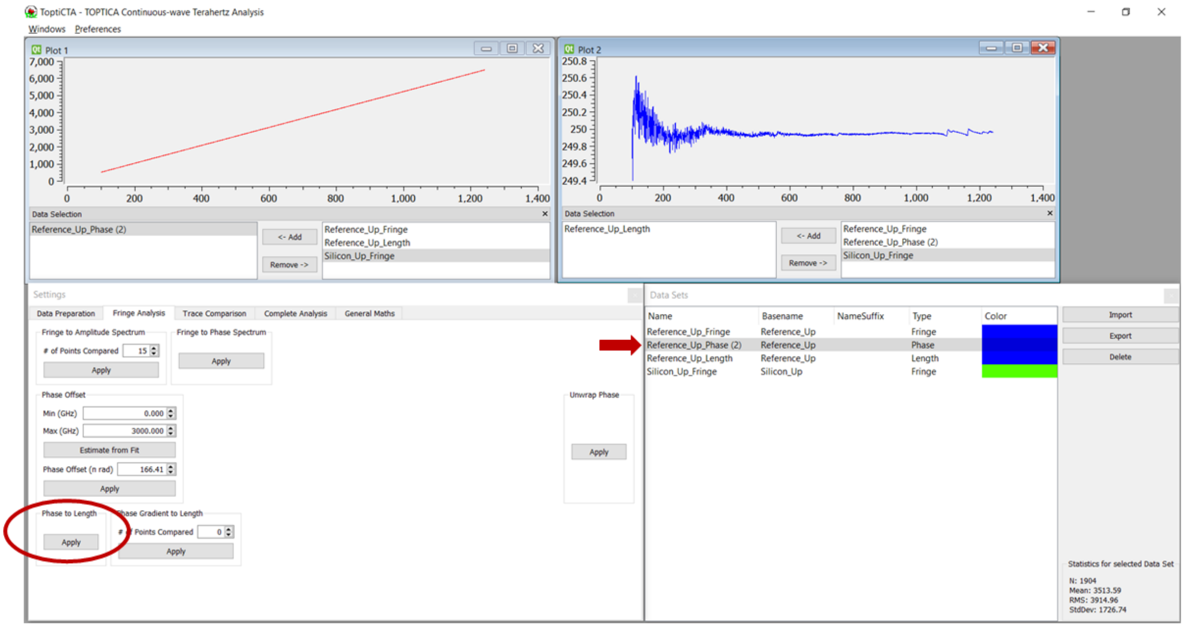


Fig. 12: Phase-to-length conversion, and resulting length plot (upper right window).

NOTE! As a guide to the eye, you can also use the function “Phase Gradient to Length” in the Settings + Analysis Window. For this conversion, the phase offset does not matter, and the first phase spectrum generated can be used as input dataset. For **# of Point Compared**, try using a value of ~ 50.

The resulting Length graph (dataset with suffix “B”) will appear noisy, but gives an indication of the value that you will reach by means of the phase offset optimization (Fig. 13).

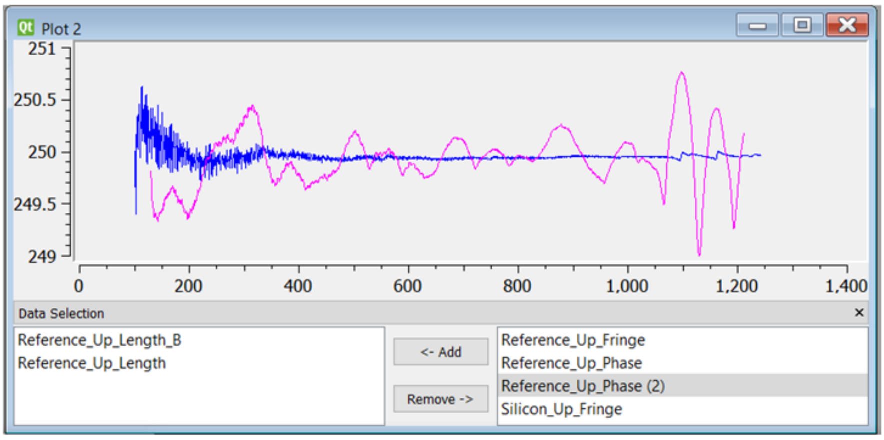


Fig. 13: Length plots using the fitted phase offset (blue curve) and the function “Phase Gradient to Length” (pink).

