

Instruction manual for T3DS software

Tool for THz Time-Domain Spectroscopy

Release 4.0



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0. Setup

The BATOP THz time-domain spectrometer comes with two panels that contain:

- USB-ports to establish a connection from your computer to the internal delay line (ZLS, Zaber linear stage), the data acquisition system (DAQ, National Instruments) and an optional voice coil for fast scans
- BNC ports for the THz emitter and detector antennas
- fiber ports to hook up the external fiber-coupled antennas
- a Mini-Din connector to plug in external stages (imaging unit or angular scanning unit)

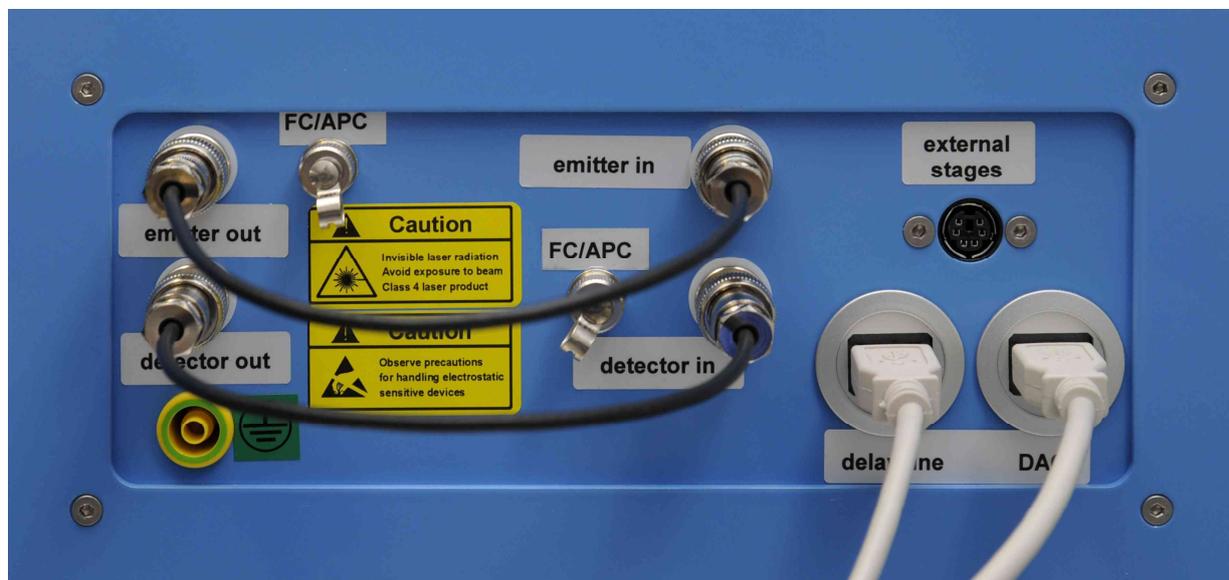


Figure 1: Panel on the right hand side of a TDS system with ports for electrical and optical connection of THz antennas, external stages (imaging unit or angular scanning unit), the delay line and the data acquisition system (DAQ). The panel shown is configured for the use of the internal free space antennas.

After setting up your equipment as described in the TDS 10XX manual, switching on the TDS system and plugging in the USB cables provided you can start the software. All connected devices and corresponding ports (delay line, data acquisition system, voice coil and external setups) are detected automatically.



Attention:

Since the software has not been tested with USB hubs please connect the USB-ports one by one with the computer using the cables provided to ensure the proper functionality of the software. The basic hardware elements to be detected are the internal delay line and the data acquisition system. If one of them can't be found upon the software will shut down automatically. Additionally, the program will activate the corresponding tab for the imaging or angular scanning unit only if either two linear stages or one rotary stage is connected to the Mini-Din port. Otherwise, the external setups connected to the system are ignored by the software due to an unknown configuration.

If necessary, you can check if there is a proper connection to the delay line, the voice coil and the data acquisition system by opening the device manager and looking for active COM-ports and an active NI device (found under Data Acquisition Devices) as shown in Figure 2. The latter can also be verified using the National Instruments Measurement & Automation Explorer.

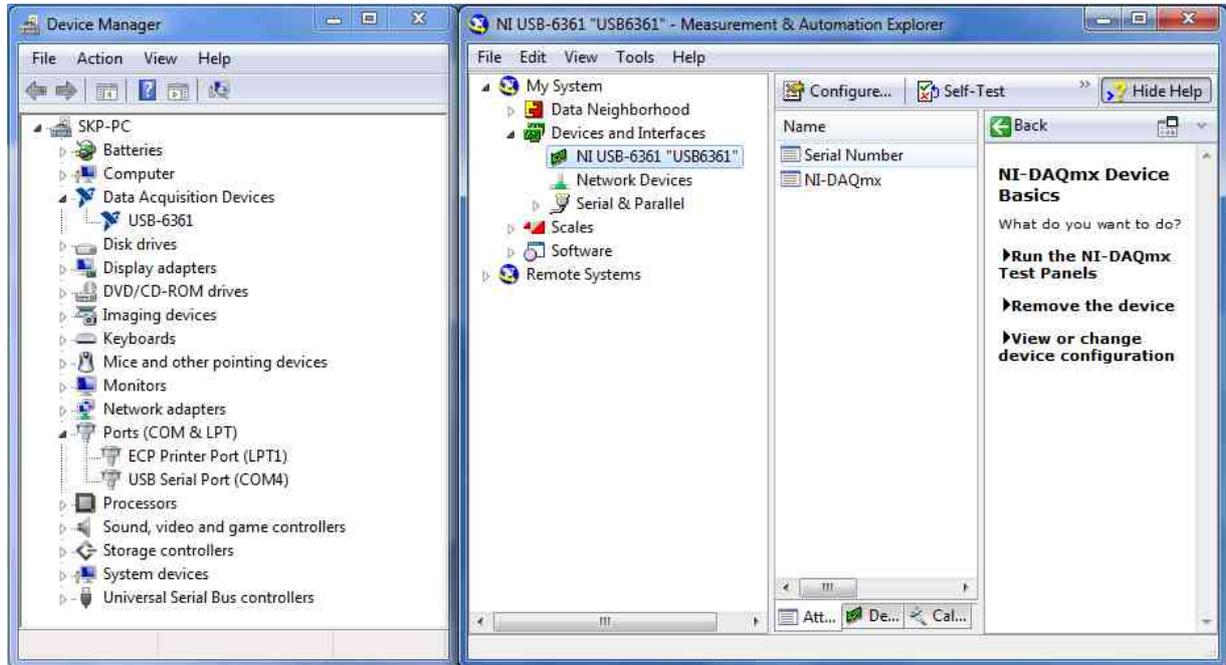


Figure 2: Device manager and National Instruments Measurement & Automation Explorer showing the active COM-ports as well as the connected NI devices.

