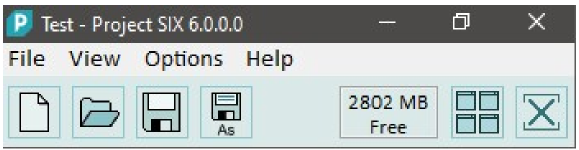
Welcome to WITec Project

Welcome to the WITec Project Data Evaluation Software Help.

Main Window	Load/Save Projects, Options, Help
Working with Projects	Managing Projects and Data, Import/Export, Project Manager
Data Objects	Different Kinds of Data Objects, Memory Requirements
Data Visualization	Handling of Image-, Graph- and Text Viewers
Data Analysis	Drop Action Dialogs, Analysis Software Concepts, Example Analysis
Math	Mathematical Definitions and Descriptions
Program Options	Viewer Defaults, Window Positioning, OpenGL Mode, Memory Strategy
Licensing	Licensing Information, Software Activation

Press the **F1 key** anywhere in the software to open the
context help or browse the Help Menu to open the help contents.

Main Window



Test - Project FIVE
The title of the application shows the current file name and the application name.
If the project has been changed and not saved, an asterisk "*" character is displayed left from the file name.

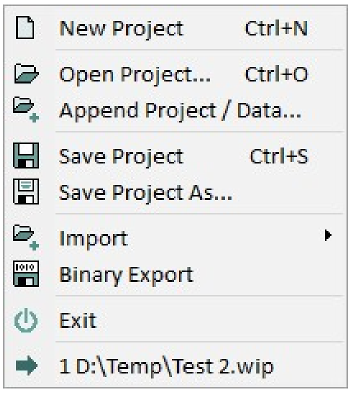
Tool Buttons

- New Project
- Open Project
- Save Project
- Save Project as

- Memory Information
- Reset Viewer Positions
- Close all Viewers

Memory Information
Hovering the memory information with the mouse shows the following memory information:
PM = Amount of free space in physical memory
PF = Amount of free space in page file
AS: Amount of free space in address space in percent
Free: Amount of free space in address space in Megabytes
If the text gets red, you should consider saving the file and creating a new project.

File Menu



New Project
Creates a new, empty project.

Open Project
Opens an existing project from file. See Loading or appending a Project.

Append Project/Data
Appends all data from a selected project file to the current project. See Loading or appending a Project.

Save Project
Saves the current project and overwrites the existing file. See Saving a Project.

Save Project As
Saves the current project and asks the user for a filename. See Saving a Project.

Import (Sub Menu)
See Import Overview.

View Menu

Drop Actions Window
Shows or hides the drop action window.

Cursor Manager Window
Shows or hides the cursor manager window. Here you can see all different cursor positions, e.g. spatial, spectral, CCD counts, ...

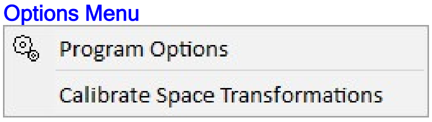
Graphic Export/Editor
Opens the graphic export window which can be used to export a bitmap to a desired image file format.

Close All (Sub Menu)
Here you can close all windows of a certain kind with one click. E.g. close all image viewers.

Reset Viewer Positions
This will realign all your viewer windows.

Point Viewer Window
Only visible in WITec Control.
Shows the point viewer for Raster Sample measurements.

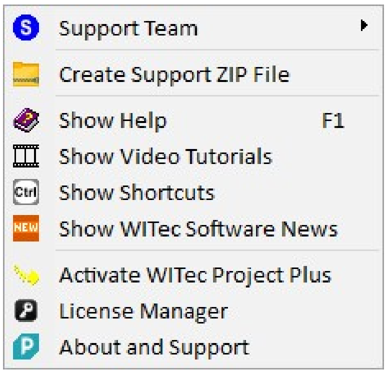
Options Menu



Program Options
Shows the program options window.

Calibrate Space Transformations
For special systems: lets you define a spatial transformation for non-calibrated scan table measurements.

Help Menu



Support Team (Sub Menu)
Contains some special functions that should be used only by a WITec employee.
To send log files and further information to WITec, the sub menu-item "Create Support ZIP File" can be used.

Create Support ZIP File
Collects information about your system and saves it into a compressed ZIP file.
Used for WITec Support Team to help fixing software issues.

Show Help
Shows this help manual. You can press F1 anywhere in the software to open the context help:
The help for the window which has the focus will be shown.
In the Video Window: the help for the component which is under the mouse pointer will be shown.

Show Video Tutorials
Opens the Web page for WITec Video Tutorials.

Show Shortcuts
Shows the shortcut viewer

Show WITec Software News
Shows the latest news about new features in the software.

Activate WITec Project Plus
Shows the WITec Project Plus Activation licensing information.

License Manager
Shows the License Manager. Here you can add new or remove expired licenses.

About and Support
Shows the About Dialog. This will show the following information:

- Software Version Number
- Presence of Plus License
- System ID and Service ID for support
- OpenGL Hardware Acceleration
- Operating System Version
- Memory Information
- Buttons for sending emails to the support.

Working with Projects Overview

A "**Project**" contains measurement data, with all additional information necessary for interpreting the data and further processing; also viewers and their current settings are stored in a Project.

A Project is stored in one .wip file.

Manage Projects

To learn how to manage projects, see Save and Load.

Manage Data

You can manage your Data Objects using the Project Manager.

Export and Import

Several export and import features are available, most of them via the Project Manager.

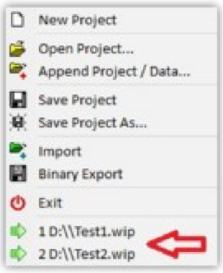
Save and Load

Loading or Appending a Project

You can load a Project by using the main menu "**File > Load Project**".
Note that the currently opened Project will be closed and all data will be lost if you don't save the Project before (a dialog may ask you before).

If you want to add all data from another Project to your currently opened Project you can append it using the main menu "**File > Append Project**".

Loading Recent Projects



You can load recently opened Project files by using the main menu "File" and selecting a file at the bottom of the menu.
Note that files which no longer exist on the hard drive will not be shown here.

Saving a Project

Save the entire Project

You can save your Project by using the main menu "**File > Save Project**" (or "**Save Project As...**") to save all your data on a hard drive or flash drive. All data will be saved in one .wip file (WITec Project File).

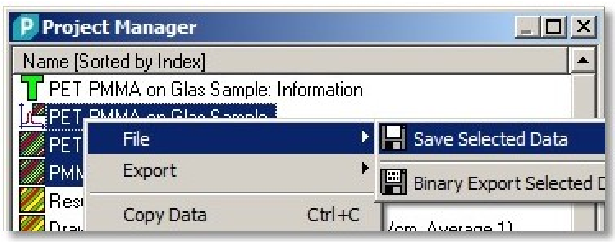
What will be saved when saving a Project?

- All data listed in the Project Manager are saved (including Data Objects that are not currently shown in the Project Manager, e.g. Transformation or Interpretation Objects).
- Viewer windows such as Image-, Graph-, Text- Viewers and their settings.
  The position and size of the Viewer windows are also saved but the windows will be automatically repositioned upon loading. You can deactivate this feature in the Viewer Positioning Options.
- Filter Viewers with their current filters. Preview windows of the filter Viewers are not saved.
  Only the drop action/analysis window is saved with the project.

What will NOT be saved:

- Currently opened **Drop Action Dialogs** and their temporary preview results and Viewers will **NOT** be saved.

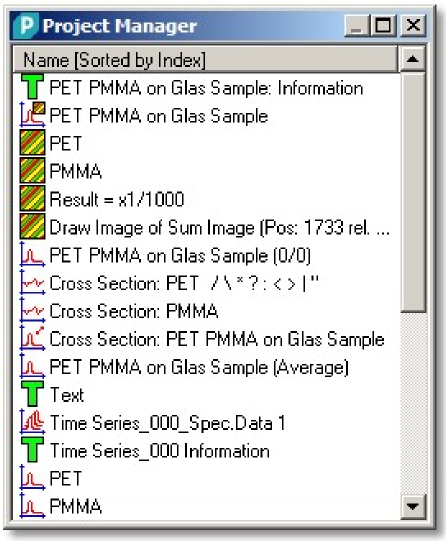
Save or append several Data Objects (not the entire Project)



It is possible to save one Data Object only or even a selection of several Data Objects into a .wid file (WITec Data File). This action can be performed by selecting several Data Objects in the Project Manager and opening the context menu **"File > Save Selected Data"**.

It is possible to append a previously saved data file to the current Project using the main menu "**File > Append Data**".

Project Manager Overview



Description

The Project Manager shows all measurement Data Objects as well as the results from the performed analysis. It is also the tool best suited to organize, visualize or analyze measured data.

The Project Manager is automatically created upon starting the program. Another Project Manager window can be added using the main menu **"Add > Project Manager"**.

Features

- Copy and Paste Data Objects
- Delete Objects
- Rename Caption

You can also show or hide data categories, change the sort mode or start data analysis via the
- Project Manager Circle Menu

To change the default behavior, also have a look at the
- Program options for the Project Manager.

You can also have a look at the context menu:
- Project Manager Context Menu

Data Visualization

To visualize a Data Object, double-click on it or select one or multiple Objects and press the enter key.

For more information see Data Visualization.

Data Analysis

A Data Analysis is performed via the so-called Drop Action dialogs: You can drag and drop one or multiple selected Data Objects from the Project Manager onto one of the drop action buttons. Alternatively start the analysis via the Circle Menu "Actions".