9. Repeat steps 7 and 8 (a) – (d) for the **sample** measurement. The fit will likely yield a slightly different phase offset.

10. Select the Trace Comparison tab of the Settings + Analysis Window. Chose the reference length dataset in section Length to Length Difference. In the Data Selection Window, highlight the sample length dataset, then click the **Length to Length Difference** button (Fig. 14). Plot the resulting “Lengthdiff” graph.

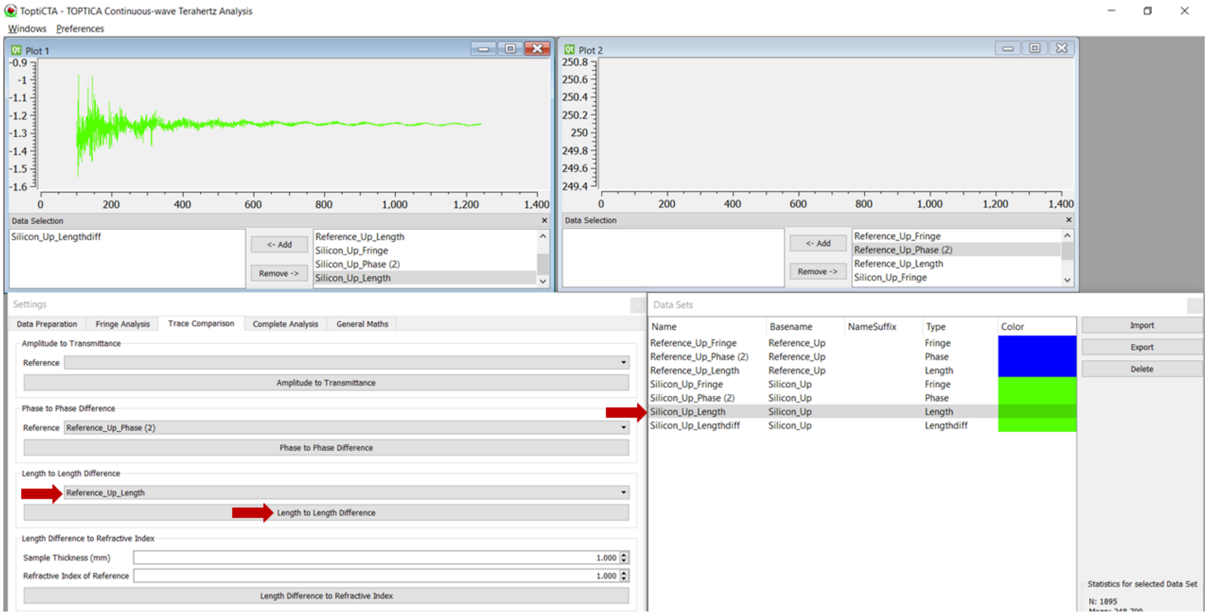


Fig. 14: Calculation of the length difference introduced by the sample in the beam.

Don’t be surprised if the length difference is negative; this means that the sample *reduces* the deviation from zero path difference at the receiver. (In this case, the terahertz beam path is – most likely – rather short.)