In case you ordered a system without enclosure and a separate Fast Scan Unit a D-Sub to USB adapter will be provided in order to connect the voice coil controller to the computer (see Figure 3). The data acquisition system and the Zaber linear stage (delay line) are supplied with USB cables which can be hooked up directly to your computer. Similar to a system with enclosure you have to connect the external stages in series with the delay line using the Mini-Din cables provided. Once everything has been set up and plugged in you can start the T3DS software.



Figure 3: D-Sub to USB adapter for connecting the voice coil controller.

1. Start-up

Once you have set up and connected all hardware you can start the software (double-click the T3DS.exe file). At first the software will detect all hardware and may initialize the linear stages as shown in Figure 4. This has to be done if the ZLS was switched off since the software was last used (always the case if you have turned off the spectrometer or disconnected the power supply of the ZLS). Please keep your hands off the stages during this procedure in order to avoid injuries.

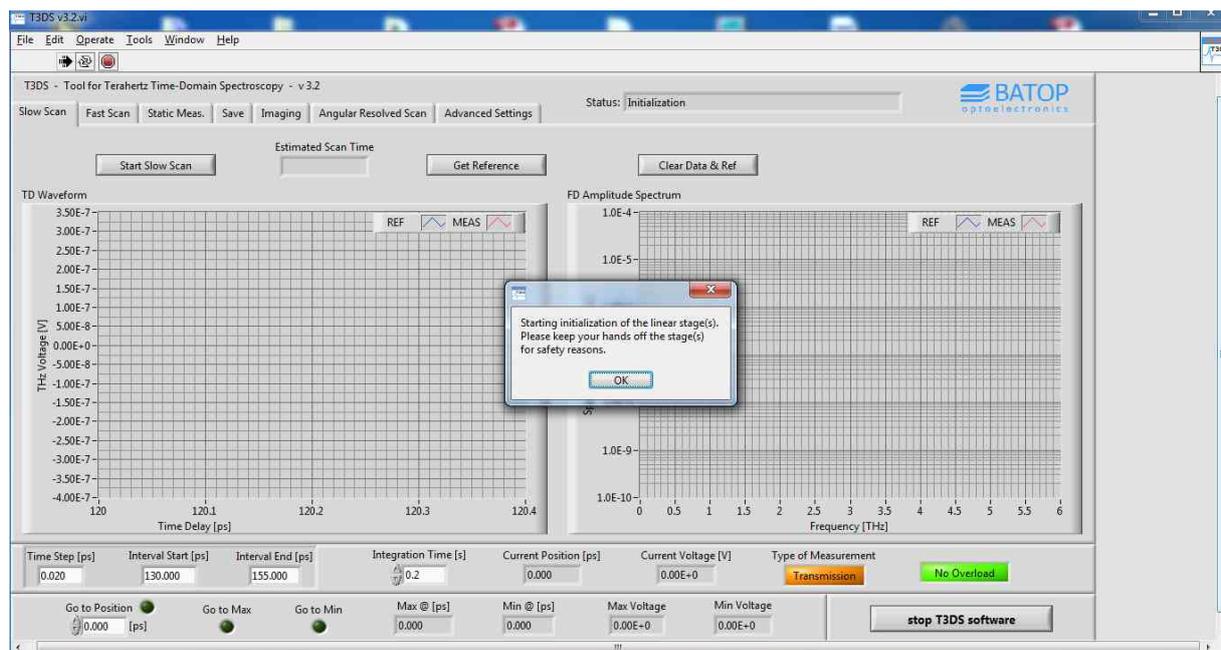


Figure 4: Start of T3DS software with automatic detection and initialization of linear stages.

During initialization (and all other measurements / processes) the program will display the current status at the top of the window. Please wait until the initialization has been executed and the status changes to "idle". Once the software is ready you may set the measurement parameters, start your measurements, change the folder where the data shall be stored, save the results of your measurements, save the current setup / parameters or move the linear stage to a certain position.



Attention:

Please note that the data acquisition system requires a 15 minute warm-up period before any measurements should be started. You may also want the laser to warm up for a few minutes. Therefore, you can switch on the spectrometer and the laser at the same time. Please wait the suggested time period in order to ensure accurate and stable measurements.

2. Input parameters and delay line control

Upon start-up the software loads a set of default values from the T3DS_settings.dat file. These values can be changed within the software but will only be “remembered” if they are stored using the button “save all settings” on the advanced settings tab (see Figure 5). On this tab you can set a few basic parameters that are typically fixed (the frequency and voltage of the AC signal applied to the emitter antenna, the phase for the software lock-in, the input range of the data acquisition unit, the window applied to the time-domain data before the Fast Fourier transformation).



Caution: Always check that the emitter voltage does not exceed the specifications of the antenna. Otherwise your antenna may be damaged permanently.