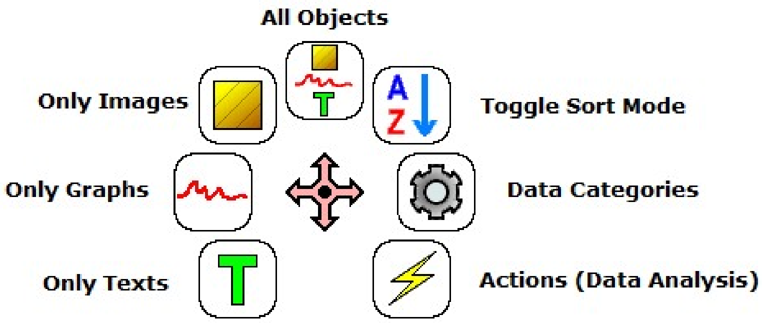
For more information see Data Analysis Overview.

Data Objects

To learn more about the different kind of Data Objects, see Data Objects Overview.

Project Manager Circle Menu

Use the Circle Menu (keep right mouse button pressed) for fast access to certain features:



All Objects
Shows Images, Graphs and Text Objects.

Toggle Sort Mode
Toggles between sort modes:

- Sort by Index (the newest Data Object is at the bottom of the list)
- Sort by Name
- Sort by Category

(You can also click on the "Name" heading of the Project Manager's list box in order to change the sort type.)

Data Categories
Opens a dialog for changing the visibility of data categories and the sort mode.

Actions
If Data Objects are selected, certain actions can be performed with them (see Drop Actions Window).

Only Texts
Shows only Text Objects.

Only Graphs
Shows only Graph Objects.

Only Images
Shows only Image Objects.

Copy and Paste Data Objects

It is possible to copy a selection of Data Objects into the Windows clipboard. You can do this by opening the Project Manager's context menu item "Copy Data" (shortcut Ctrl-C).

Note that the clipboard will be cleared upon starting any WITec Project or WITec Control instance. If you intend to copy data from one instance of WITec Project into another, you must open the second instance before you copy your data.

Simply use the Project Manager's context menu item "Paste Data" (shortcut Ctrl-V) to append the copied data to the Project.

If you would like to copy and paste multiple Objects make sure you paste them in one step; otherwise some analysis features will not work due a missing relation between between the single Objects.

Pasting Bitmaps
It is also possible to copy bitmap data such as screenshots into the Project using the "Paste Bitmap" function. A new bitmap object without transformation will be created and appended to the Project.

Delete Objects

You can delete one or multiple selected Data Objects using the context menu item "Delete Data" (shortcut Delete).

Be careful:

- Deleting Data Objects can NOT be reversed!
- Deleting Transformation or Interpretation Objects that are still used by Image- or Graph-Objects will lead to data loss and therefore inconsistent data; i.e. the data possibly can no longer be used for visualization or analysis. Please only delete Data Objects if you are certain they will no longer be used.

Rename Caption

You can rename a single Data Object by using the context menu item "Rename" (shortcut F2).

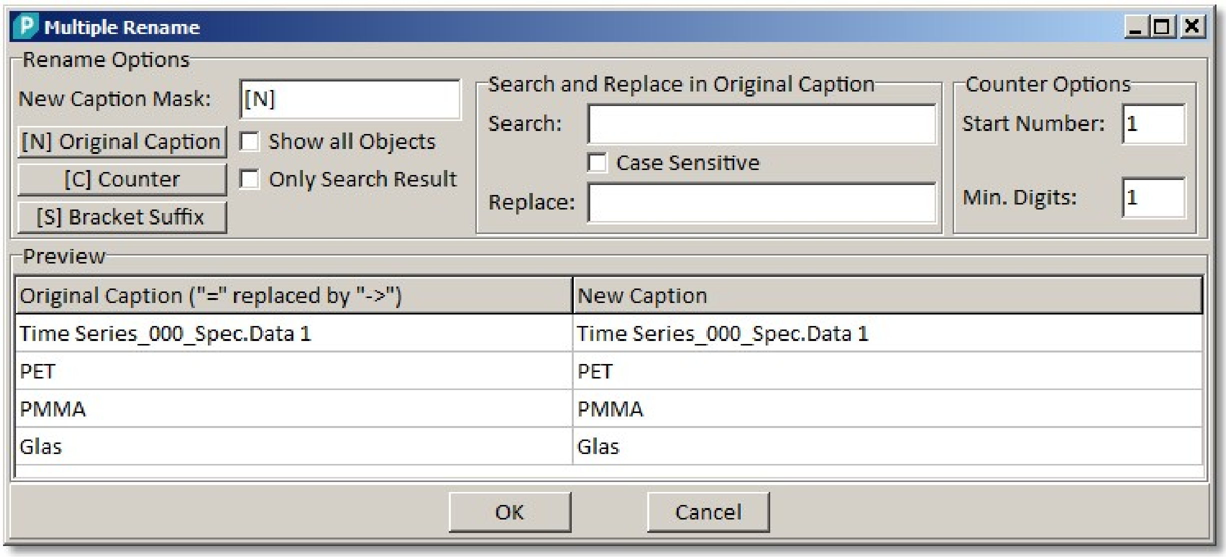
It is also possible to rename multiple Data Objects using the context menu item "Multiple Rename" which will open the Multiple Rename Tool.

Multiple Rename

Description

The Multiple Rename tool allows the changing of the caption/name of multiple Data Objects using a mask or by using search and replace. It's also possible to modify each caption separately after the caption-generation process.

User Interface



Rename Options

New Caption Mask
Enter a mask for the new caption; you can use the following variables for the mask:

[N] Original Caption
Inserts the original caption of the Data Object.

[C] Counter
Inserts a counter value.

[S] Bracket Suffix
Inserts all strings written in brackets in order to preserve information regarding data analysis results.

Show all Objects
If checked, all Data Objects in the complete Project are shown and renamed, otherwise only the selected objects are shown and renamed. Please only use this feature if you use search and replace. Save your project before renaming all data.

Only Search Result
If checked, the new caption mask is only applied on names that contain the current search string.

Search and Replace
Enter a search and replace string in order to replace all occurrences of the search pattern by the replace string.

Counter Options

Start Number
Define the start number for the counter value variable [C].

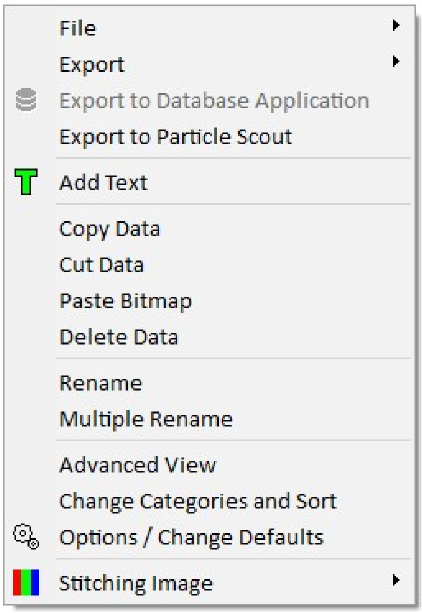
Min # of Digits
Define the minimum number of digits for the counter value (for preceding zeros).

Preview

The preview shows you the original caption and also the new caption which is created by changing the above mentioned Rename Options. You can also change the new caption in the second column to define a completely custom string, but be careful: this string is overwritten upon changing any Rename Options.

Project Manager Context Menu

The Context Menu of the Project Manager contains several management features. It can be opened by clicking and releasing the right mouse button anywhere in the Project Manager.



File
The File Menu enables a selection of Data Objects to be saved in a WITec Project file or exported through the WITec Binary Export file format.

Export
You can export one or multiple Data Objects using one of the export features.

Export to Database Application
Depending on the Database Export Options, the selected single spectrum data object(s) will be opened in an external database application such as the WITec TrueMatch Database Software or ACDLabs. Also see Database Search in WITec Project .

Export to Particle Scout
Exports a Video Image or a Stitching Image to the WITec ParticleScout.

Add Text
Adds a new text data object for adding custom notes.

Copy/Cut/Paste Data
Copies/Cuts/Pastes the selected Data Objects into/from the windows clipboard.

The clipboard is cleared when starting a new WITec Project instance; data is temporarily stored on the hard drive in a WITec Temp Directory. When copying Data Objects the corresponding internal helper Data Objects (e.g. transformations) are also copied automatically.

Delete Data
Deletes the selected Data Objects.

Rename
Renames the currently selected Data Object.

Multiple Rename
Opens the multiple rename dialog which enables to rename multiple Data Object at once.

Advanced View
This will show all internal Data Objects (transformations, interpretations, ...). Please, use this feature only if you really know what you are doing. Deleting internal data objects can lead to data loss or crashes.

Change Categories and Sort
Opens the quick menu for changing Data Categories and the sort mode. You can also click on the Name column header of the project manager to change the category or open that quick menu via the circle menu.

Options / Change Defaults
This will open the program options for the Project Manager.

