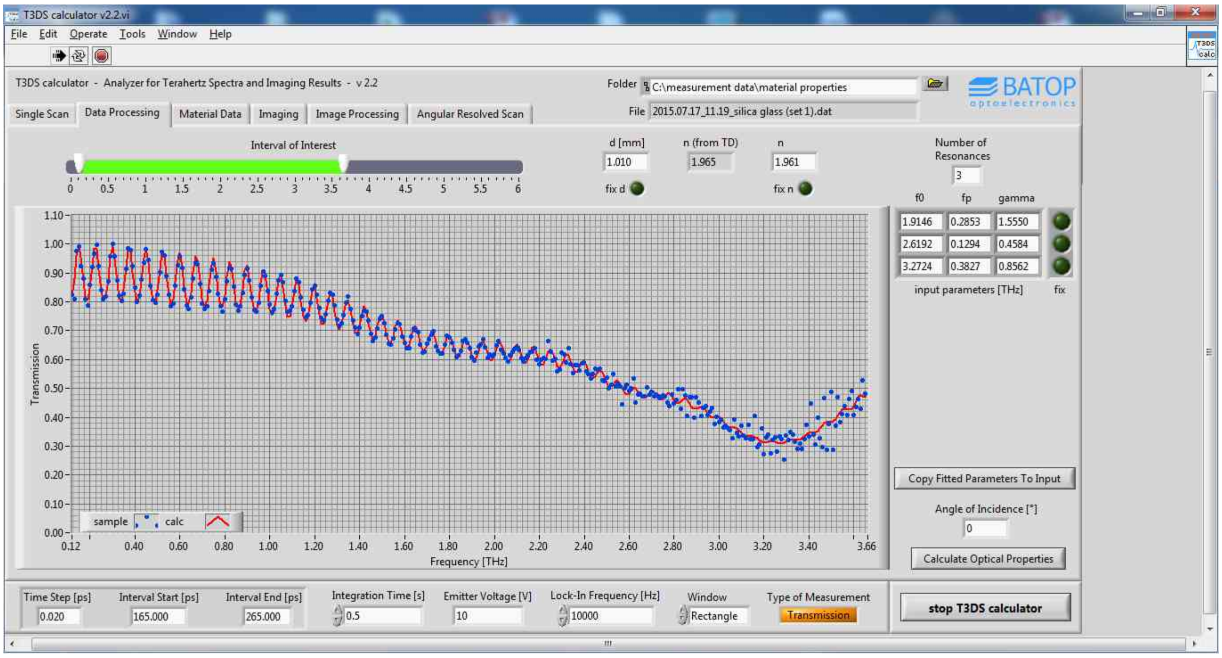
Instruction manual for T3DS calculator software

Analyzer for terahertz spectra and imaging data

Release 2.4



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0. Preliminary remarks

Attention:

All software versions up to T3DS calculator v1.8 assume a bulk material when calculating the material properties. They neglect any secondary reflections / interferences in the transmission / reflection spectrum. Starting with the release of the T3DS calculator v2.0 the software employs the correct formulas to handle interferences created by very thin samples / samples with a very low absorption.

The software now applies a dispersion model in order to calculate a fit for the dielectric function:

$$N(f)^2 = \varepsilon(f) = \varepsilon_\infty + \sum_j \frac{f_{p,j}^2}{f_{0,j}^2 - f^2 - i \times f \times \gamma_j}$$

With
- f – frequency
- ε_∞ – high frequency limit of the dielectric function $\varepsilon(f)$
- f_0 – resonance frequency
- f_p – plasma frequency
- γ – damping constant

The dispersion formula ensures that the real and imaginary parts of the dielectric function – and consequently also of the refractive index - are related according to the Kramers-Kronig relation.

The frequency spectra of the reference and the sample are used in order to determine the absolute numbers for the transmission / reflection of the sample investigated. The software will then fit the calculated data with the formulas that correspond to the measurement setup. For more detailed information on the determination of the material properties please have a look on our website:

http://batop.de/products/terahertz/THz-spectrometer/benchtop-terahertz-spectrometer.html

Attention:

In order to determine material properties you need to conduct a reference measurement first. Otherwise, the transmission / reflection cannot be calculated. Additionally, please be aware that the software assumes an s-polarized THz beam for reflection measurements. All TDS systems are equipped with polarizers in order to ensure a well defined polarization state. If your plan on building your own terahertz setup for reflection make sure to polarize the THz beam accordingly.

1. Analyzing material properties

1.1 Loading data

The T3DS calculator v2.2 is capable of determining the material properties of solid samples, measured in transmission or reflection. On the first tab you may load the data of a static measurement, a “pixel” of an imaging measurement or one scan of an angular resolved measurement. The most important thing to remember is that the software requires a reference measurement. Otherwise, the material properties cannot be analyzed.