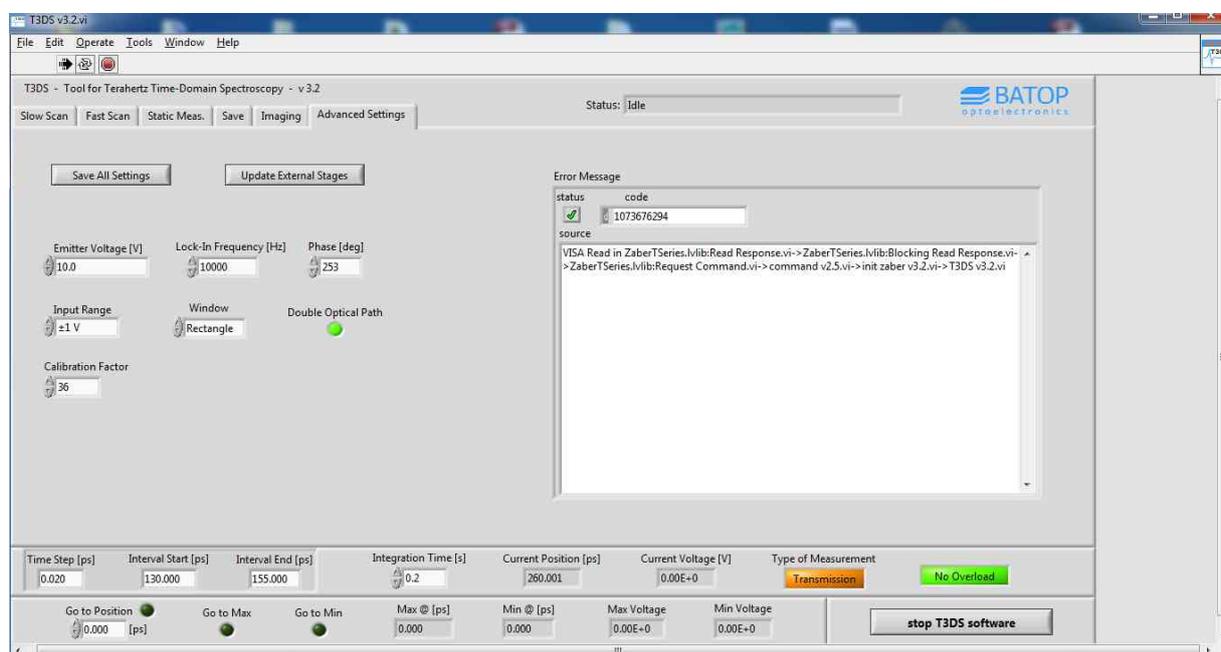


Figure 5: Advanced settings tab with the button to save all settings.

On the advanced settings tab you'll also find a calibration factor. This factor is used to calculate the voltage that the terahertz detector antenna actually delivers. Since there is a preamplifier in the NI-USB device, it will measure a higher voltage internally. You can check if the calibration factor is correct by applying a known square-wave voltage to the input of the NI-USB device while using the static measurement mode (e.g. you can use the AC voltage provided by the NI-USB device for the emitter antenna and scale it down to a few mV using a voltage divider). Make sure that the voltage provided to the device is well below 1 % of the chosen input range because the pre-amplification can be up to 100.

Additionally, there is one button / LED called “double optical path” that tells the software about the hardware configuration. This button indicates that the optical path changes by 2x (or 1x) the length travelled by the internal linear stage (delay line). For a regular THz system with two mirrors mounted to the linear stage the LED has to light up. In contrast, for an all-fiber setup with the emitter mounted to the stage the LED has to be off.

Starting with T3DS v3.2 an additional button can be used in order to automatically detect if any external setups have been connected / disconnected.

At the bottom of the front panel you'll find the basic measurement parameters for the time-domain scan, three buttons to move the internal linear stage, a button to tell the software about the measurement mode (transmission / reflection), current results of a measurement (maximum / minimum and their position) and an indicator for an overload that may have occurred during the measurement.



Attention:

In case of an overload (voltage higher than 90 % of input range), the system will stop the measurement immediately, independent of the measurement mode. You may then switch to a higher input range and restart the measurement. Please choose your input voltage range carefully and do not touch the hardware during the measurement. Otherwise an electric discharge may cause an overload.

For most measurements you will only need to adjust five parameters:

- time step – sets the resolution of the THz pulse in the time-domain which directly determines the maximum frequency in the Fourier-transformed spectrum (the smaller the time step, the higher the maximum frequency); ideally you should choose a time step much smaller than the time delay between the maximum and minimum; we recommend using the time step that the T3DS system came with
- interval start and interval end – set the range of the time-domain scan, which directly correlates to the frequency resolution in the Fourier-transformed spectrum (increasing the interval length results in a higher frequency resolution but in a decreasing spectral bandwidth); make sure your interval covers the reference pulse as well as the pulse(s) when putting in a sample; starting 10 ps before the reference pulse is recommended
- integration time – in order to decrease the noise level we recommend an integration time of 0.5 s or more
- Transmission / Reflection – this button indicates the measurement type and has to be set manually; the type of measurement is saved with the data and it is used in the T3DS calculator software in order to choose the right formulas for calculating the material properties

3. Slow scan measurement

The “Slow Scan” measurement mode on the first tab is the feature used for most standard measurements. If you already know the position of the peak of the THz signal you may chose a small time step (< 0.05 ps), resulting in a broad frequency spectrum. However, if you start searching for a THz signal a time step of ≥ 0.05 ps and a short integration time of 0.05 s are recommended. You can then scan the full distance between start and end position in a reasonable amount of time.

If you want to calculate the maximum distance between start and end position (in picoseconds) it is helpful to know that 1 ps is equal to 300 μm in air (hence, 1000 ps are equal to 300 mm). The optical path on the delay line (ZLS) counted twice for a TDS system because of the light being redirected by two mirrors (see the manual of the spectrometer). As a consequence, a delay line with a travel length of 100 mm results in a maximum distance equal to about 650 ps. Now that this limit is known, you may choose the start and end position accordingly (the absolute limits of the interval have been set by the software upon detection of the delay line).

Once a slow scan measurement is started, the time-domain graph will be filled slowly with the axes being scaled automatically. The current position as well as the measured voltage are updated continuously and shown at the bottom of the window. After the measurement has been carried out the corresponding frequency spectrum is calculated and displayed in the right graph as shown in Figure 6.