Data Object Sub Menu ("Stitching Image")
If **one** Data Object is selected, at the bottom of the context menu there is a special sub menu for this Data Object. The contents of this sub menu depends on the kind of data object which is selected.
See Graph Data, Image Data, Bitmap Data

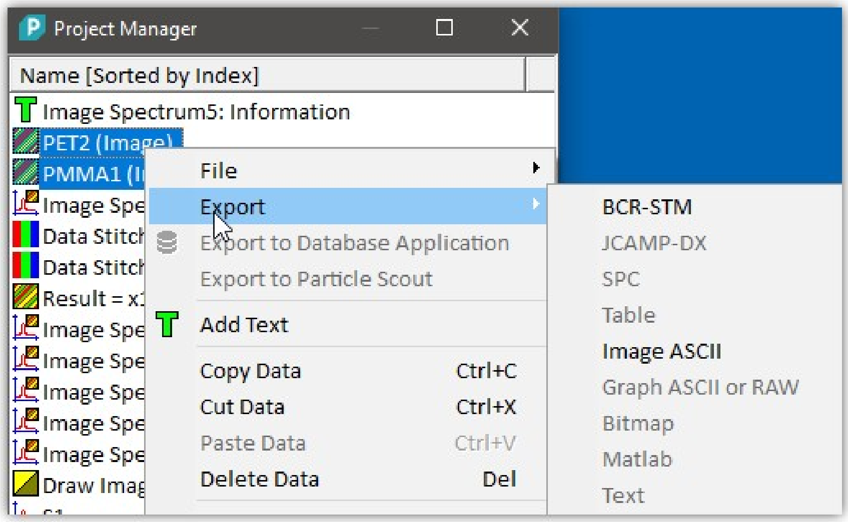
Export Overview

You can export your data in several ways:

- Export Data Objects into one or multiple files or the clipboard.
- Export the current **drawing/bitmap** or even the ASCII data from a **Viewer.**
  See Graph Viewer Export or Image Viewer Export.
- Binary export into the custom and public WITec Binary Export Format.
  To perform a binary export of the whole project, select from the main menu "**File > Binary Export**".
  To perform a binary export of selected items in the Project Manager, open the Project Manager's Context Menu and select "**File > Binary Export Selected Data**".

Export Data Objects

You can export one or several Images, Graphs or Text Data Objects into one or several files using the context menu of the Project Manager:



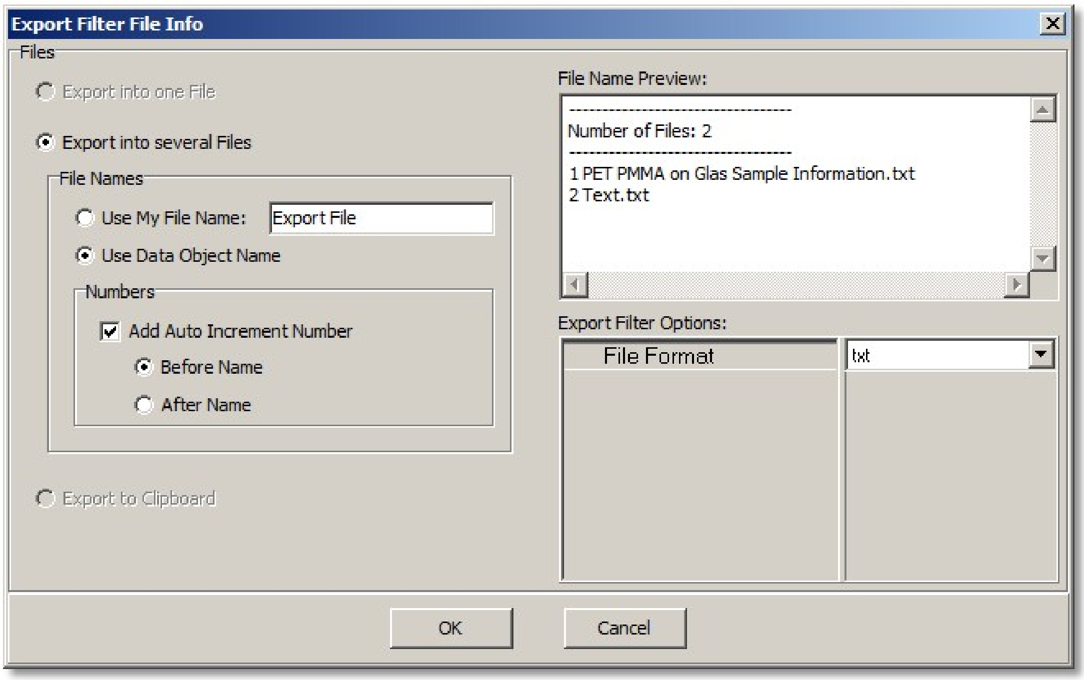
Available Formats

The following export formats are available:

- BCR-STM
- JCAMP-DX
- SPC
- Table (ASCII)
- Image ASCII
- Graph ASCII or RAW
- Bitmap
- Matlab
- Text

Export Dialog

The following dialog will open upon selecting one of the export features:



"Export Into One File":
Exports one or several Data Objects into the same file.
Available for certain export filters.

"Export Into Several Files":
Exports one or several Data Objects into several files.
Available for certain export filters.

"Export To Clipboard":
Exports one or several Data Objects into the clipboard.
Available for certain export filters.

File Names

"Use My File Name":
Define your own file name. All output files will use this file name together with an auto increment number.

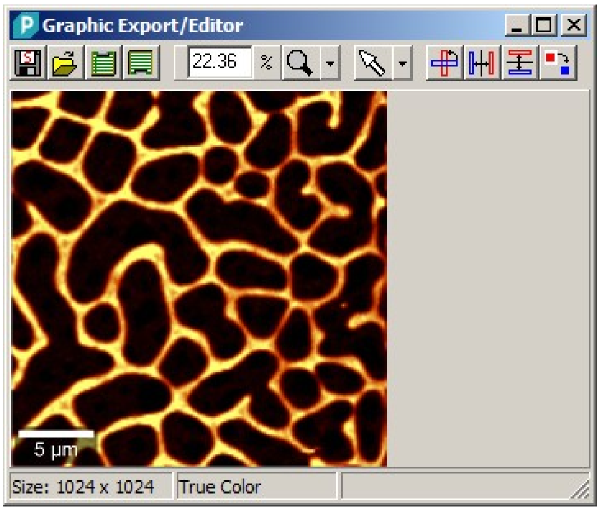
"Use Data Object File Name":
Uses the caption of the exported Data Object as file name.

"Add Auto Increment Number":
If checked, an auto increment number is added to the file name. You can choose between adding the auto increment number before or after the file name. This feature is automatically used when using a single file name.

"File Name Preview":
Shows a preview of all file names that will be exported.

"Export Filter Options":
Here you can change some export options; each export filter uses different export options, i.e. the Text Export function for example has file format options allowing files to be saved in ASCII or Rich Text Format.

Graphic Export / Editor



Description of Tool Buttons (from left to right):

Save Graphic:
Saves the current graphic into a graphic file.

Load Graphic:
Loads graphic from a graphic file.

Copy Graphic To Clipboard:
Copies the current graphic as bitmap into the clipboard.

Copy Graphic From Clipboard:
Copies a bitmap from the clipboard into the graphic editor.

Zoom:
Changes the zoom of the graphic.

Mouse Mode:
- Drag
- Select
- Move Text

Rotate Image:
Rotates the graphic.

Flip Vertical:
Flips the image vertically.

Flip Horizontal:
Flips the image horizontally.

Auto Crop White Border:
Removes the white border around the image.

WITec Binary Export Format

This chapter will describe the WITec Binary Export file format in detail. With this format it is possible to export WITec Project objects (graph, image, bitmap and text objects) as binary data in a straightforward and flexible format. The Binary Export format allows storing multiple objects in one file: Not only the data itself is stored but also all information that is needed to interpret the data, such as dimensions, transformations, additional meta information etc.

In the first section some basic information about the component technique of the file format can be found. In the second part, the file header is described. Finally, the storage of data in general and in particular how WITec Project objects are stored in the Binary format is explained.

Please ask the WITec Support Team for the C header files and example pseudocode!

Structures, Pointers and Data

The WITec Binary Export format consists of several components:

- Structures **(C structs), that simply can be loaded into memory using the structure size. These structures hold information necessary to read the data from the file, e.g. what data is stored in the file, what is the file position of the data, what kind of data is stored and more.**

- File pointers, which are part of all structures and which are 64 bit pointers that point to a file address at which another structure or data value can be found. All file pointers are absolute pointers inside the file.
- Data values, which can have different data types - multiple values are stored sequentially.

It is possible to create instances of structures inside the memory and fill them by reading <structure size> bytes from the file into this structure.

The structures use structure packing, i.e. that small memory gaps are used between the variables to optimize performance and therefore the structure size is not necessarily the sum of all variable sizes (see „Data Structure Alignment" on the web). A pack size of 8 bytes (?) is used in all structures. Most C/C++ compilers use 8 byte structure packing or at least have a possibility to change the pack size (e.g. by a #pragma pack(n) statement).

Header

The exported binary file starts at file position 0x00 with a header - the TWITecBinExportHeader structure - which is the only static positioned structure in this format. Other structures can be stored anywhere in the file and to find the position of the structures their file positions must be read from file pointers first.

```
struct TWITecBinExportHeader
{
    char Identifier[8];
    unsigned int Version;
    TWITecBinExportDataInfo GlobalMetaStringDataInfo;
    FILE_POINTER FirstObjectInfoFilePointer;
};
```

- Identifier:
  Describes a file format identifier (ASCII). When starting an import the identifier should be compared with the identifier in the WITecBinaryExport.h header file (8 bytes without null termination).
- Version:
  Represents an unsigned integer which means the version of this file format. If the version number changes it can be expected that some structures changed and therefore are no longer compatible to older export formats. The read version number should just be compared with the version in the WITecBinaryExport.h header file.
- GlobalMetaStringDataInfo:
  Is a TWITecBinExportDataInfo structure which holds information about a meta information string. The TWITecBinExportDataInfo structure is used for all kind of data (also for strings) and is described later on in this documentation. This meta information string contains global information like:
    - the original file name of the WITec Project file that was opened before exporting the data objects
    - the number of exported data objects
    - the export date.
- FirstObjectInfoFilePointer
  Is a 64 bit unsigned integer which stores the address of the first object information Structure (TWITecBinExportObjectInfo). In order to load the first object info structure a TWITecBinExportObjectInfo structure must be created and filled with the bytes from the file at this file pointer position.