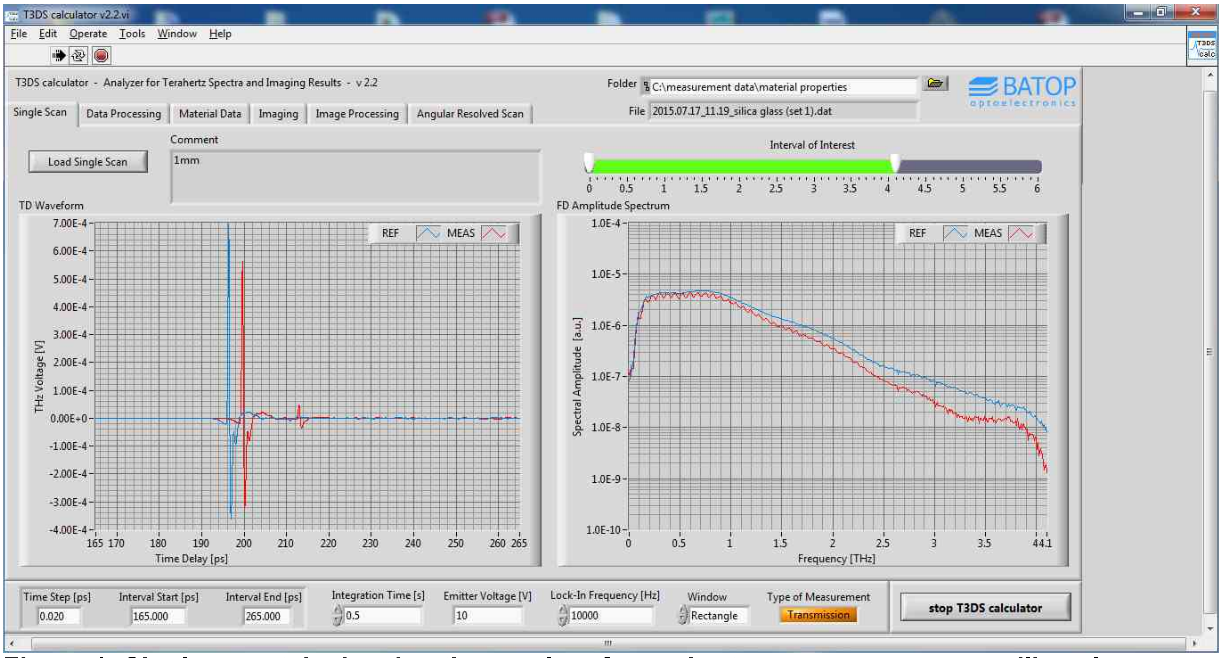

Figure 1: Single scan tab showing the results of a terahertz measurement on a silica glass.

The T3DS calculator software displays the time-domain data and the frequency spectra much the same way as the T3DS software with frequency spectra including the baseline subtraction before the Fourier transformation (if a baseline was acquired).

Upon loading the data the program also reads most of the scan parameters and displays them in the bottom line of the main window. Since the fields are not read-only you can change for example from transmission to reflection measurement (e.g. if you find that this option has been set incorrectly before saving the data). This is important as the software uses this setting to choose the right formulas to determine the optical properties on the next tab.

Attention:

If you want you can rescale the graphs manually by right-clicking the axis and setting a new upper / lower limit. Some axes may rescale automatically but you can turn off this option or reactivate it if you prefer. This procedure can be applied to all xy-graphs, similar to the T3DS software.

1.2 Data preparation

On the second tab the user needs to prepare the data for the fitting procedure. At first put in a best guess for the thickness (as measured) and the refractive index n. The latter can be estimated from the time domain graph using the first and second pulse of the measurement data.

$$n = \frac{\Delta t[ps] \times 0.3 \times \cos\alpha}{2 \times d[mm]}$$

With Δt – time shift between the first and second pulse of the sample data
α – angle of incidence (typically 30° for reflection measurements)

If there is no secondary pulse, the refractive index can only be determined for the transmission measurement using the time shift between the reference pulse and the 1st pulse of the sample data:

$$n = \frac{\Delta t[ps] \times 0.3}{d[mm]} + 1$$

This number is also calculated by the software (n from TD) for all transmission measurements.

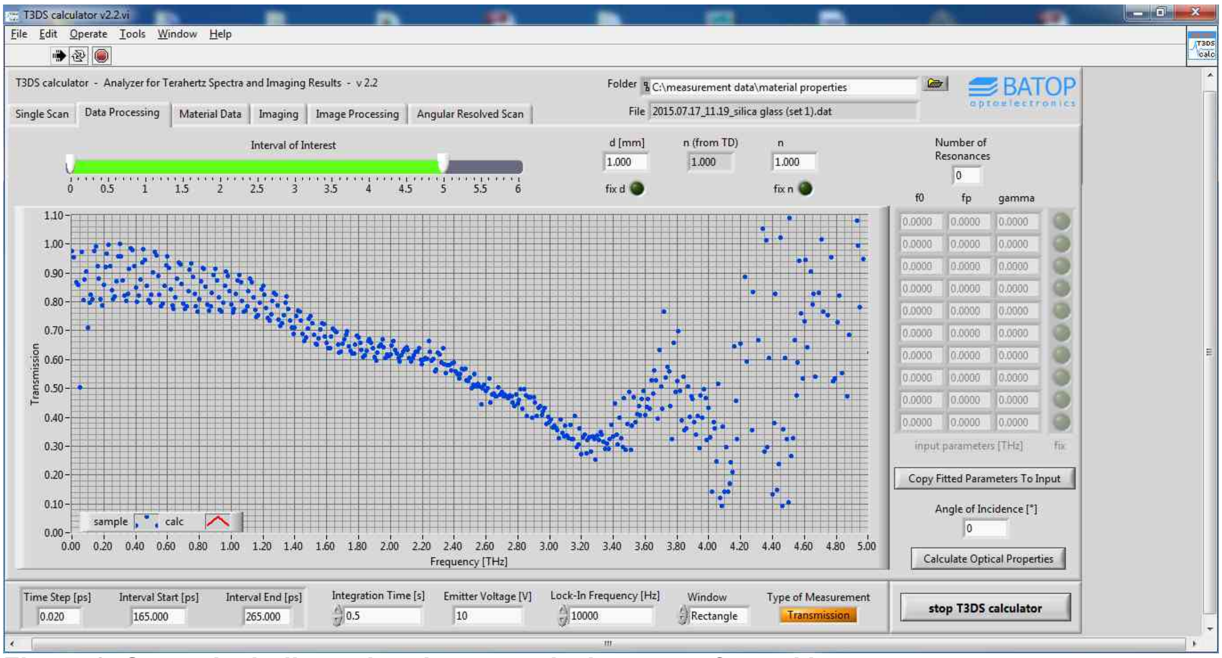

Figure 2: Second tab displaying the transmission curve for a silica glass.