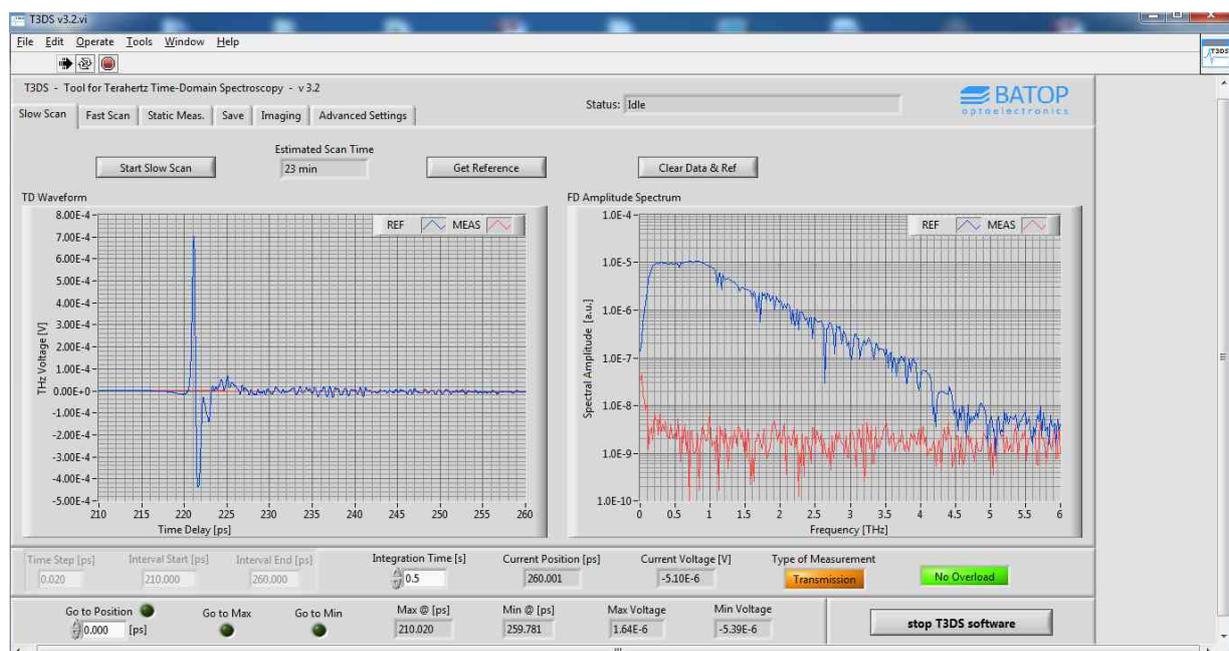


Figure 6: Slow scan tab showing the results of a background measurement (THz path blocked).

Additionally to the collection of sample data you can first measure a baseline and a reference spectrum by using the center button at the top of the tab. If you observe a large offset or some other background signal in the time-domain data, we highly recommend collecting a baseline as it helps to reduce artifacts in the frequency spectrum at low frequencies.

Once the “get reference” button is pressed, the program will ask you if a baseline measurement is required. Depending on your choice the software will start the measurement with the current settings. In order to have the same settings for the reference and sample data, the time step as well as the interval start and interval end will be fixed until the “clear data & ref” button is pressed. However, you may choose a longer integration time for the baseline and reference measurement in order to reduce the noise level.

First, you will be asked to block the terahertz path with a metallic object as shown in Figure 7 (in case you have chosen to acquire a baseline). After the baseline measurement the software will request that you remove this object in order to carry out the reference measurement.

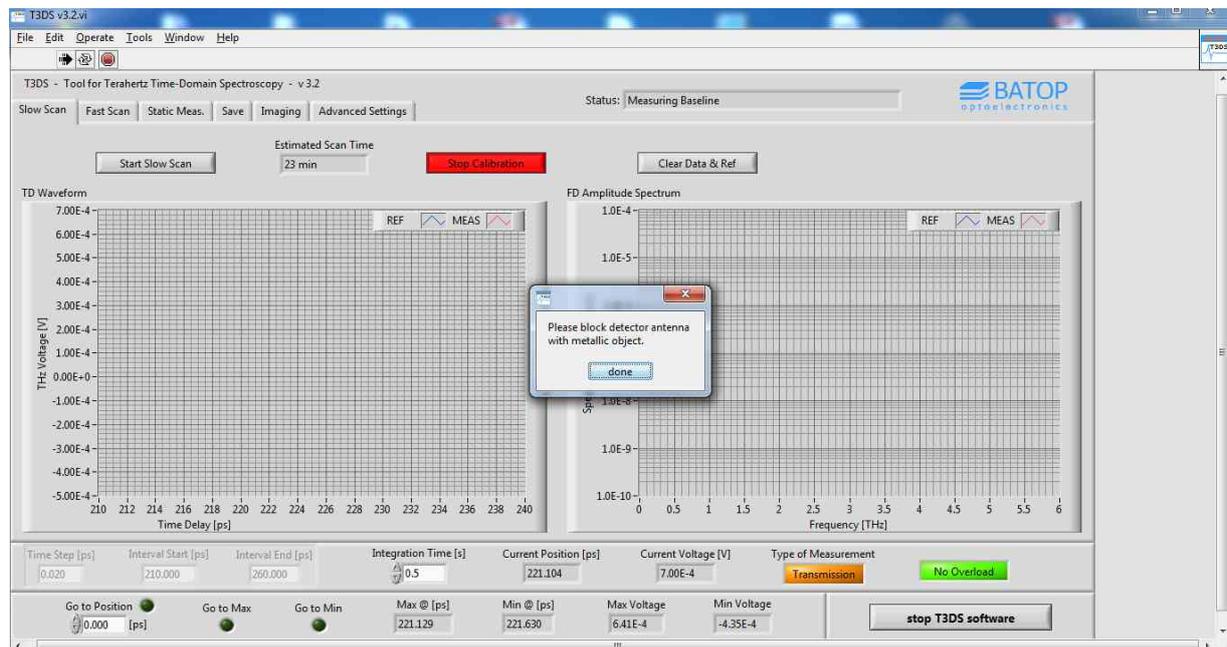


Figure 7: Slow scan tab during calibration procedure (before baseline measurement).

The baseline measurement is used to subtract the background from the reference and sample data before calculating the frequency spectrum. In order to avoid an increasing noise level, the baseline will be averaged using a moving average. Ultimately, the data of the reference measurement in combination with the sample data can be used to calculate the material properties within the T3DS calculator software.



Attention:

If you choose a long measurement interval you may start to see the absorptions lines of the water vapor in the frequency spectrum. Hence, please activate the nitrogen purge upon starting the laser and the TDS system. This ensures that the material data can be calculated correctly and is not influenced by the absorption due to water vapor.

Please note that all graphs can be rescaled after a measurement by clicking on an axis and choosing a desired upper / lower limit. This option works for all graphs in the T3DS software but it may be temporary as the software rescales some of the graphs automatically after / during each measurement. However, even this setting can be activated or deactivated.