Data

The TWITecBinExportDataInfo structure defines information about data with any number of values and any type of data. So this struct is able to store data of a WITec Project data object as well as strings that are used in other export structures in this file format, e.g. the GlobalMetaStringDataInfo in the header structure.

```
struct TWITecBinExportDataInfo
{
    unsigned __int64 NumberOfValues;
    TWITecDataType DataType;
    FILE_POINTER DataFilePointer;
};
```

- NumberOfValues
  Defines the number of data values.
- DataType
  Defines the data type and therefore the size of one data value. DataType can for example be integer or floating point values, RGB color values or even ASCII characters. TWITecDataType is an enumeration (treated as a 4 byte integer, like all enumerations) which is defined in the WITecDataType.h header file.
- DataFilePointer
  This is a 64-bit file pointer which points to the file position of the first data value. From this file position the data can be loaded by reading <NumberOfValues * sizeof(DataType)> bytes.

String Data

In case of TWITecBinExportDataInfo representing string data (DataType = ASCII) the NumberOfValues variable defines the number of characters (without null termination).
Note: If null-terminated strings are used <NumberOfValues+1> bytes of memory must be allocated and the last byte must be set to '\0'.

Meta Information

The TWITecBinExportHeader structure as well as TWITecBinExportWITecData both have variables for meta information which are struct variables of the type TWITecBinExportDataInfo. These meta information strings contain keys and values - each value string belongs to a key string.
A meta information string is one big string that can store any number of key-value string pairs. The strings are separated from each other by the two control characters CR and LF (Carriage Return 0x0D and Line Feed 0x0A). Therefore two lines represent one key-value pair. The following example shows two keys with their corresponding values:
"ExcitationWavelength[CR+LF]532.0[CR+LF]Caption[CR+LF]My Spectrum Caption[CR+LF]"

Data Objects

To allow storing more than one Data Object into one file this file format uses linked lists that can be jumped through to get all of the exported data objects.

The TWITecBinExportHeader structure exhibits a file pointer to the first TWITecBinExportObjectInfo structure of the linked list. This first object info in turn points to the first WITec Data Object structure as well as to the next object info (which is the info for the second data object).

The TWITecBinExportObjectInfo structure is defined as follows:

```
struct TWITecBinExportObjectInfo
{
      TWITecBinExportObjectType ObjectType;
      FILE_POINTER ObjectFilePointer;
      FILE_POINTER NextObjectInfoFilePointer;
};
```

- ObjectType
  The object type defines which structure is stored in this object. In case of a data object linked list (that starts with the first file pointer in the header structure) this should normally be a TWITecBinExportObjectWITecData, where information about a WITec Project data object like Graph, Image, Bitmap or Text objects is stored. Other object types are described later on in this documentation.
- ObjectFilePointer
  Points to the structure which holds all necessary information about the object.
- NextObjectInfoFilePointer
  Points to the next object info structure, which is also of type TWITecBinExportObjectInfo. If this pointer is null, there is no further data object.

The TWITecBinExportObjectWITecData structure is used to store information about one WITec Project data object:

```
struct TWITecBinExportObjectWITecData
{
      FILE_POINTER FirstTransformationObjectInfoFilePointer;
      TWITecBinExportUnitKind DataUnitKind;
      TWITecBinExportDataInfo DataUnitStringDataInfo;
      TWITecBinExportDataInfo DataInfo;
      TWITecBinExportDataInfo MetaStringDataInfo;
};
```

- FirstTransformationObjectInfoFilePointer
  Points to the first transformation object info which is of type TWITecBinExportObjectInfo. The TWITecBinExportObjectWITecData structure uses a linked list for storing multiple transformation objects. Transformations are important describing the dimensionality as well as the dimension sizes of the data and how all the data values should be interpreted.
- DataUnitKind
  This enumeration describes the data value's unit kind, like e.g. spatial, spectral, temporal etc. Each unit kind has a standard unit, e.g. the spatial standard unit is [µm], the temporal standard unit is [s] e.c. All unit kinds and the standard units for each unit kind can be found in the WITecBinaryExport.h header file.
- DataUnitStringDataInfo
  Normally the data unit string is the standard unit of the respective data unit kind, e.g. "µm". In the case of the unit kind ZValue (that is a free unit), it can be anything, e.g. "CCD cts", "Intensity", "RGB Value" or just "Arbitrary Unit" / "a.u." (can also be a user defined unit via the calculator tool in WITec Project).
- DataInfo
  This struct of the type TWITecBinExportDataInfo stores the information about the main data array of this data object: the number of data values, the data type and a pointer to the file position of the data.

  The number of dimensions and the number of data values in each dimension can either be obtained from the meta information string (see below) or by walking through all transformation informations.
  The first transformation describes the first dimension(s), the second transformation describes the next dimension(s) e.c. A transformation can have one or more dimensions.
  For example, if there is a image graph with 200 x 150 image pixels and 1024 spectral pixels, the first transformation will describe the 1024 spectral pixels, the second transformation will be a spatial transformation that has 3 dimensions with the sizes 200 for X, 150 for Y (and 1 for Z, because there is only one image layer at the moment). So the dimension sizes are 1024, 200, 150, 1.
  Therefore the data is stored in the file as follows:

(x=1, y=1) Value1, Value2, …, Value1024 (end of first spectrum)
(x=2, y=1) Value1, Value2, …, Value1024
…
(x=200, y=1) Value1, Value2, …, Value1024
- End of first line -
(x=1, y=2) Value1, Value2, …, Value1024
(x=2, y=2) Value1, Value2, …, Value1024
…
(x=200, y=2) Value1, Value2, …, Value1024

- MetaStringDataInfo
  This string describes a meta info list that contains several information about the data object.

  The meta string contains some important keys:
  - "WITecProjectObjectType" (required)
    Declares the object type like "Image", "Graph", "Bitmap" or "Text".
    If an object type is known, some things can be assumed, e.g. Bitmap or Image data is (up to now) always two dimensional and Graph data can be four dimensional (e.g. when using an image graph with a spectrum at each image pixel - the fourth dimension is 1 because there is only 1 layer). It can also be assumed that a Image or Bitmap always has one transformation, which is a three dimensional linear spatial transformation. A Graph may have one or two transformations, the first one is for the values in one graph, the second one is a 3D spatial transformation if the graph consists of more than one "Spectrum".
  - "Caption" (optional)
    Stores the caption of the data object, which is also the caption of the data object in the WITec Project "Project Manager".
  - "NumDataDimensions" (required)
    Stores the number of dimensions of the data
  - "DataDimension0", "DataDimension1" […] (required)
    Stores the number of data values in each dimension.
  - "ExcitationWavelength" (optional)
    Stores the excitation wavelenth, if the object is a spectrum (Type "Graph").

Transformations

All WITec Project data objects (except Text objects) need information about the dimensionality and the sizes of each dimension as well as the interpretation of the dimension axes. This information is stored in so called "Transformations" (if the interpretation and transformation is not needed, it may be sufficient only to read the dimensions from the meta string, see above).

The TWITecBinExportObjectWITecData has got a pointer to a linked list of Transformation objects. More precisely, the pointer points to a TWITecBinExportObjectInfo, which in turn points to an object of the type TWITecBinExportTransformationInfo. The object info also has got a pointer to the next object which will be the next object info containing a pointer to the next transformation info.

```
struct TWITecBinExportTransformationInfo
{
      TWITecBinExportUnitKind TransformationUnitKind;
      TWITecBinExportDataInfo TransformationUnitStringDataInfo;
      TWITecBinExportTransformationType TransformationType;
      FILE_POINTER TransformationFilePointer;
};
```

- TransformationUnitKind
  Defines the unit of the axis, which is described by the transformation. See DataUnitKind of TWITecBinExportObjectWITecData.
- TransformationUnitStringDataInfo
  Stores the string of the transformation unit, e.g. "nm". See DataUnitStringDataInfo of TWITecBiNExportObjectWITecData.
- TransformationType
  Defines the type of the transformation (see below).
- TransformationFilePointer
  A file pointer to a structure of a type which is selected by the TransformationType enumeration.

Transformation Types

At the moment, there are two different types of transformations:

- Lookup Table
  A lookup table transformation is a structure of the type TWITecBinExportDataInfo. It stores a value for each data value to define the x position of this data value (so the number of values of the Lookup Table is the number of data values for this dimension).
  E.g. the table stores 1024 wavelength numbers (in [nm]) for each pixel in a spectrum, while the 1024 data values itself represent the intensity in CCD cts for each pixel.
- Linear Transformation

```
struct TWITecBinExportTransformationLinear
{
      unsigned int NumberOfDimensions;
      FILE_POINTER DimensionArrayFilePointer;
```

```
    FILE_POINTER BinOriginFilePointer;
    FILE_POINTER OriginFilePointer;
    FILE_POINTER ScaleMatrixFilePointer;
    FILE_POINTER RotationMatrixFilePointer;
};
```

- NumberOfDimensions

The linear transformation can be one dimensional, e.g. when describing a graph which x axis represents the time or a phase. There is also a three dimensional linear transformation, for example representing 3 spatial dimensions X/Y/Z to define the position, scale and rotation of an image layer. With such a 3D transformation it is possible to calculate the real world position by a given pixel number in each dimension (see below)

- DimensionArrayFilePointer

Points to an unsigned integer array with <NumberOfDimensions> unsigned integers that describe how many data values are stored for each dimension.