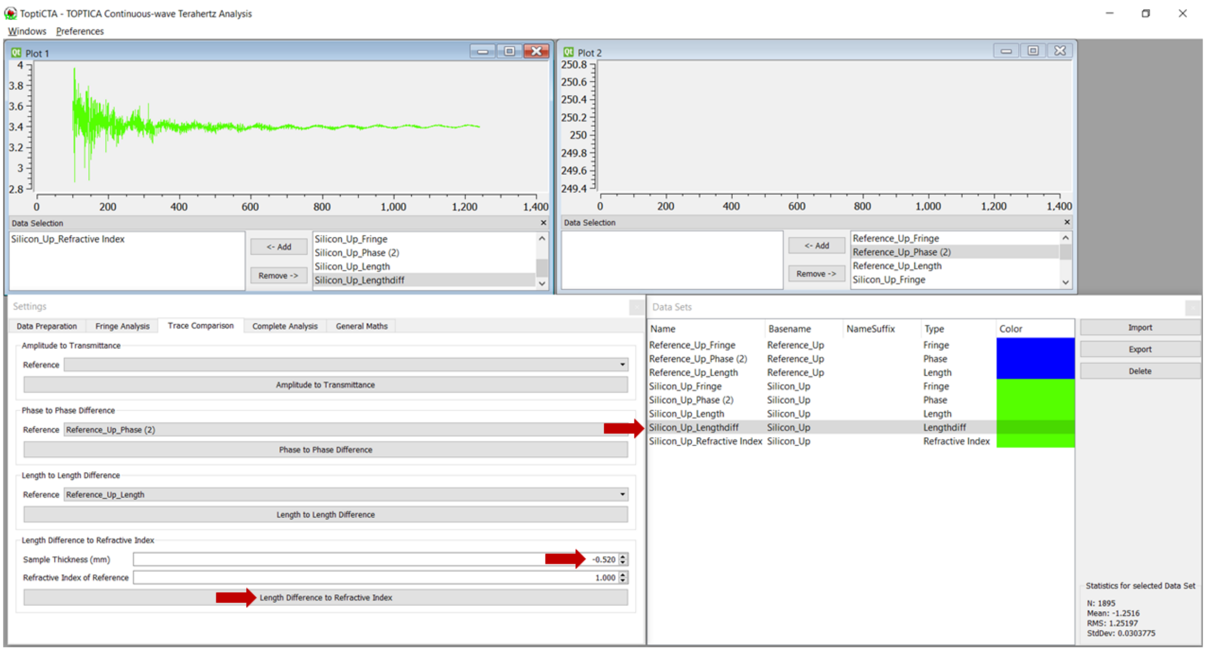


Fig. 15: Refractive-index calculation. Note the negative value for the sample thickness. The graph in Plot 1 shows the refractive index of silicon, with “wiggles” due to multiple reflections of the terahertz beam in the sample.

11. In section Length Difference to Refractive Index, enter the geometric thickness of the sample (in mm) and the refractive index of the reference measurement. If the reference comprised a spectrum with an empty aperture, use 1.0 for the refractive index of air.

NOTE! If the length difference is negative (step 10), then you need to enter a *negative* value for the sample thickness.

12. Make sure that the dataset of type “Lengthdiff” is highlighted in the Data Selection Window. Click **Length Difference to Refractive Index** to obtain the frequency-dependent refractive index (Fig. 15).

2.2 <u>One-hundred Percent Lines and the Effect of Trace Averaging</u>

A “one-hundred percent line” denotes the ratio of two spectra acquired under the same conditions. The calculation is identical to that of a transmittance spectrum (steps 1-5 in section 2.1).

Trace averaging is an established method to reduce statistical errors. While you can apply trace averaging to raw data of type “Fringe”, it is not advisable to do so, since in the case of a phase drift, this step will reduce the amplitude of the signals. However, trace averaging is often very useful for amplitude spectra, i.e. datasets of type “Amplitude”.

The following steps present an example of trace averaging for the computation of a one-hundred percent line. Eight scans each are used as “reference” and “sample” measurements.

1. Load all of the datasets into the Data Selection Window (Fig. 16).

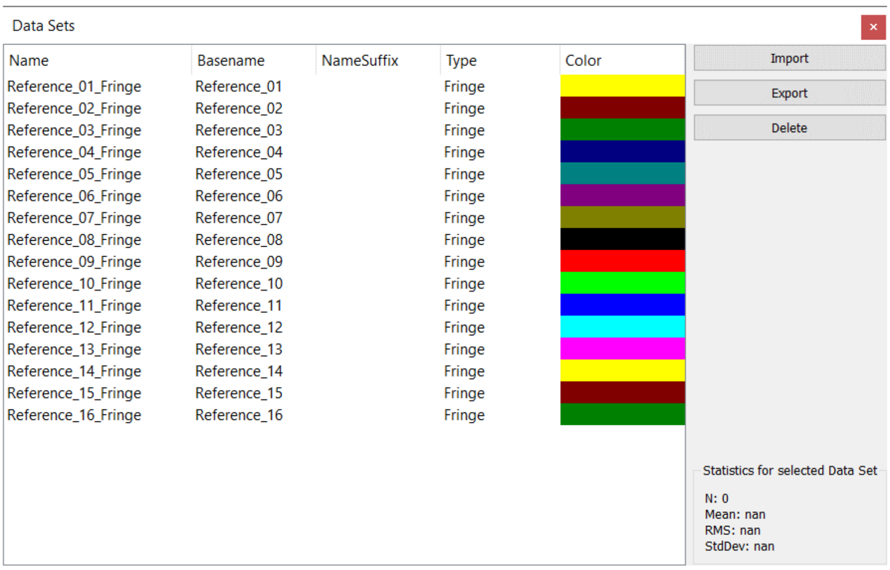


Fig. 16: Data selection, with 16 measurements loaded.