4. Fast scan measurement

Complementary to the slow scan mode you may use the fast scan mode to measure a signal more quickly. In this mode of operation a voice coil is used in order to change the length of the optical path more rapidly than with the linear stage. The signal data is read continuously at a high rate until the measurement is stopped and the voice coil ends its oscillation. Because of the very fast data acquisition the signal-to-noise ratio and band width of the frequency spectrum are not as good as for the slow scan measurement. Hence, this mode of operation is not meant for sample characterization but rather as an additional option to optimize the signal strength while having a live picture of the THz pulse (for signal optimization please see the chapter on the static measurement mode).



Attention:

In order to use this mode of operation the computer has to be connected to the controller of the voice coil via USB before start-up of the software. Otherwise the fast scan tab will not show up.

The data obtained during the oscillations can be averaged to improve the SNR and the band width of the frequency spectrum. Two different options are available:

1. Mean – all scans since the last reset are averaged
2. Forget – the new data and the already collected data are weighted using the weighting factor; the lower the weighting factor, the longer it takes till the old data is “forgotten”, thus leading to a lower noise level

Figure 8 shows the data collected during a fast scan measurement. While the current data (red) has a large noise component the averaged data (blue) already begins to look like the data in Figure 6 after a few seconds of data acquisition.

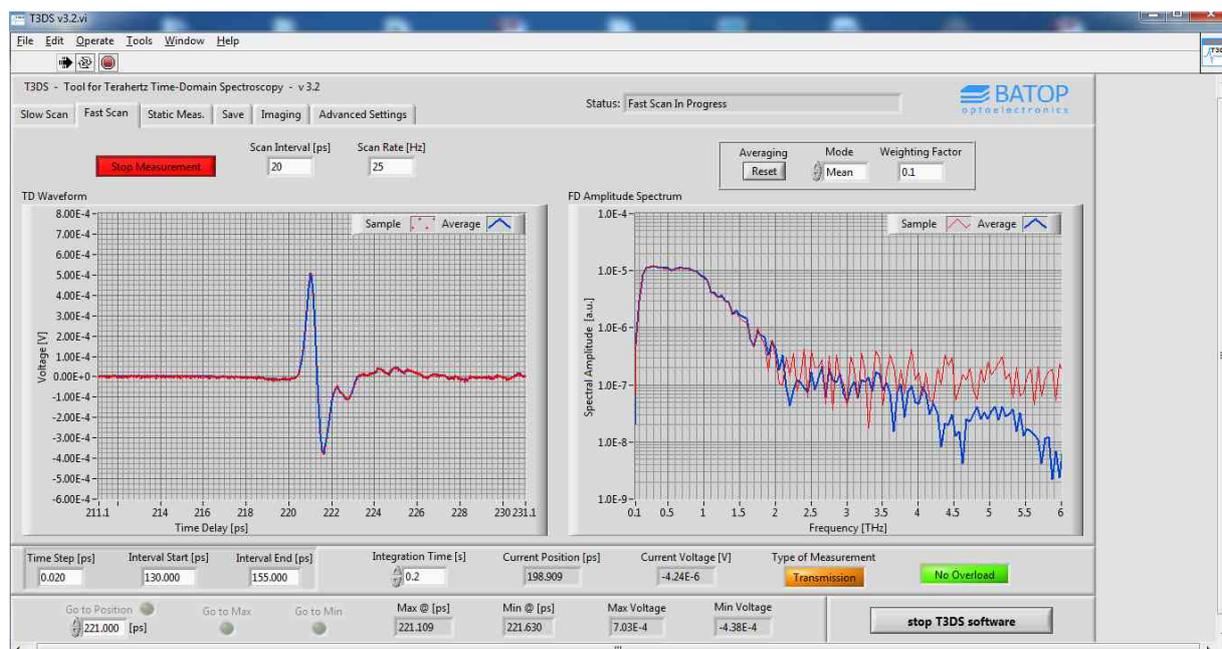


Figure 8: Fast scan tab during the oscillation of the voice coil.

As the acceleration on the mirrors mounted to the voice coil scales with the square of the frequency and linearly with the oscillation magnitude the software limits the scan rate and the scan interval for safety reasons and practical purposes. The software will tell you if the acceleration would exceed 5g or if the resolution on the time scale will be worse than 0.1 ps. A poor resolution on the time scale would lead to the flattening of the THz peak and has therefore to be avoided. For recommended combinations of the scan rate and the scan interval please see the following table.

Table 1: Suggested combinations of scan rate and scan interval for the fast scan measurement mode.

| | | | | |
|--------------------|-----|----|----|----|
| scan rate [Hz] | 100 | 50 | 25 | 10 |
| scan interval [ps] | 5 | 10 | 20 | 40 |

5. Static measurement

Contrary to the slow scan mode the static measurement mode is executed, as the name indicates, with the delay line (ZLS) predominantly staying at the same place. This mode is recommended if you want to improve signal strength by adjusting the optical and terahertz path. Using this mode of operation you can simultaneously watch the signal strength (measured voltage) as you change the alignment of the laser or terahertz beam.

Before you can use this mode, it is necessary that you have found a first (weak) signal using the slow scan mode. Once this has been achieved, you should move the ZLS to the largest peak (maximum or minimum) using the buttons at the bottom of the window. Subsequently, you can start the static measurement mode. At this point you will see the data points building up in the diagram. The lower the integration time the faster the diagram will be filled. Up to 100 points are shown at the same time in order to have a reasonable overview (older data points will not be displayed).

At first you should optimize the phase shift and the timing (ZLS position) by clicking the corresponding buttons at the right hand side (see Figure 9). Please note that for optimizing the timing a fixed time step of 0.02 ps is used. This small time step will suffice even for very narrow peaks.



Figure 9: Static measurement mode showing the signal strength as a function of time after adjustment of the optical and terahertz path (T3DS v3.2).

After the timing and the phase shift have been optimized, you can start fine tuning the optical and terahertz path as described in the spectrometer manual. Because no changes in the phase and only small changes in the timing are expected for transmission setups, it is typically sufficient to press the corresponding button once in a while. However, if you use a reflection setup you may need to use the “optimize timing” button more frequently. If the signal is lost completely you need to stop the static measurement and conduct a slow scan with a length of a few 10 ps. This should be sufficient to find the peak position and return to the static measurement mode. If you do not find a peak but have a rather high offset the phase may need to be changed manually by about 90 degrees. This effect typically occurs if the signal strength is within the same order of magnitude as the offset / background.