As a second step we recommend choosing an interval where there is little noise on the calculated transmission / reflection in order to simplify the fitting procedure for the T3DS calculator. For the example displayed in Figure 2Figure 2Figure 2Figure 2 you may choose the interval between 0.1 – 3.6 THz.

1.3 Fitting transmission data

The transmission curve in the chosen example displays three (maybe more) characteristic resonances at about 1.8 THz, 2.5 THz and 3.3 THz. Besides the resonance frequency you need to set a plasma frequency (typically 0.01 – 0.1 *f_0) and a damping constant. The latter is roughly the full width at half maximum / minimum of the resonance – which is basically half the total width of the absorption minima. If you now fix all preset parameters the software can calculate a first “fit” as a test.

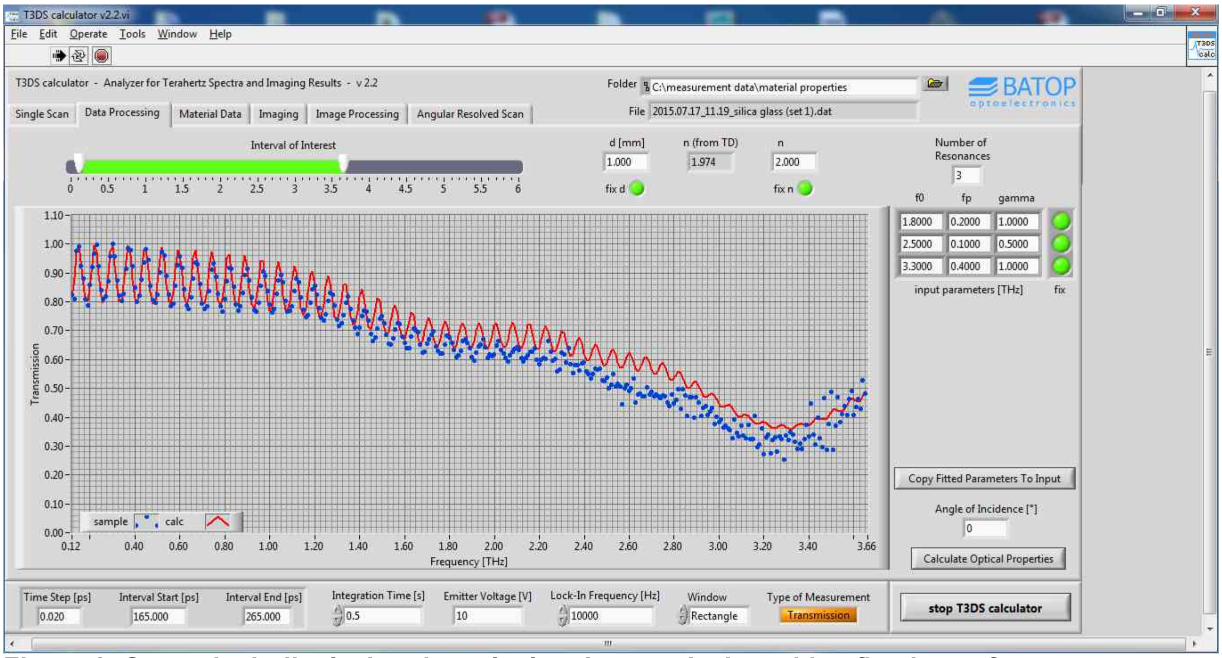

Figure 3: Second tab displaying the calculated transmission with a fixed set of parameters.

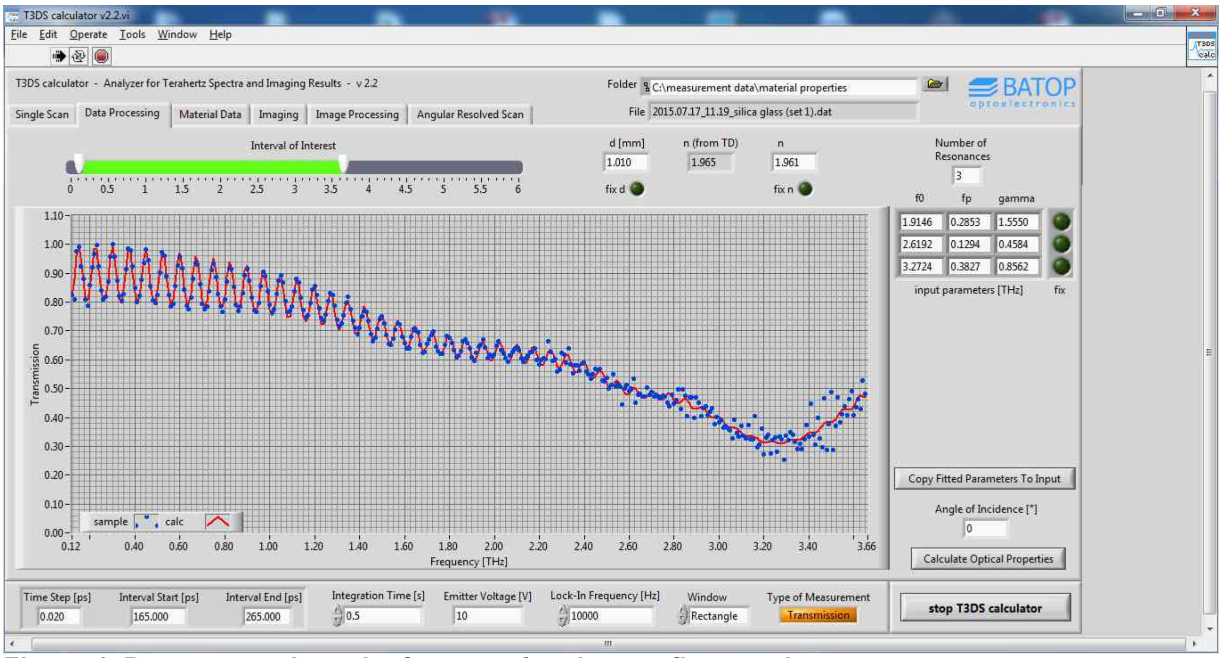

Figure 4: Data processing tab after completed curve fit procedure.