2. Successively, select each dataset and convert it to an amplitude spectrum (Settings + Analysis Window, tab Fringe Analysis, section Fringe to Amplitude Spectrum). Make sure to use a suitable value for **# of Points Compared.**

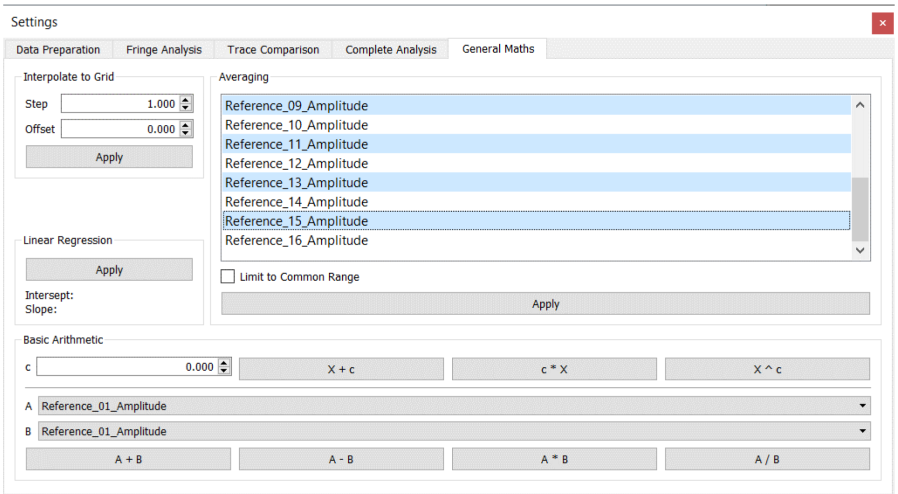


Fig. 17: Trace averaging. In the example, the "uneven" amplitude files are selected for averaging.

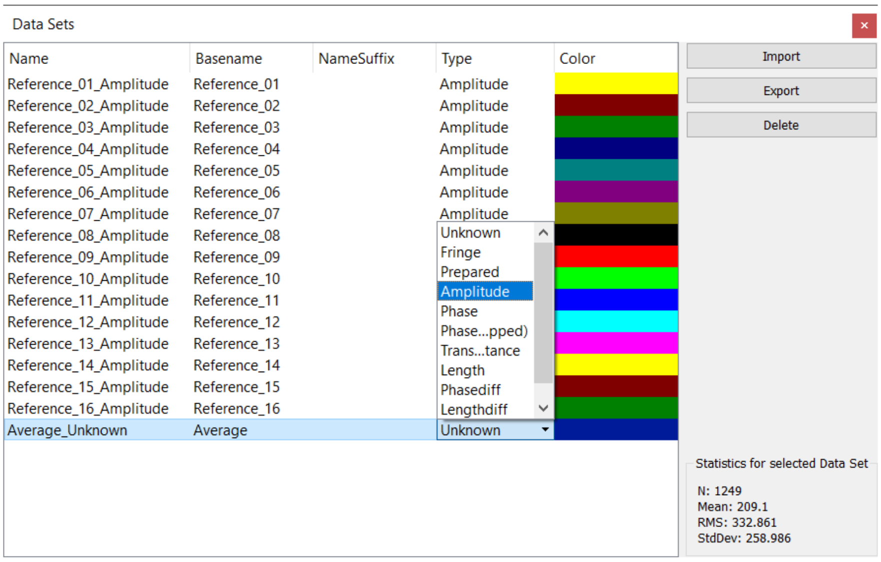


Fig. 18: Changing the file type of the averaged dataset.

3. Open the General Maths tab in the Settings + Analysis Window (Fig. 17). Select the "reference" files that you wish to average, then click the **Apply** button beneath the selection window.

4. The averaged dataset appears in the Data Selection Window, as yet of type "Unknown". Change the type to "Amplitude" (Fig. 18).