- BinOriginFilePointer

Points to a double array with <NumberOfDimensions> double values that describe the pixel numbers that correspond to the real world origin, which is stored in OriginFilePointer

- OriginFilePointer

Points to a double array with <NumberOfDimensions> double values that describe the real world origin for the corresponding BinOrigin

- ScaleMatrixFilePointer

Points to a double array with <NumberOfDimensions*NumberOfDimensions> double values that represent the scale matrix which defines the size of a pixel in each dimension in the real world (normally only the main diagonal is used)

- RotationMatrixFilePointer

Points to a double array with <NumberOfDimensions*NumberOfDimensions> double values that represent the rotation matrix which defines the rotation of the data in all dimensions in the real world.

For example, if there is an single graph 1024 pixels, the origin is 500.0 nm and the bin origin is 512, then the graph values can be interpreted from 0 µm to 1000 µm (assuming the scale is 1.0).

The following formula can be used to get the position of a pixel in the real world:

$$\vec{x} = R \cdot S \cdot (\vec{b} - \vec{b}_0) + \vec{x}_0$$

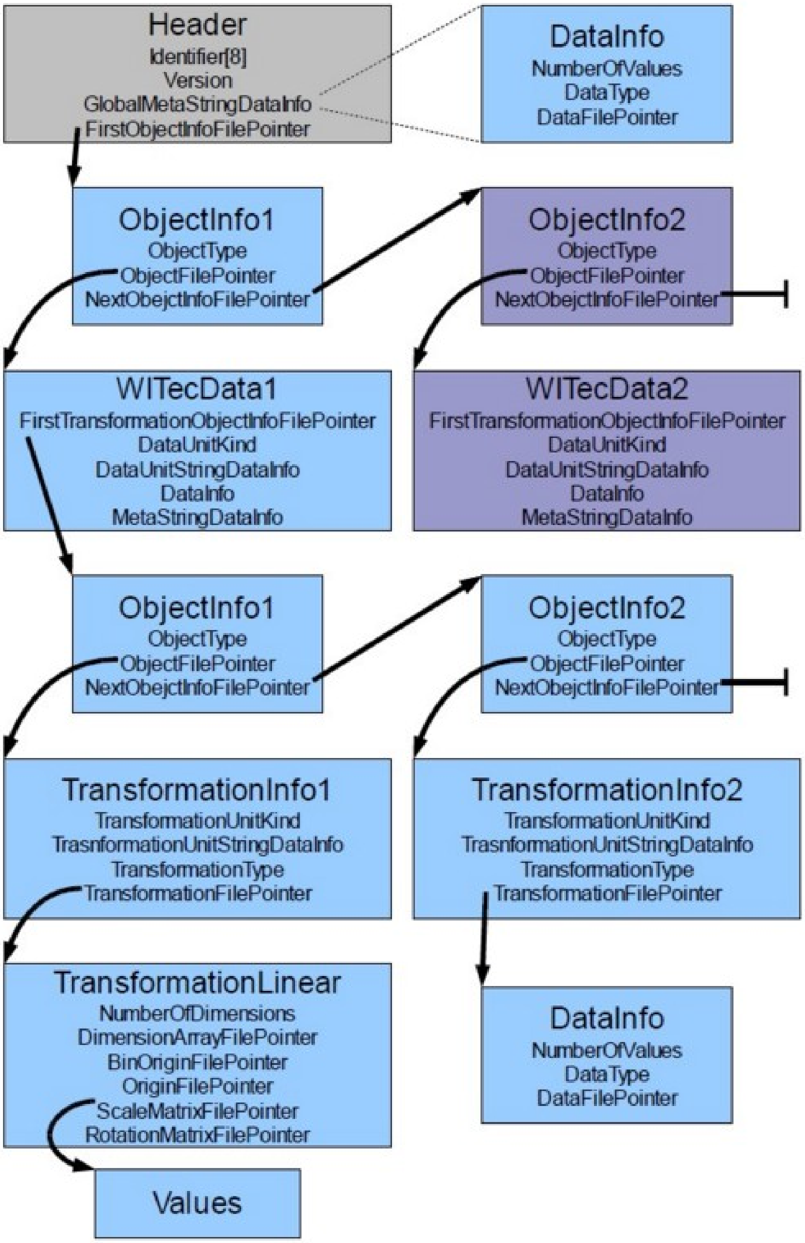
$$\vec{x} = Real\ World\ Position$$
$$\vec{x}_0 = (Real\ World)\ Origin$$
$$\vec{b} = Pixel\ Number$$
$$\vec{b}_0 = (Pixel)\ BinOrigin$$
$$R = RotationMatrix$$
$$S = ScaleMatrix$$

When using a three dimensional (spatial) linear transformation, the memory alignment of matrices is defined as follows:

$$R = RotationMatrix = \begin{pmatrix} Value[0] & Value[3] & Value[6] \\ Value[1] & Value[4] & Value[7] \\ Value[2] & Value[5] & Value[8] \end{pmatrix}$$

$$S = ScaleMatrix = \begin{pmatrix} Value[0] & Value[3] & Value[6] \\ Value[1] & Value[4] & Value[7] \\ Value[2] & Value[5] & Value[8] \end{pmatrix}$$

The following diagram might help understanding the object structure of this file format.



Export BCR-STM

Description

The BCR-STM format is a very old format for storing STM images. It is also used to store AFM images.

Input and Output

Input:
One or multiple (floating point) image objects.

Output:
One or multiple BCR-STM files, each containing one image.

Format

The format contains an ASCII header with some properties of the image. The header size is exactly 2048 characters. The image data is stored as binary data (floating point 32 bits per value).
In general one image is stored in one file, but you can export multiple images in one step into multiple files.

Export JCAMP-DX

Description

The JCAMP-DX format is a pure ASCII file format. It is used to export different kinds of spectra.
There is no clear specification for this format because the header attributes are defined differently by each organization.

Input and Output

Input:
One or several spectral data objects (of any dimension).

Output:
- One or several files, each containing all spectra of each selected data object
- One file containing all spectra of all selected data objects
- All data can be exported to Windows Clipboard

Format

The file contains different header information followed by the spectral values, separated by spaces.
The x-axis values are equidistant.

Export Filter Options

X Unit:
The unit of the exported x-axis data.
Can be: rel. cm 1/cm, 1/cm, nm and µm.

Interpolation Type:
When the x-axis values are converted into equidistant values, the y-axis values have to be interpolated.
This parameter defines how the y-axis values are interpolated.
It can be a cubic spline or a linear interpolation.

Number of Points Type:
The number of exported supporting points / x-values can be defined in 3 different kinds.
For each type there is one parameter that you can change, see the following parameter descriptions.

Oversampling Factor:
The smallest distance between two x-values is calculated. This distance has the number of supporting points defined in this parameter.

Fixed Number of Points:
Defines exactly the number of x-values.

Wanted Data Spacing:
Defines exactly the data spacing (defined in the selected unit) of the x-values.
The actual spacing can vary slightly because the first and the last point of the spectrum are exactly on a supporting point.

Export SPC

Description

The SPC format is a binary file format for different kind of spectra.
See https://en.wikipedia.org/wiki/SPC_file_format

Input and Output

Input:
One or multiple spectral data objects (with any dimension).

Output:
One or multiple files, each containing all spectra of each selected data object

Export Filter Options

X Unit
The unit of the exported x-axis data.
Can be rel. 1/cm, 1/cm, nm and µm.

Export Table

Description

The export table format exports any kind of graph data objects into ASCII Tables.

Input and Output

Input:
One or multiple graph data objects (with any dimension).

Output:
- One or multiple files, each containing all spectra of each selected data object
- One file containing all spectra of all selected data objects (if all objects share the same x-axis values)
- All data can be exported to Windows Clipboard

Format

The first column of the table always contains the x-axis values (in the selected unit).
All other columns are y-values of the graph objects.

Export Filter Options

Column Delimiter:
The separation character used to separate the columns.
Can be Tabulator, Semicolon, Comma and Space.

Text Qualifier:
Column Labels and Column Units are surrounded by the text qualifier.
Can be nothing, quote sign or inverted comma.

Decimal Separator:
Can be point or comma.

Decimal Precision:
Defines the number of decimal places. The exponential format is used, e.g. 1234567 with a precision of 3 is exported as 1.23E+06.

Export Column Label:
Exports the name of the data object as a table header.
If a graph object contains multiple spectra, the spectrum number is added as a suffix.

Export Column Unit:
Exports the unit strings of the x- and y-axis values as a table header.

X Unit:
The unit of the exported x-axis data. Can be all x-units that WITec Project can handle (see Interpretation Data).

Export Image ASCII

Description

The Image ASCII format exports floating point image data objects into an ASCII file.
Can be used as a compatible export from the ASCII export options in older software versions.

Input and Output

Input:
One or multiple (floating point) image data objects.

Output:
- One or multiple files, each containing one image
- Single images can be exported to Windows Clipboard

Format

The ASCII header gives some information about the image like the number of pixels and the scan size and position.
The image values are stored line by line as exponential floating point strings with a selected separator.

Export Filter Options

Export Header
Defines if the header should be exported, or only the image values.

Column Delimiter:
The separation character used to separate the columns.