You may now choose to loosen the restrictions on the different parameters in order for the software to fit the measurement data properly. We recommend starting with the resonance parameters, followed by the refractive index and – at last – the thickness. As the software does not allow the parameters to change arbitrarily you should copy the fitted parameters of the resonances to the second tab by pressing the button. This way you can iterate the parameters towards the best fit by alternating the curve fit procedure and copying the results. You will note that upon freeing the refractive index and the thickness that these parameters will be rewritten with automatically.

Once the calculated data fits the measurement data you can fix the parameters, zoom in on a certain part of the spectrum and calculate the numbers again in order to get a more detailed view.

Attention:

If you rescale the spectrum using the slider above the graph the next fit will only apply to the new interval. Hence, if you want to avoid that the software calculates a new set of parameters they need to be fixed.

Depending on the chosen interval the software calculates the real and imaginary part of the refractive index with every fit and displays it on the third tab. You can also zoom in on the data displayed using the slider above. However, the whole range of calculated data points will be stored when clicking the “save optical data” button. The file with the material data uses the original file name, extended by “material properties”. It contains all fit parameters, the sample transmission / reflection, the calculated transmission / reflection, the refractive index and the extinction coefficient.

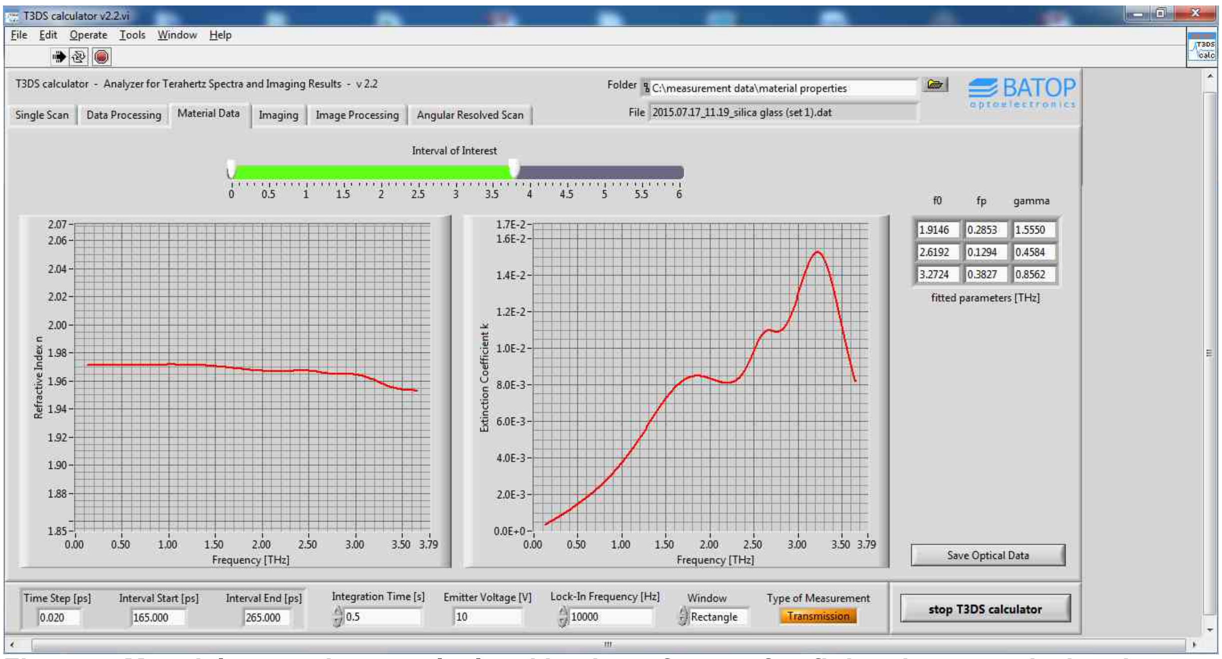

Figure 5: Material properties as calculated by the software after fitting the transmission data.

1.4 Fitting reflection data

As mentioned before it is more complicated determining a refractive index in advance for fitting reflection measurements. Contrary to a transmission measurement the reflection also increases with absorption but the features are much less pronounced compared to a transmission measurement. This further complicates to choose the parameters for starting the fitting procedure. Ideally, you may have some data from transmission measurements in order to have an idea about the number of resonances and the corresponding set of parameters.