The static measurement mode is also used to measure the noise voltage required for determining the dynamic range. To do so please follow these steps:

- Move delay line to THz maximum
- Block the THz beam
- Right click the graph on the static measurement tab and clear the diagram
- Start a static measurement with an integration time of 0.5 s and wait till **at least 1000 samples** have been acquired

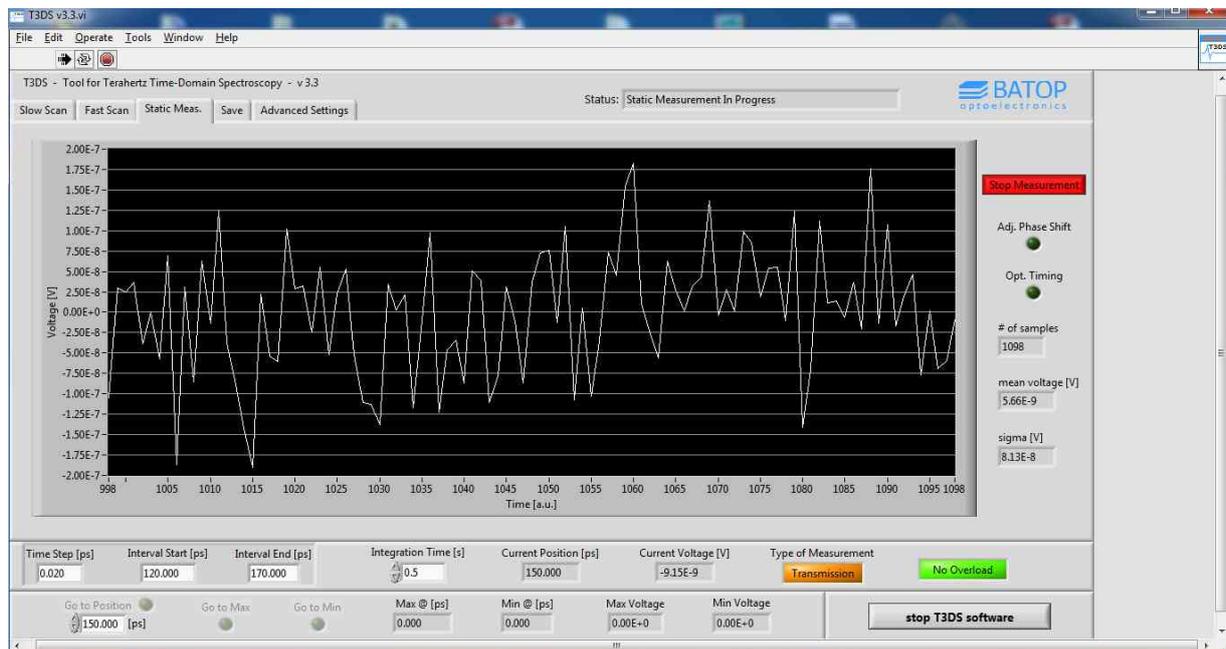


Figure 10: Static measurement to determine the noise voltage (sigma).

At the right hand side you will find the average voltage and sigma – the noise voltage – calculated from all samples collected since the measurement was started. If you choose a smaller sample size you will get a larger noise voltage – the same is true for a shorter integration time.



Attention:

After stopping the measurement you have to right click the graph and choose to scale the x-axis automatically. This option allows you to see whether or not any events such as an electric discharge may have occurred which would render the results useless. Hence, please make sure that the data collected is valid.

Now that the noise voltage is known the dynamic range (DNR) can be determined as follows:

$$DNR = 20dB \times \log \frac{V_{\max}}{\sigma}$$

With σ being the noise voltage and V_{\max} being the maximum absolute voltage of the THz signal. The result can then be compared with the specifications given in the test report.

6. THz Imaging

The imaging mode of operation can be used to record the THz signal not just for one point of an object but for multiple points on a plane. You can choose the pixel size (resolution of the image) as well as the starting point and the size / length of the image in x- and y-direction. Please note, that the second linear stage (connected to the delay line via the side panel) is the designated x-axis, while the third linear stage (last in line) is the designated y-axis (for more information please see the manual on the external stages). In order to get an idea about the time consumption of the measurement, an estimated imaging time is calculated beforehand. This value gives an indication whether you will be dealing with minutes, hours or even days, depending on your measurement parameters.



Attention:

In order to activate this mode of operation two additional linear stages (ZLS) have to be connected to the first stage in a daisy chain configuration before the software is started. Otherwise, this tab will not be activated and you can't use the imaging mode. However, you can also hook up the imaging stage afterwards and click the "update external stages" button on the advanced settings once the software is running.

Since acquiring a 2D array of full THz spectra requires a very long time, it is recommended to reduce the length of one measurement (distance between the start and end position) to a few picoseconds, reduce the integration time and / or increase the time step. You can also choose the start and end position to be identical. In this case only one data point is collected in the time-domain at each point of the 2D scan. Though this setting saves time, the THz signal is reduced to one point and therefore no frequency spectrum can be calculated.

Generally, we recommend making a slow scan first in order to have an idea for the position of the peaks that are characteristic for your sample. Depending on your needs it might be also useful to acquire the baseline and reference data. Additionally, you should check if the object is roughly in plane with the movement direction of the linear stages, especially for the reflection setup. Characteristic peaks should occur at roughly the same time at different xy-positions on the sample. If this is not the case please realign the object. If you choose not to, peaks may be cut off during the imaging measurement or you have to increase the time between start and end position in order to compensate for the tilted object plane. Consequently, this would increase the measurement time considerably.

Once all preparations have been taken care of, you can start the imaging. For a high xy-resolution of the 2D scan it is necessary to use a focused THz beam. Otherwise the beam diameter is in the same range as the diameter of the TPX lens. Hence, only with a focused beam a pixel size in the order of a millimeter makes sense.

During measurements the software displays a picture with one of the following parameters:

- the peak to peak voltage of every scan
- the peak shift between the pulses at different positions (earliest pulse has a black pixel)
- the integrated THz spectrum of every scan

Over time you will see that the image colors change. This happens because the values shown have been normalized. Hence, if a new point sets a new maximum / minimum all pixels are recalculated.