Can be Tabulator, Semicolon, Comma and Space.
Is not used for column labels and column units, if no text qualifier is used.

Text Qualifier:
Column Labels and Column Units are surrounded by the text qualifier.
Can be nothing, quote sign or inverted comma.

Decimal Separator:
Can be point or comma.

Decimal Precision:
Defines the number of decimal places. The exponential format is used, e.g. 1234567 with a precision of 3 is exported as 1.23E+06.

File Suffix:
Only defines the suffix of the file name.

Export Graph ASCII or RAW

Description

The Graph ASCII or RAW export exports graph data objects into several ASCII or binary files.
Can be used as a compatible export from the ASCII export options in older software versions.

Input and Output

Input:
One or multiple graph data objects.

Output:
Up to 3 files per data object (Header, X-Axis, Y-Axis)

Format

The ASCII header gives some information about the image like the number of pixels and the scan size and position. It is stored in an extra file.
The x-axis and y-axis values are also stored in extra files. The y-axis data first contains the spectral dimension, then the other dimensions (e.g. space line by line). Values are exported as exponential floating point strings with a selected separator or as binary 4-byte floating point values.

Export Filter Options

Export Header:
Defines if the header should be exported into an extra file.

Export X-Axis:
Defines if the x-axis values should be exported into an extra file.

Export Mode:
Graph ASCII - Exports all numbers as ASCII text
Raw as Float - Exports all numbers as 4-byte floating point numbers (binary export)

Text Qualifier:
Column Labels and Column Units are surrounded by the text qualifier.
Can be nothing, quote sign or inverted comma.

Decimal Separator:
Can be point or comma.

Decimal Precision:
Defines the number of decimal places. The exponential format is used, e.g. 1234567 with a precision of 3 is exported as 1.23E+06.

X Unit:
The unit of the exported x-axis data. Can be all x-units that WITec Project can handle (see Interpretation Data).

File Suffix:
Only defines the suffix of the file name.

Export Bitmap

Description

The Bitmap export allows to export color bitmap data objects into the graphic file formats PNG, BMP, JPG.
The maximum bitmap size is 4096 x 4096 pixels.

Input and Output

Input:
One or multiple color bitmap data objects.

Output:
One or multiple graphic files.

Export Filter Options

Keep Aspect Ratio:
If not set, the pixel size in the result image are quadratic.
If set, the color bitmap transformation is taken into account. This makes sense if the scan size ratio is different to the pixel size ratio.

File Format:
Can be .bmp, jpeg, png.

Export MATLAB

Description

The MATLAB export format exports any kind of graph data objects into a MATLAB structure or DSO format.
The export is limited to 2 GB of data. More data can be exported using the Graph ASCII or RAW Export.

Input and Output

Input:
One or multiple graph data objects (with any dimension).

Output:
One or multiple files, each containing all spectra of each selected data object

Format

Depending on the MATLAB export type "DSO" or "Matlab Structure", the format is one of the following.

DataSetObject (DSO 6.0)

This format is specified by "Eigenvector". A MATLAB package can be downloaded there.
See http://www.eigenvector.com/software/dataset.htm
It contains MATLAB functions, that can be used on the DSO data format. It is for free (BSD-License).
It only supports simple functions for the display of data.
The DSO is created as a MATLAB object mat-file, see http://www.mathworks.com/help/pdf_doc/matlab/matfile_format.pdf
A description of each DSO field is available under http://wiki.eigenvector.com/index.php?title=DataSet_Object
or in the downloaded package.

DSO Fields:

Name:
Contains the graph object name in the WITec Project project manager.

Type:
The type of the graph object. "image" if its an 2D graph object, otherwise "data".

Date:
Current date as yyyy.mm.dd hh.mm.ss

ModDate:
Same as Date. Will be changed if MATLAB changes the file.

ImageSize:
Null for 0d and 1D graph objects, SizeY and SizeX for 2D graph objects

ImageMode:
1 if its a 2D graph objects, otherwise 0

Data:
Contains the graph data. For single graph objects the graph data is saved as a row vector.
For 0D and 1D graph objects (e.g. / time series / line scan) the graphs are saved as sequential row vectors.
The data is stored in a matrix with <NumberOfSpectra> rows and <SpectrumSize> columns.
For 2D graph objects the matrix has SizeY*SizeX rows and <SpectrumSize> columns.

The image columns are stored sequentially, then the rows.

Label:
Is always null.

AxisScale:
The graph scale is stored in a cell with 2x2 elements. For this the X Unit setting in the export filter options is used.
For 1d graphs (e.g. time series), the cell element (1,1) contains the series scale (e.g. the time scale). The cell element (1,2) is the string of the unit of the series (e.g. "seconds").
For single spectra the cell elements (1,1) and (1,2) are empty.
The cell element (2,1) is always the graph x-axis scale, the cell element (2,2) is the unit string of the x-axis scale (e.g. "rel. 1/cm").

ImageAxisScale:
The image axis scale is stored in a cell with 2x2 elements. A standard unit is used.
For 0D and 1D graph objects the elements are empty. For 2D graph objects element (1,1) contains the scale of the image columns, element (2, 1) contains the scale of the image rows, element (1, 2) and (2, 2) contain the unit string of the x/y scale (e.g. µm).

Title:
Is always null.

Class:
Used for MATLAB to recognize the file as a DSO format. Contains "dataset".

Include:
Used to set an image- or graph mask to tell MATLAB which pixels should be used. WITec Project always sets all pixels in the mask.
The field is a cell with 2 elements. Element 1 has the image mask as row vector with <SizeY*SizeX> elements.
Element 2 has the graph mask as row vector with <SpectrumSize> elements.

ClassLookUp:
Is always null.

AxisType:
Can be used to characterize the spectral axis scale (data will not be changed by this). Can be "none", "continuous" and "discrete".
WITec Project uses "none".

ImageAxisType:
See AxisType, but for the image axis scale.

Description:
Is always null.

UserData:
Is always null.

DataVersion:
WITec Project uses DSO 6.0, so "6.0" is written.

History:
Contains "Created by WITec Project (Version XXX)".

UniqueID:
For each graph object a unique ID is generated from the caption + date.

Usage of DSO in MATLAB

The download package contains a folder @dataset. To open an exported DSO file in MATLAB, the file must be in the same folder than the folder @dataset (or the file must be a sibling of this folder).
In the MATLAB window "Current Folder" the file can be double clicked or via command "load('filename_dso-file').
MATLAB shows it then in the MATLAB window "Workspace". You can list the DSO fields in the command window of MATLAB by entering the DSO file name.
You can use the fields by using "dso-filename.fieldname". Fields with multiple values like AxisScale can be addressed via e.g. "dso-filename.axisscale{2,1}". For the DSO the functions in the folder @dataset can be used.
There is a documentation on http://wiki.eigenvector.com/index.php?title=DataSet_Object_Methods

MATLAB Structure

This is a custom structure format defined by WITec.
The fields Name, Date, Data, AxisScale, ImageSize, ImageAxisScale are the same like the DSO format.

Usage in MATLAB

You can double-click the exported file in the "Current Folder" window of MATLAB or via the load command.
The structure is shown in the MATLAB window "Workspace". You can double-click on the structure to show the fields, they can also be double-clicked.

The fields "date", "data" and "imagesize" are matrices, which can be addressed using brackets, e.g. structurename.data(1,:) returns the first line of data that means the first spectrum of the dataset.
The fields "axisscale" and "imageaxisscale" are cells and are addressed via curly brackets, e.g. structurename.axisscale{2,1} returns the line vector of the spectral axis scale.
You can also press the tabulator-key to show the possible fields after typing "structurename." .

Here are some examples to plot graph objects in MATLAB. Just copy one of the functions in the gray boxes into a MATLAB file (filename.m) and load it in MATLAB:

```
function PlotGraph(aGraph, aImagePosition, aYLim)
% Plots a single graph from the whole dataset in a 2d coordinate system.
% aGraph: struct from WITec Project Export
% aImagePosition: x- and y- image coordinates of the graph, e.g. [30,50] means x=30, y=50
% aYLim: lower and upper limit of the spectral y-axis, e.g. [-5,250] plots the graph in a range of -5 to 250
% Note that the Rayleigh-Peak may make your important raman peaks invisible due to automatic scaling.

aSpectrum = aGraph.data(aImagePosition(1) * aGraph.imagesize(1) + aImagePosition(2),:);
aXAxisscale = aGraph.axisscale{2, 1};
plot(aXAxisscale, aSpectrum);
aXLabel = sprintf('[%s]',aGraph.axisscale{2, 2});
xlabel(aXLabel)
ylabel('CCD cts.')
ylim(aYLim)
aTitle = sprintf('%s (y = %i, x = %i)',aGraph.name, aImagePosition(2), aImagePosition(1));
title(aTitle)
end
```

```
function PlotAverageGraph(aGraph, aYLim)
% Plots the average spectrum
% aGraph: struct from WITec Project Export
% aYLim: lower and upper limit of the y-axis

aAverageSpectrum = mean(aGraph.data);
aXAxisscale = aGraph.axisscale{2, 1};
plot(aXAxisscale,aAverageSpectrum)
aXLabel = sprintf('[%s]',aGraph.axisscale{2, 2});
xlabel(aXLabel)
ylabel('CCD cts.')
ylim(aYLim)
aTitle = sprintf('%s (Average Spectrum)',aGraph.name);
title(aTitle)
end
```

```
function PlotImage(aGraph)
% Plots the intensity image
% aGraph: struct from WITec Project Export

aSizeY = aGraph.imagesize(1);
aSizeX = aGraph.imagesize(2);
aSumImage = sum(aGraph.data,2);
aImage = zeros(aSizeY,aSizeX);
for x=1:aSizeX
for y=1:aSizeY
aImage(y, x) = aSumImage((x - 1) * aSizeY + y);
end
end
figure
aXAxisScale = aGraph.imageaxisscale{2, 1};
aYAxisScale = aGraph.imageaxisscale{1, 1};
imagesc(aXAxisScale, aYAxisScale, aImage)
%colormap(gray)
colormap(hot(256))
aTitle = sprintf('%s (Intensity image)',aGraph.name);
title(aTitle)
aXLabel = sprintf('[%s]',aGraph.imageaxisscale{2, 2});
xlabel(aXLabel)
aYLabel = sprintf('[%s]',aGraph.imageaxisscale{1, 2});
ylabel(aYLabel)
end
```

```
function SpectrumToImage(aGraph, aSpectralPosition)
% Plots the intensity image of the specified spectral position
% aGraph: struct from WITec Project Export
% aSpectralPosition: spectral position

aSizeY = aGraph.imagesize(1);
```