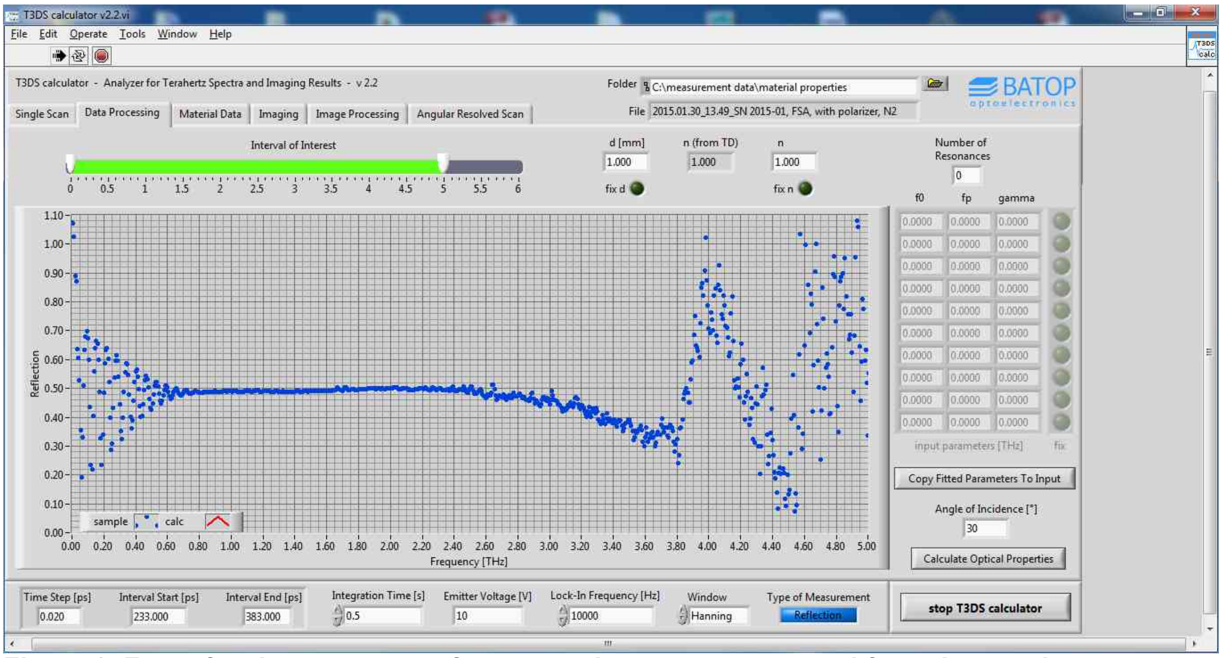

Figure 6: Full reflection spectrum of a glass substrate as calculated from the raw data.

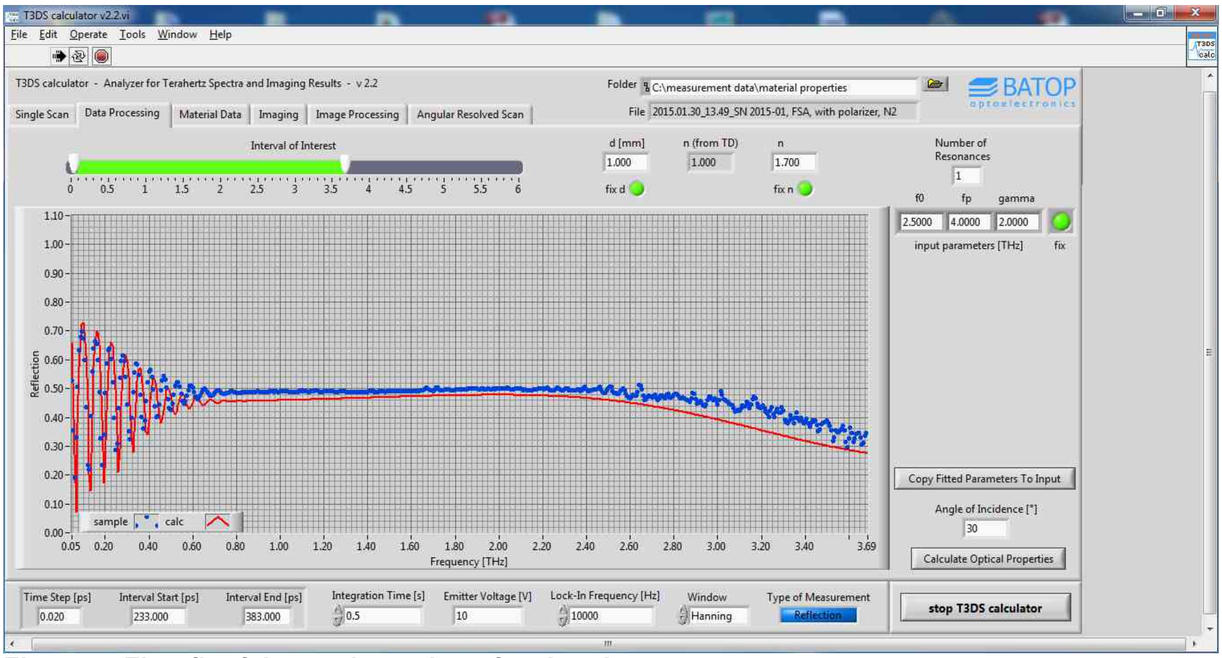

Figure 7: First fit of the model to the reflection data.

As can be seen in Figure 6 there is a slight reflection maximum at about 2.5 THz, indicating a strong absorption at this frequency. The interferences vanish at around 0.5 THz giving a full width at half maximum of about 2 THz. The absorption is much stronger than for transmission measurements. Hence, the plasma frequency f_p is much higher – we'll assume 4 THz in the given example.