5. Repeat steps 3-4 for the "sample" files.

6. Calculate the transmittance as described in Section 2.1, step 5. Use the first average dataset as reference and the second dataset as sample.

Fig. 19 shows one-hundred percent lines without averaging (i.e., taking the ratio of two amplitude spectra), and with averaging of 8 + 8 scans.

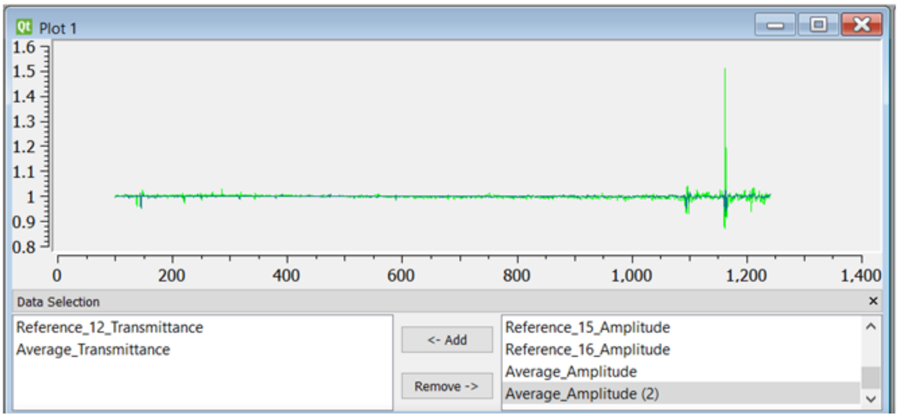


Fig. 19: One-hundred percent lines without averaging (black trace) and with 8 + 8 traces averaged (green). Note the difference in particular at the water vapor absorption frequencies around 1.1 THz and 1.16 THz.

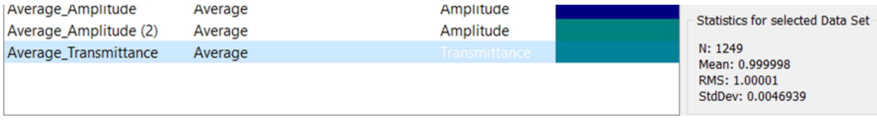


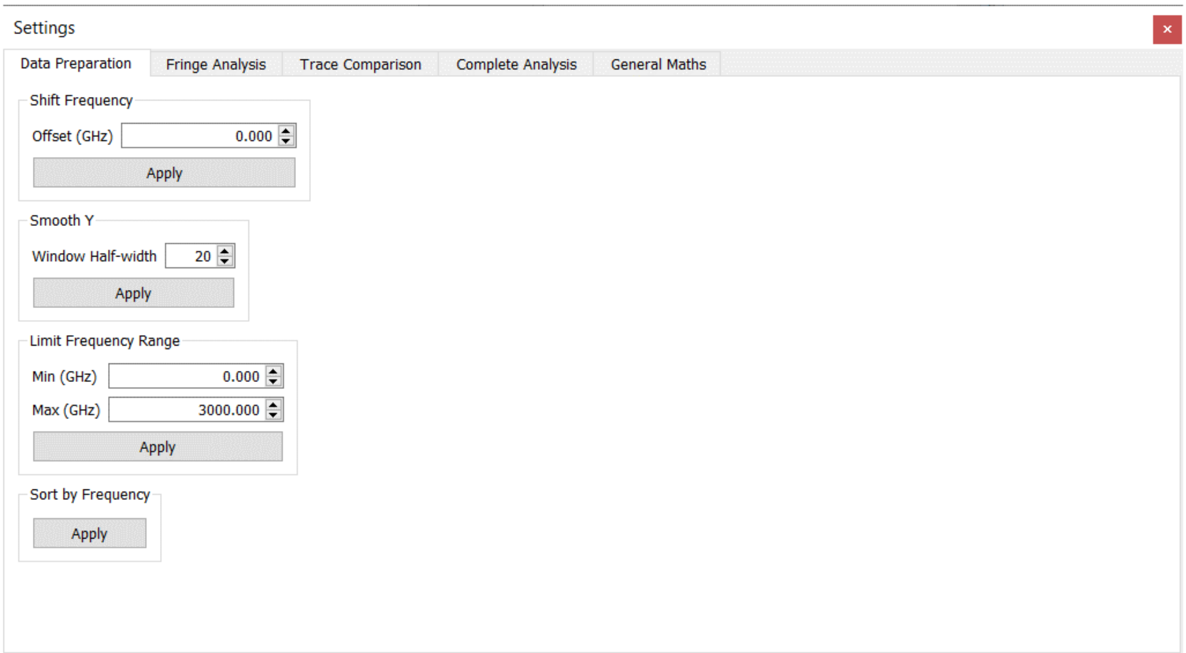
Fig. 20: Statistical information about a data set.