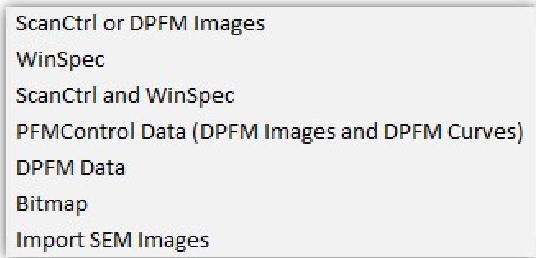
```
aSizeX = aGraph.imagesize(2);
aSumImage = sum(aGraph.data(:,aSpectralPosition),2);
aImage = zeros(aSizeY,aSizeX);
for x=1:aSizeX
for y=1:aSizeY
aImage(y, x) = aSumImage((x - 1) * aSizeY + y);
end
end
figure
aXAxisScale = aGraph.imageaxisscale{2, 1};
aYAxisScale = aGraph.imageaxisscale{1, 1};
imagesc(aXAxisScale, aYAxisScale, aImage)
%colormap(gray)
colormap(hot(256))
aTitle = sprintf('%s (Intensity image)',aGraph.name);
title(aTitle)
aXLabel = sprintf('[%s]',aGraph.imageaxisscale{2, 2});
xlabel(aXLabel)
aYLabel = sprintf('[%s]',aGraph.imageaxisscale{1, 2});
ylabel(aYLabel)
end
```

Export Filter Options

Matlab Export Type:
Can be DataSetObject (DSO 6.0) or Matlab Structure.

X Unit:
The unit of the exported x-axis data. Can be all x-units that WITec Project can handle (see Interpretation Data).

Import Overview



ScanCtrl or DPFM Images
Imports Data from the old WITec software "ScanCtrl".

WinSpec
Imports Data from the WinSpec software.

ScanCtrl and WinSpec
Imports Data combined from ScanCtrl and WinSpec.

PFMControl Data (DPFM Images and DPFM Curves)
Imports PFM Data.

DPFM Data
Imports DPFM Data. The dialog allows you to select in detail the DPFM curves that you would like to import.

Bitmap
Imports one or multiple bitmap files from hard drive as new bitmap data objects to the project.

Import SEM Images (only available if license present)
Imports TIF or PNG image files that were created using a scanning electron microscope.
TIF must have the format 8/16-bit gray scale or 8-bit color.

Data Objects Overview

Data Categories

WITec Project and WITec Control feature several Data Object categories. In general, only Image, Graph, Bitmap and Text objects are required.

- Image Data

- Bitmap Data
- Graph Data
- Text Data

Internally, the following Data Object categories are used (and can be made visible for advanced users):

- Color Profile Data
- Transformation Data
- Interpretation Data
- Cursor Data
- Filter Data (deprecated)

Common Data Properties

All different kind of Data Objects contain of:

- **A data caption / name**
  Can be changed by the user; has no effect on the operation of the software
- **A unique Index** (used for "Sort by index" in Project Manager)

Some Data Objects are linked to other Data Objects in order to use shared information, e.g. two images from different channels that were created by the same measurement may link to the same spatial transformation

Data Objects are created by WITec Control during measurements, via a Drop Action Dialog or the Filter Viewer/Filter Manager in WITec Project/Control.

Memory Consumption

Please also have a look at the Data Object Memory Consumption in order to be able to estimate the size of a measurement.

Graph Data

Graph Data Objects contain:

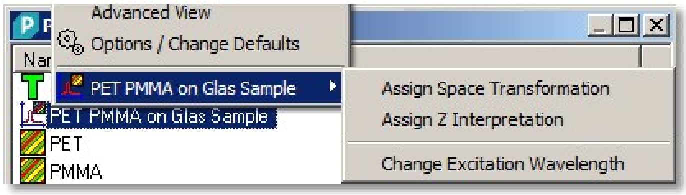
- the graph data: a 3D array of floating point numbers; the three dimensions represent the following values:
  a. SizeGraph ("spectral" dimension, typically 1024 or 1600 pixels for spectra)
  b. SizeX (= 1 for single spectra, > 1 for image graph objects or line graph objects)
  c. SizeY (= 1 for single spectra or line graph objects, > 1 for image graph objects)
- a link to a spatial transformation (defines the graph object's position and size in physical space)
- a link to a z-value interpretation (defines the unit of the graph values. This can be virtually anything, e.g. "CCD cts")
- a link to an x transformation (defines the graph object's x-axis scale, e.g. pixel to wave numbers)
- a link to an x interpretation (defines the unit of the x-axis, e.g. rel. 1/cm - can be switched to other units, see Interpretation)

Different kinds of Graph Data Objects:

- **Single Spectrum:**
  Contains 1 spectrum, SizeX = 1, SizeY = 1;
  e.g. created by single spectrum measurement or average graph drop action.
- **Line Graph Object:**
  Contains n spectra, SizeX = n, SizeY = 1;
  e.g. created by the line scan, time series or the cross-section drop action.
- **Image Graph Object:**
  Contains n*m spectra, SizeX = n, SizeY = m;
  e.g. created by the image or large area scan.

Graph Objects are visualized in the Graph Viewer, which can be opened by double clicking the object in the Project Manager.

Data Object Context Menu:



Assign Space Transformation:
This feature allows you to assign a space transformation to the selected Graph Data Object.
Please only use this feature if you exactly know what you are doing.

Assign Z Interpretation:
This feature allows you to assign a z-interpretation (defining the value unit) to the selected Graph Data Object.
Please only use this feature if you exactly know what you are doing.

Change Excitation Wavelength
If the Graph Data Object contains spectral data, it's possible to change the excitation wavelength, see Interpretation Data (Spectral Interpretation).

Image Data

Image Data Objects contain:

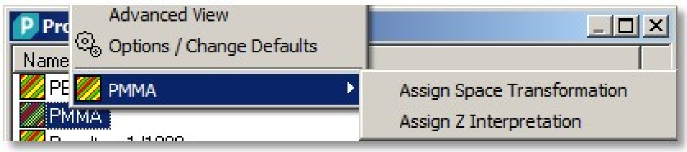
- the image data: a two-dimensional array of floating point numbers
- a link to a spatial transformation (defines the image's position and size in physical space)
- a link to a z-value interpretation (defines the unit of the image's values. This can be virtually anything, e.g. "CCD cts")

Examples for Images:

- Sum Image (one image pixel value is the CCD count sum of a number of CCD pixels of the corresponding spectrum)
- T-B Image (one image pixel value is the voltage of the T-B A/D Converter)
- Mask Image (one image pixel value is 0.0 or 1.0, the image is used as a mask)

Images are visualized by the Image Viewer using a false color mapping (Color Profile). The viewer can be opened by just double clicking the object in the Project Manager.

Data Object Context Menu:



Assign Space Transformation:
This feature allows you to assign a space transformation to the selected image;
please only use this feature if you exactly know what you are doing.

Assign Z Interpretation:
This feature allows you to assign a z-interpretation (defining the value unit) to the selected image;
please only use this feature if you exactly know what you are doing.

Bitmap Data

Bitmap Data Objects contain of:

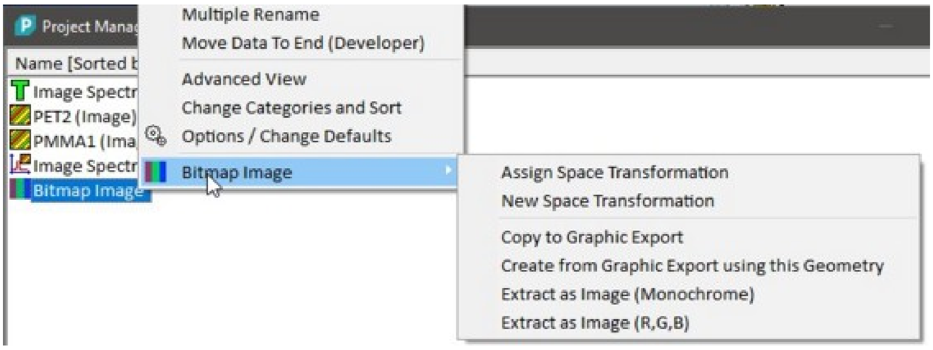
- the bitmap data: a two-dimensional array of RGB color values (24 bit)
- a link to a spatial transformation (defines the bitmap's position and size in physical space)

Examples for Bitmaps:

- Video Image
- Imported Windows Bitmap
- Texture Bitmap created by the Image Viewer

Bitmaps are visualized in the Image Viewer, which can be opened by just double clicking the object in the Project Manager.