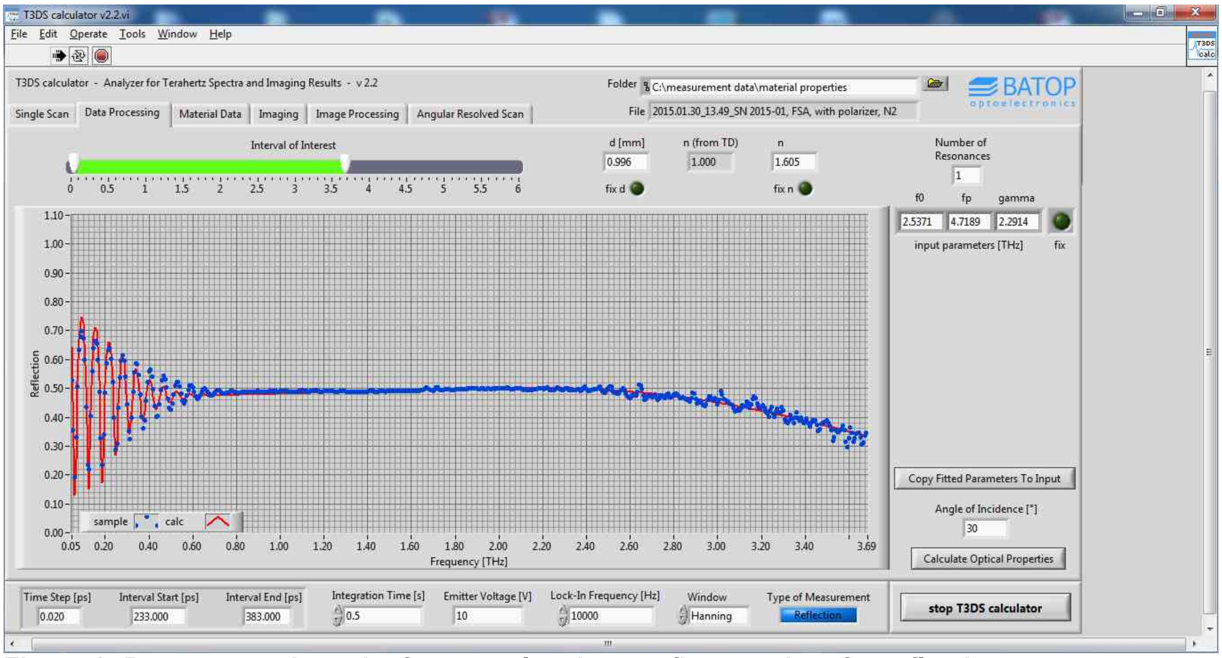

Figure 8: Data processing tab after completed curve fit procedure for reflection measurement.

Again, we suggest that you now loosen the restrictions on the fitting parameters, starting with the resonance parameters. With every fit you may copy the new fitting parameters to the second tab and loosen another parameter.

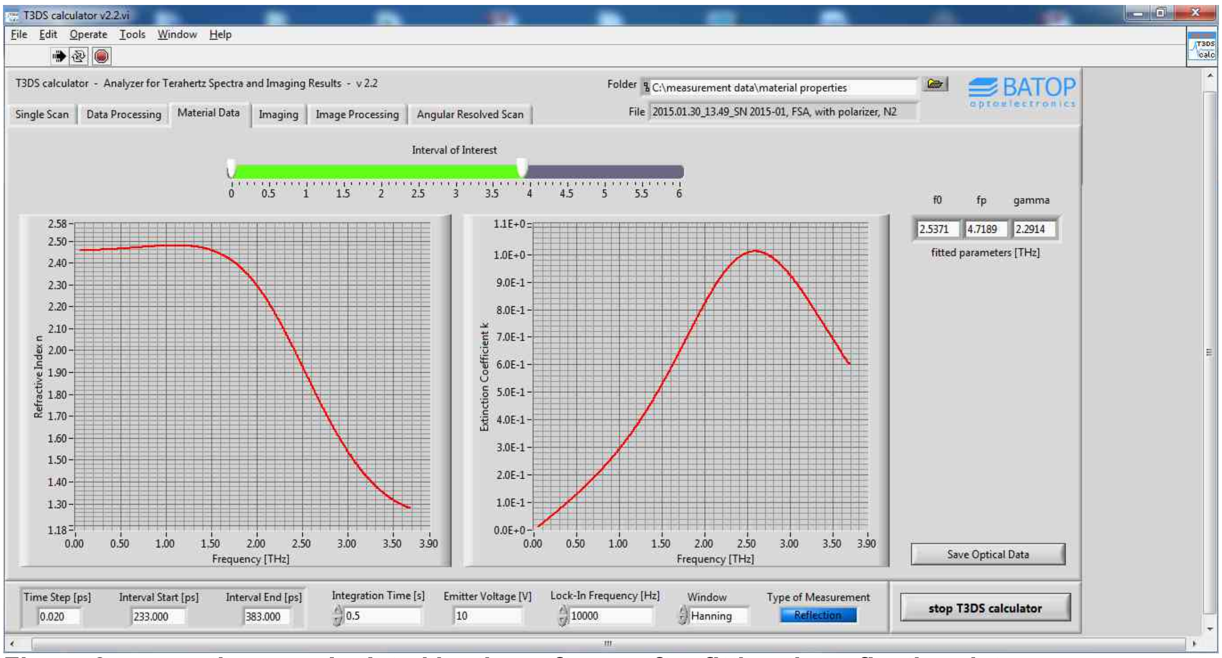

Figure 9: properties as calculated by the software after fitting the reflection data.

Similar as for the transmission measurement you'll find the calculated material properties on the third tab. If you now compare the data to the transmission measurement you can see that there is significant more absorption for the regular glass than for the silica glass measured in transmission.

You can also see that there is a significant change in the refractive index, contrary to the silica glass where it is almost constant. Additionally, the fitted reflection spectrum does show some deviation at low frequencies. Hence, another resonance at 1 THz might be required.

2. Analyzing imaging data

2.1 Loading images

The fourth tab of the T3DS calculator allows loading and displaying the results of imaging measurements. As you can see in Figure 10 there are four images displayed at the bottom of the “Imaging tab”. These will be visible once you have loaded the data and clicked the “calculate images” button. The first image displays the relative peak to peak voltages obtained for all xy-positions. Similar to the T3DS software, black corresponds to a value of zero and light blue corresponds to a value of one.