Please note that the choice of the displayed parameter has to be made beforehand and cannot be changed during the measurement. If your time-domain data contains just one point only the measured voltage can be displayed.

After every pixel the slow scan tab will display the time-domain data and frequency spectrum of the last scan. If you abort the imaging measurement you will find that the program will not end immediately but complete the scan at the next position. Depending on your measurement settings this will take a few minutes.

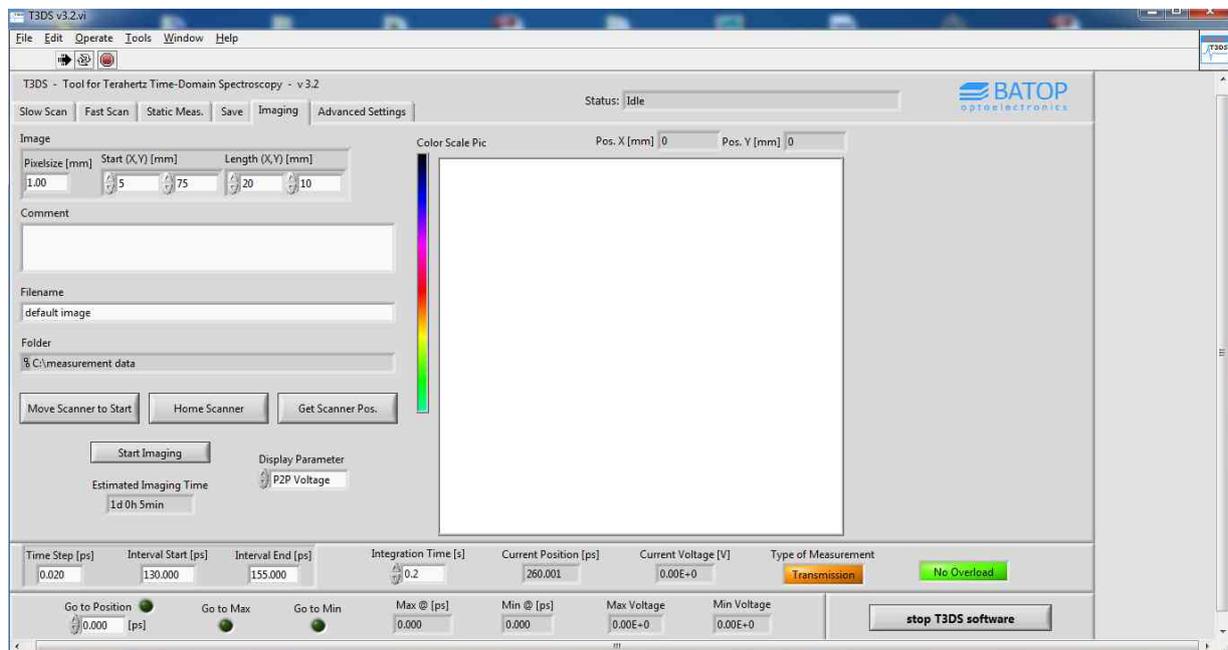


Figure 11: Imaging tab of the T3DS software.

Contrary to regular measurements the imaging mode saves all data while the measurement is being carried out. Hence, you should put in the designated sample name beforehand. For every point in the 2D scan a separate file will be created that contains a similar set of data as for a regular scan. In order to avoid filling the designated data folder with numerous files, a subfolder with the same name as the sample name is created. In this subfolder all files of the 2D scan are saved. The file names of the 2D scan contain the xy-position of each measurement as a prefix in the following way: YYYY_XXXX_sample_name. Additionally, the reference data and the measurement parameters are saved in two separate files within the same folder.

7. Angular resolved scanning

The reflection setups of the imaging unit and the internal sample compartment typically operate at a fixed angle of reflection of about 30° . In contrast, by using the T2T setup it is possible to record the THz signal of a reflected pulse for various angles of incidence. In this setup the sample is fixed at the center of rotation while the antennas move symmetrically to the chosen angles.



Attention:

In order to activate this mode of operation the Zaber rotation stage has to be connected to the first stage in a daisy chain configuration before the software is started (similar to the imaging unit). Otherwise, this tab will not be activated and you can't use the angular scanning mode. However, you can also hook up the rotary stage afterwards and click the "update external stages" button on the advanced settings once the software is running.

On the "angular resolved scan" tab you can choose the interval of interest, move the antennas to a designated angle or align the antennas in a transmission configuration. The angular resolved measurement consists of a number of slow scans, similar to the imaging measurement. Hence, a time estimate is given in order to let you reconsider your settings.



Caution:

The system limits the range of angles that can be set to $15\text{--}90^\circ$ (at 90° the antennas line up in a transmission configuration). This is necessary because the antenna packages may otherwise collide with other parts of the equipment. Hence, we do not recommend using the manual knob while the antennas are mounted to the stage.

In order to optimize the signal there are two possible options. Either you use the transmission configuration or you choose a certain angle of incidence and optimize in a reflection configuration. You have to note that at large angles of incidence part of the THz beam might be cut off / will not be reflected. Once the antenna and the sample have been set up you can record the THz signal, move the delay line to the signal maximum and start the static measurement to improve the signal strength. From there on the signal optimization is similar to any other fiber-coupled setup.



Attention:

Please note that because of the larger distance to the object compared to the imaging setup there is a shift in the THz pulse position of about 230 ps. This is due to the longer focal length of the THz lenses (67 mm instead of 32.5 mm for the standard lenses)

After rotating your sample into the designated position and starting the measurement the system will do a slow scan at every angle. Every time a slow scan has been completed the 3D plot will be updated and the last scan is displayed on the slow scan tab. If you choose to stop the measurement you have to wait till the next scan is completed. Depending on your measurement parameters this may take a few minutes.