A useful feature in this context is the information displayed in “Statistics for selected Data Set” in the bottom-right corner of the Data Selection Window (Fig. 20). In the example of the one-hundred percent lines shown in Fig. 17, the standard deviation (StdDev) is 1.9% for the unaveraged ratio, and 0.005% for the averaged ratio, roughly consistent with an improvement proportional to the square root of the number of averages.

3) Overview of Analysis Functions

This section provides an overview of the functions in the Settings + Analysis Window.

Data Preparation Tab



Shift Frequency: Adds or subtracts an offset to a selected dataset. You can enter positive or negative values in the input field. Changes take effect by clicking **Apply**.

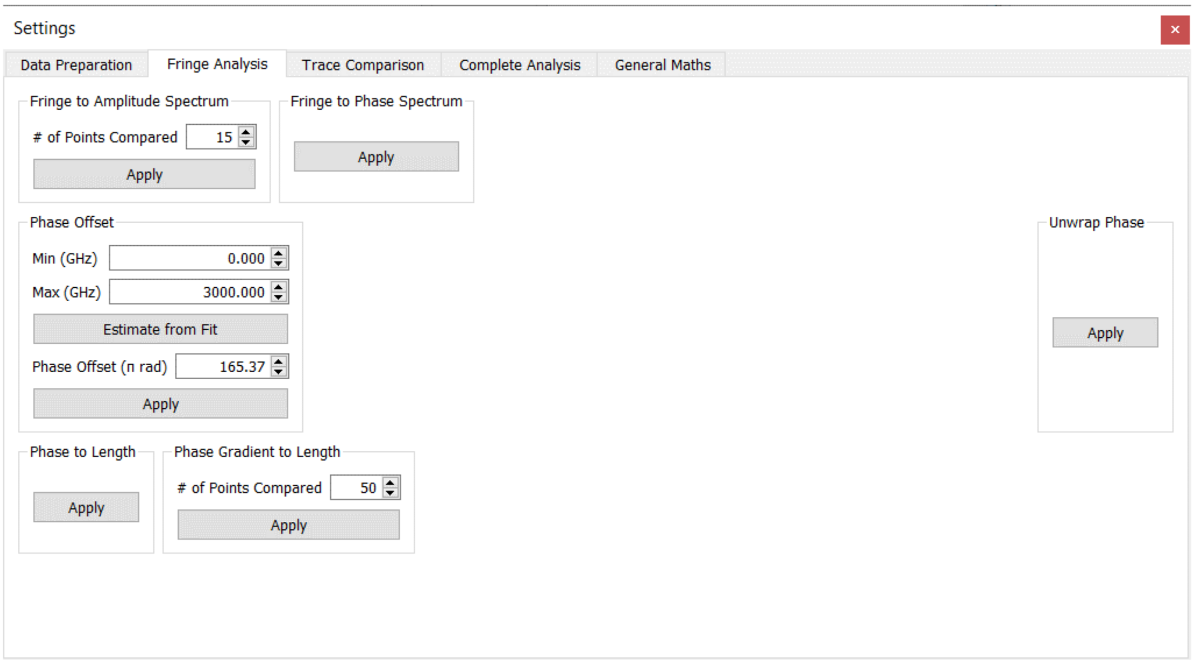
Smooth Y: Applies a moving average to a selected dataset. **Window Half-width** defines the halfwidth of the moving average. Changes take effect by clicking **Apply**.

Limit Frequency Range: Generates a new dataset containing only data of a restricted frequency range, which is defined via **Min (GHz)** and **Max (GHz)**. This is useful e.g. if values at high frequencies only comprise noise. Changes take effect by clicking **Apply**.

NOTE! The default setting is a minimum frequency of 0 GHz and a maximum of 3000 GHz. If the selected dataset comprises a smaller range, then only the frequencies of the dataset are evaluated.