In image number two the relative time shift delta t between the peaks with the highest voltage is displayed. The xy-position where the largest peak comes first serves as a reference for all other xy-positions. The image may give you an idea about the tilt between the image plane and the movement directions of the xy-stage or the surface features of a reflecting object.

The third image allows integrating the frequency spectrum for each xy-position within a certain frequency band (as chosen by the slider). Hence, the result directly corresponds to the area under the curve which can be used as a measure for the transmission / reflection of the material, depending on the measurement setup. However, also surface features may change the signal strength and hence, the frequency spectrum.

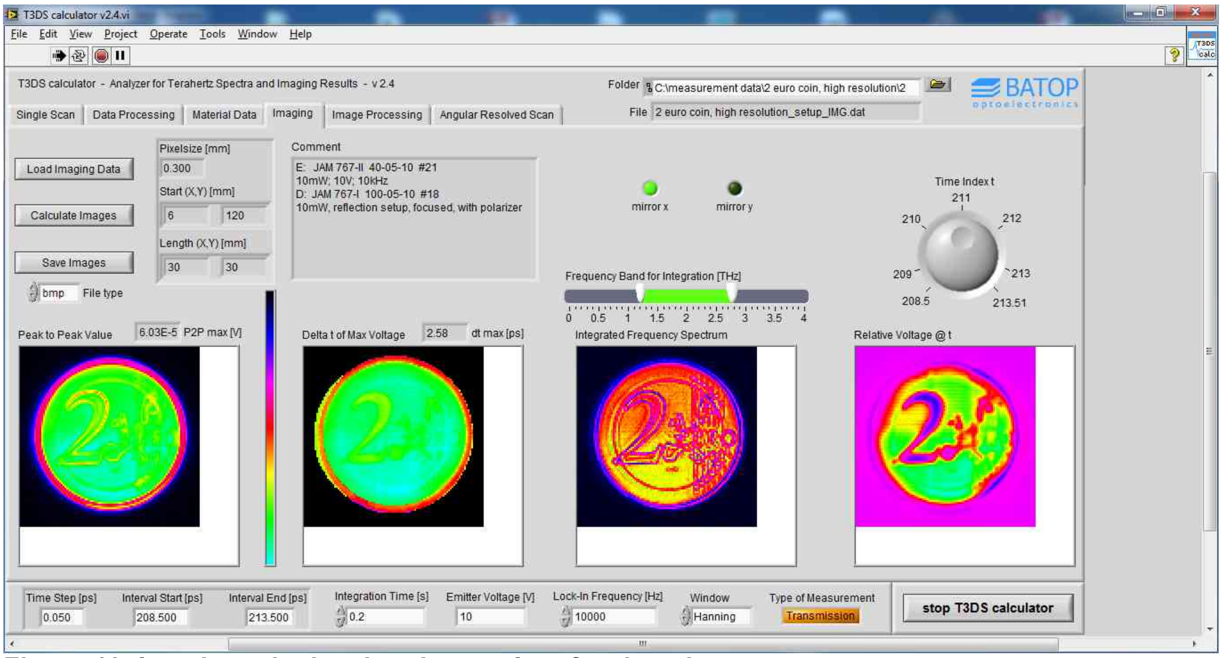

Figure 10: Imaging tab showing the results of an imaging measurement.

The last image on the second tab displays the voltage at a certain time t (given in picoseconds). As the data is loaded the time index will be set to the first point of the scan. Uniform regions indicate that the sample properties are constant within that area.

In order to flip the images horizontally or vertically you may use the two buttons at the top of the tab. The images displayed can be saved as bmp, jpg and png files using the “Save Images” button. They are found in the same folder as the measurement data that has been loaded.

2.2 Processing images

Even if you take good care of arranging your object, the plane of the xy-stage may not be totally parallel to the surface of the object. Hence, it may be necessary to recalculate the time delay for each point of the object, especially if the image has been recorded using the reflection setup. In order to do so please select three reference points that will be used to calculate the time shift for each point of your image. By default the software chooses three points at the corners of the picture but you may choose differently.

The graph on the left will display the time-domain data for the chosen points which can be shifted in time using the corresponding buttons and input windows (see Figure 11). By shifting the data you can manipulate the picture in a way that characteristic peaks occur at the same time. Please choose your points wisely in order to conduct this procedure.