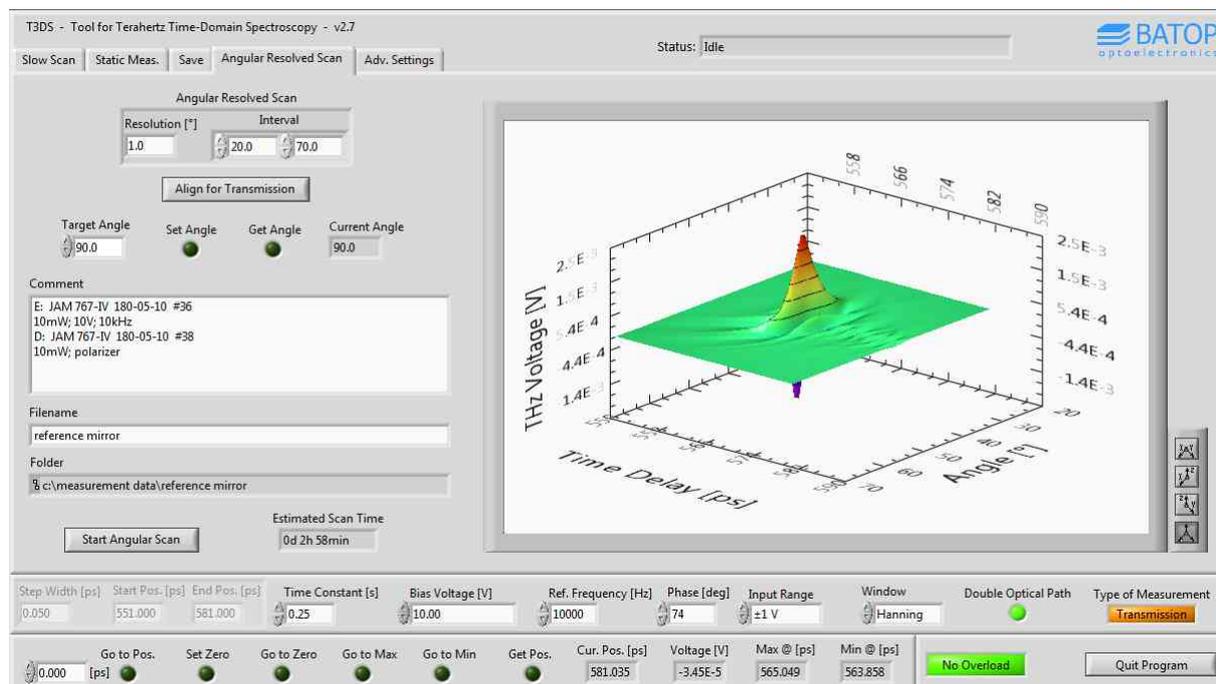


Figure 12: Tab for angular resolved measurements using the rotation stage (image taken from an older T3DS version).

Similar to the imaging mode all data is saved while the angular resolved scan is being carried out. Hence, you should put in the designated sample name beforehand. For every angle a separate file will be created that contains a similar set of data as for a regular scan. In order to avoid filling the designated data folder with numerous files, a subfolder with the same name as the sample name is created. In this subfolder all files of the angular scan are saved. The file names of the angular scan contain the angle of each measurement as a prefix in the following way: XXX.Xdeg_sample_name. Additionally, the reference data and the measurement parameters are saved in two separate files within the same folder.

8. Saving results

The data that was acquired during the last slow scan measurement can be saved using the button “save dataset” on the “Save” tab of the main window. You can choose the folder / path as well as the name of the file. Please note that the software will automatically add the date and time in the following way: YYYY.MM.DD_HH.MM

The time-domain data will be saved in the raw format, giving you the opportunity to analyze the original data before modification, subtract the baseline or compare the sample data and the reference spectrum in more detail. Additionally, the displayed frequency spectra are saved – they therefore include the subtraction of the baseline. The saved file also contains some data about the measurement parameters (e.g. time step, bias voltage, reference frequency, sampling rate, type of window for Fourier transformation). Additionally, you can provide comments that will be put in the file header in order to have more details on the setup or sample.

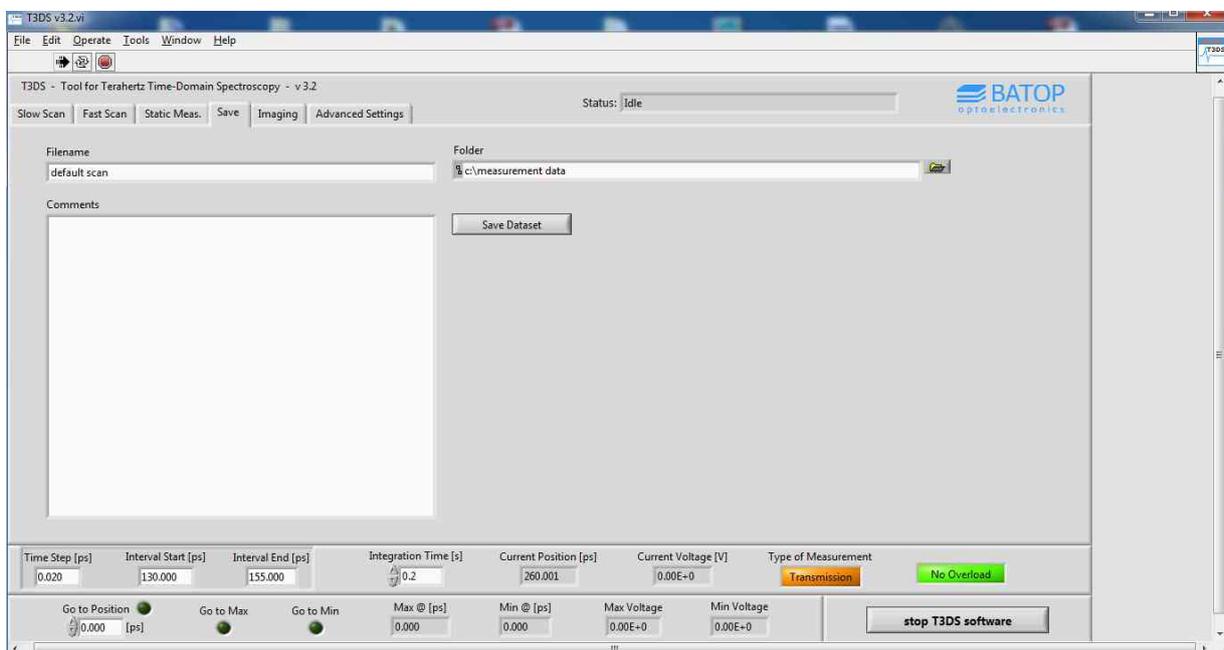


Figure 13: Save tab of the T3DS software.

9. Contact details

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

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