Sort by Frequency: Clicking **Apply** rearranges a dataset as “up” scan, i.e. with frequencies in rising order.

Fringe Analysis Tab



Fringe to Amplitude Spectrum: Converts a dataset of type "Fringe" to an amplitude spectrum, by analyzing the maxima and minima of the phase fringes.

> **# of Points Compared:** This value should equal (at least roughly) the number of datapoints in a fringe halfwave.

Fringe to Phase Spectrum: Generates a phase spectrum from fringe data.

Phase Offset: This is an option to correct the offset of a phase spectrum. A phase offset can either be entered manually (Parameter **Phase Offset**) or determined via a linear fit.

> **Min (GHz)** and **Max (GHz)** restrict the linear fit to a user-defined frequency range.
>
> **Estimate from Fit** initiates the fit routine. The result is displayed in the field underneath, **Phase Offset**, in units of [rad] as multiples of π. This value can still be modified manually.
>
> Clicking **Apply** creates a new dataset for the offset-corrected phase spectrum.

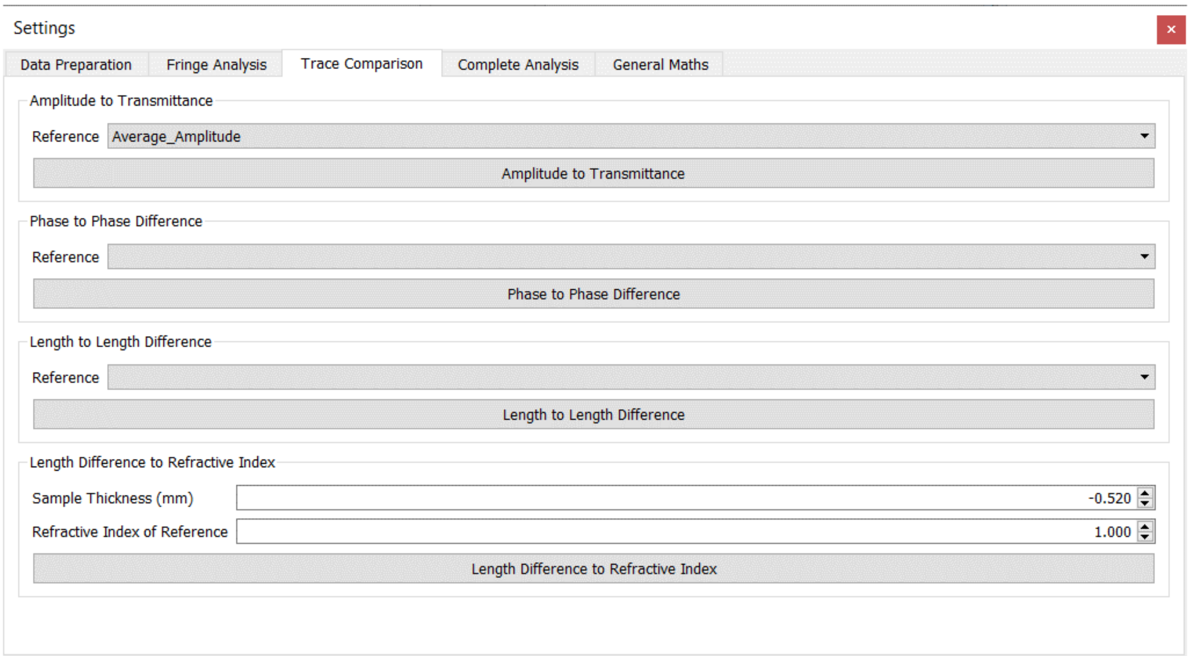
Phase to Length: Converts a phase spectrum to a length plot.

Phase Gradient to Length: Approximate calculation of the length, based on the phase gradient rather than the complete phase spectrum.

> **# of Points Compared:** Number of the phase fringes (i.e., zero crossings) considered for the gradient calculation.

Unwrap Phase: Unwraps phase data measured with a fiber stretcher setup.

Trace Comparison Tab



Amplitude to Transmittance: Compares two datasets of type Amplitude and calculates the transmittance, i.e. the *squared* ratio of the amplitudes.

Reference opens a pull-down menu to select the reference file.

The **Amplitude to Transmittance** button starts the analysis, using the dataset highlighted in the Data Selection Window.