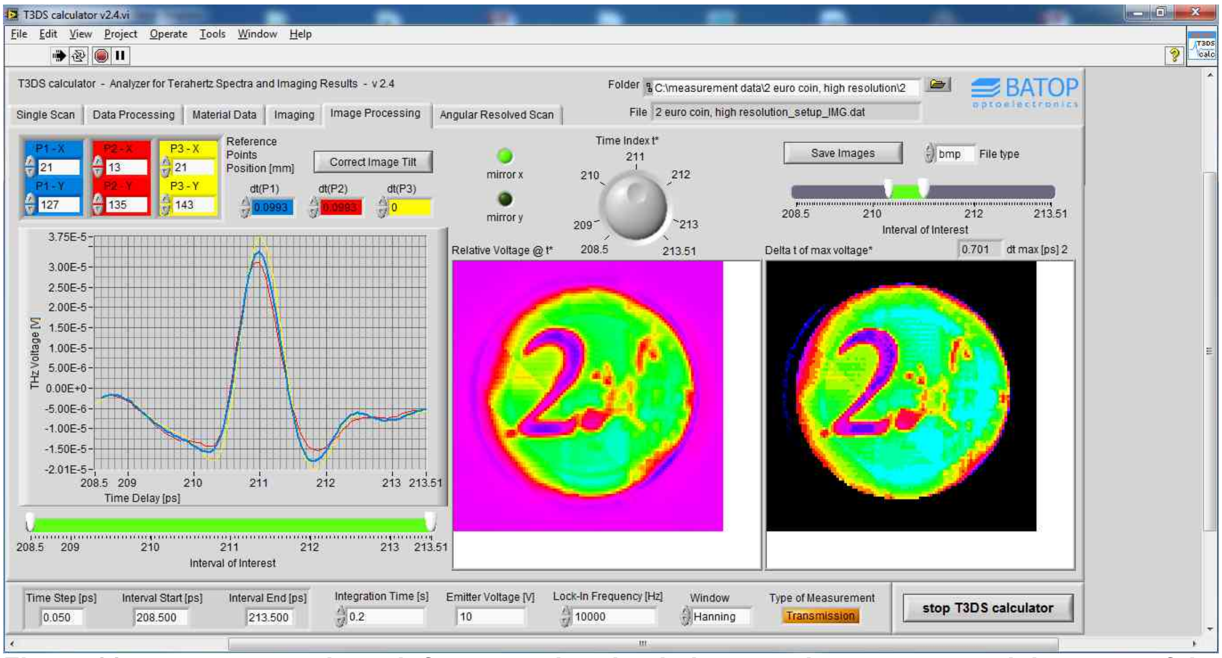

Figure 11: Image processing tab for correcting the tilt between image plane and the plane of the xy-stage.

After choosing the reference points and adjusting the time shift you can click the “correct image tilt” button. At this point a new data array will be created in order to maintain the original data. On the two images to the right you will find the processed data for the voltage at a given point in time as well as the time delay between the points with the largest peak. For the latter picture there is another slider in order to focus on a smaller time interval.

If you have large, flat and homogeneous surfaces you will find corresponding areas of similar color in your image after you corrected the tilt. However, if material properties change locally or the surface is rough the image may not contain homogeneous regions even after correcting the tilt.

Finally, you can save the two pictures and the parameter set used for the correction of the image tilt using the “Save Images” button at the top. The name of the picture files will indicate that the data was processed before saving in order to distinguish the results from the unprocessed data displayed on the “Imaging tab”. Additionally, a text file is created that contains details on parameters used to correct the image tilt.

3. Loading results of angular resolved scans

On the last tab of the T3DS calculator software you can load the results of an angular resolved scan. Similar to other measurement types the program will display the parameters used for the scan as well as the collected data. By clicking on the buttons that are attached to the graph you can change the contour plot to a 2-dimensional graph and back again. Additionally, you can revolve the 3D plot in order to get a better angle of view on the results. Once you are done adjusting the view you can save the 3D plot as an image.

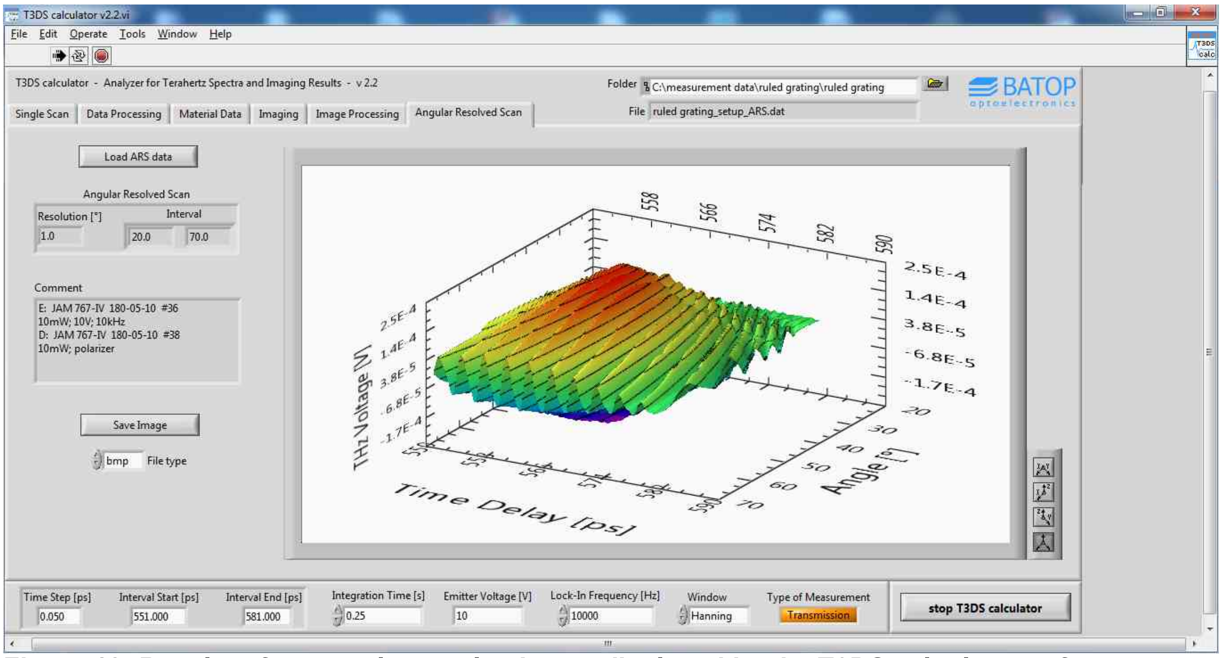

Figure 12: Results of an angular resolved scan displayed by the T3DS calculator software.

Please note that the 3D contour plot may not yield a smooth surface because the software connects all data points with lines rather than interpolating what is in between.

4. Contact details

If you have any further questions or remarks, please do not hesitate to contact us.

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