Phase to Phase Difference: Compares two datasets of type Phase and calculates the phase difference.

Reference: Enables selection of reference file.

The **Phase to Phase Difference** button performs the analysis for a dataset chosen in the Data Selection Window.

Length to Length Difference: Compares two datasets of type Length and calculates the length difference introduced by a sample in the terahertz beam.

Reference: Enables selection of reference file.

The **Length to Length Difference** button performs the analysis for a dataset chosen in the Data Selection Window.

Length Difference to Refractive Index: Calculates the refractive index from the (frequency-dependent) length difference.

Sample thickness: Input field for sample thickness, in mm.

NOTE! If the length difference is negative (step 10), then you need to enter a *negative* value for the sample thickness.

Refractive Index of Reference: Should be 1.0 if the reference comprises a spectrum with empty aperture. Otherwise, insert the refractive index of the reference material.

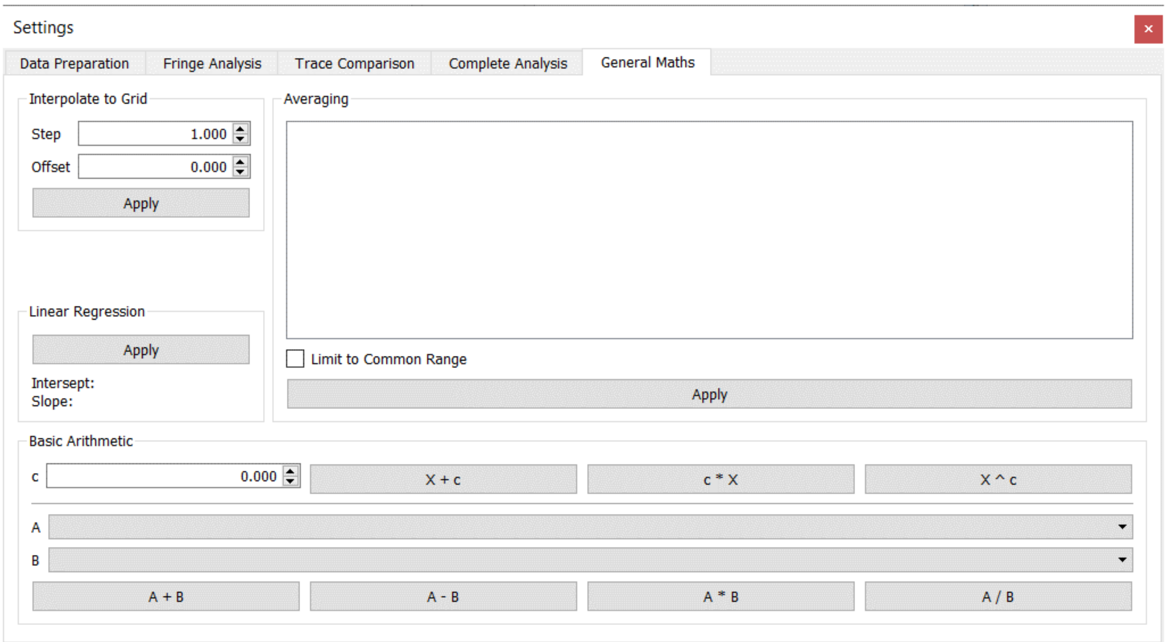
The **Length Difference to Refractive Index** button performs the analysis for a dataset chosen in the Data Selection Window.

NOTE! All these functions can be applied to any data set in the Data Selection Window. The result will only be meaningful if the correct input data type is chosen.

Complete Analysis Tab

Not implemented yet.

General Maths Tab



Interpolate to Grid: Interpolates a dataset to a frequency grid, defined by **Step** and **Offset.**

Averaging: Enables averaging of an arbitrary number of datasets, which are selected in the window in this tab.

Limit to Common Range: Restricts the average to a frequency range common to all of the selected datasets.

Apply generates a new dataset that comprises the averaged data.

Basic Arithmetic: Enables arithmetic operations for a dataset, or a combination of two datasets.

You can perform an addition, a multiplication, or exponentiation with a constant (input field **c**). Note that the dataset (**X**) has to be chosen in the Data Selection Window.

Moreover, you can perform an addition, subtraction, multiplication or division of two datasets **A** and **B**, which are selected via the respective pull-down menus.

If you have feedback or comments regarding the software or this documentation, please write to

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