Data Object Context Menu:



Assign Space Transformation
This feature allows you to assign a space transformation to the selected bitmap;
please only use this feature if you exactly know what you are doing.

New Space Transformation
Creates a new custom space transformation and assigns it to this bitmap.

Copy to Graphic Export
Copies the bitmap to the Graphic Editor / Export window.

Create from Graphic Export using this Geometry
Creates a new bitmap object from the Graphic Export window and uses the transformation / geometry from this bitmap.

Extract as Image (Monochrome)
Create a monochrome floating point image (Intensity = 0.299 * R + 0.587 * G + 0.114 * B).

Extract as Image (R, G, B)
Create 3 Floating Point Images (R, G and B) using the bitmap's color channels.

Text Data

Text Data Objects contain text in rich text format (RTF).

Measurements in WITec Control create text objects containing measurement information.

Text objects can be visualized and edited with the Text Viewer, which can be opened by just double clicking the object in the project manager.

You can add a new empty text object via main menu "Add > Text"

Data Object Memory Requirements

The required memory size for a Data Object depends on the dimensionality/size of the scan:

Size in Bytes = Pixels per Row * Rows in Image * Number of Channels * 4 [Bytes]
Size in MB = Size / 1024 / 1024

Examples:

Raman Image Scan with 128 x 128 Spectra (CCD Camera with 1024 Channels):
Size = 128 * 128 * 1024 * 4 = 64 MB

AFM Image Scan with 512 x 512 Pixels 4 Channels (T-B, R-L, Aux1, Aux2):
Size = 512 * 512 * 4 * 4 = 4 MB

Color Profile Data

Color Profiles are used by the Image Viewer to convert the image floating point numbers to colors.

The color scale can be defined in the Image Viewer:

- **Top Color Scale Value:**
  Defines the image value that will get the "furthest right" color of the color table (in most color tables this will be the brightest color).

- **Bottom Color Scale Value:**
  Defines the image value that will get the "furthest left" color of the color table (in most color tables this will be the darkest color).

Color Profile objects have the following properties:

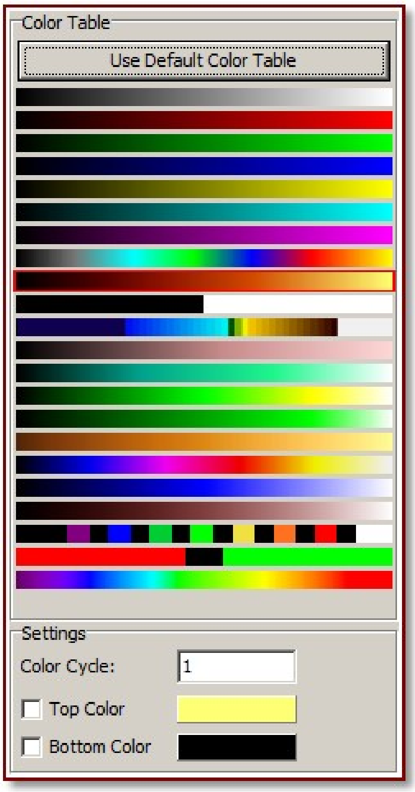
- **A Color Table:**
  Defines the RGB color values. You can choose the desired table via the Color Profile Editor.

- **Color Cycle:**
  With this option it's possible that color tables are repeated multiple times, e.g. a cycle of 2 leads to:
  

- **Top Color:**
  If top color is turned on, the defined top color will be used if the image value is higher than the defined top color scale.

- **Bottom Color:**
  If bottom color is turned on, the defined bottom color will be used if the image value is lower than the defined bottom color scale.

Use the Color Scale Circle Menu in the Image Viewer in order to change the Color Profile:



Transformation Data

Transformation Data Objects are used to convert from a pixel position to a real physical position.

There are different kind of transformation objects:

- **Spatial Transformation:**
  Converts image/bitmap/graph-image pixel positions (x,y) into real spatial coordinates;
  uses the space interpretation (see Spatial Transformation (Math)).

- **Spectral Transformation:**
  Converts x-axis pixel positions of spectral Graph Objects into a spectral unit (e.g. relative wave numbers);
  uses the spectral interpretation.

- **Linear Transformation**

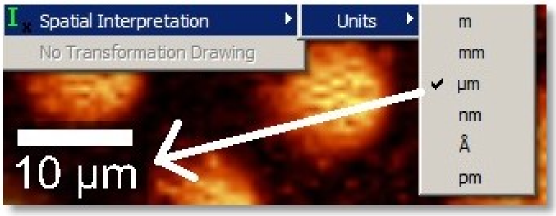
Converts x-axis or line graph pixel position of Graph Objects into a real unit;
uses e.g. time, frequency, phase interpretation.

Interpretation Data

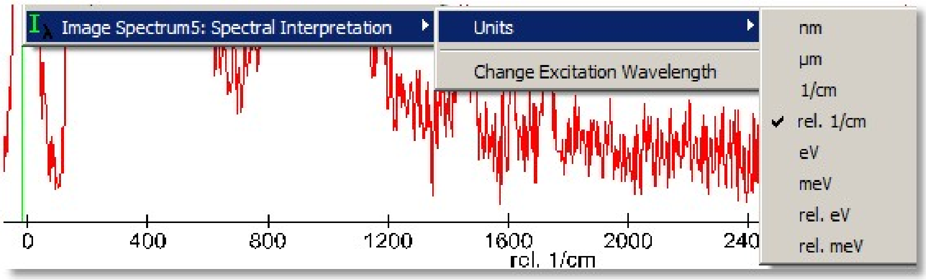
Interpretations can convert between physical units.

To change the unit, use the **context menu** of a viewer that uses this interpretation, open the submenu of the interpretation object and again open the "Units" submenu, then select a unit.
This will affect all viewers that use this interpretation object.

Example Image Viewer:



Example Graph Viewer:



There are different kind of interpretation objects:

- **Z Interpretation:**
  Used to define the unit of image or graph floating point values, e.g:
  CCD cts, Volts, microns (Topography), e.c.
  Unit is static here, i.e. you can not convert between units.
- **Space Interpretation:**
  Standard unit is µm;
  can convert between: m, mm, µm, nm, Å, pm.
- **Inverse Space Interpretation:**
  Standard unit is 1/µm;
  can convert between: 1/m, 1/mm, 1/µm, 1/nm, 1/Å, 1/pm.
- **Spectral Interpretation:**
  Standard unit is rel. 1/cm;
  can convert between: nm, µm, 1/cm, rel. 1/cm, eV, meV, rel. eV, rel. meV.

  For relative units ("rel."), a reference wavelength is used. It is stored in the spectral interpretation.
  Thus it is possible to compare spectra with different wavelengths.
  To change the excitation wavelength after a measurement the Spectral Interpretation context menu "Change Excitation Wavelength" or the Graph Data Object Context menu (see Graph Data) can be used.
  Please avoid using this feature by doing a correct configuration of the spectrometer before doing the measurement!
- **Time Interpretation:**
  Can convert between: h, min, s, ms, µs, ns, ps, fs
- **Frequency Interpretation:**
  Can convert between: µHz, mHz, Hz, kHz, MHz, GHz, THz.
- **Phase Interpretation:**
  Can convert between: rad, mrad, °, grad, mgrad.

Cursor Data

Cursors are used to send mouse positions (in physical units) from one software component or window to other components or windows. This allows e.g. to show the corresponding spectrum from a spectral image scan in a graph viewer window when clicking on a pixel in the image viewer.

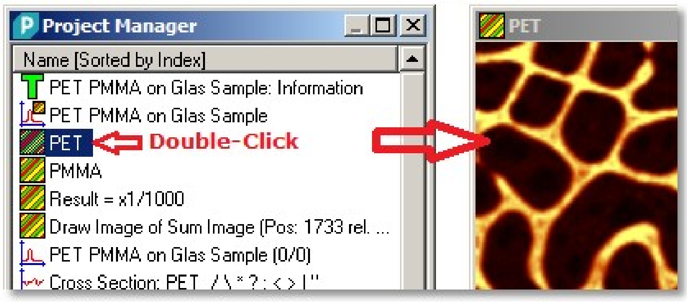
The cursor object is also used in the [Listen Cursor Mechanism.]

Cursor Positions are shown in the status bar of image- and graph-viewers.
You can also show more detailed cursor position information using the cursor manager window (press 'P' in Viewers).

Data Visualization Overview

How to visualize

You can visualize Data Objects by simply doing **double click** on a Data Object in the Project Manager.
It is also possible to select one or multiple Data Objects first and to press the **Enter key**.



Viewers

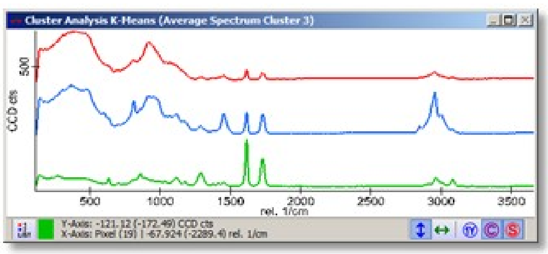
There are different kind of viewers for showing images, bitmaps, graph and text objects:

- Image Viewer

  shows Floating-Point-Images as False-Color-Image and Bitmaps.

- Graph Viewer

  shows one or multiple Graph/Spectral Data objects.



- Text Viewer

  shows Text Objects (using Rich Text Format).

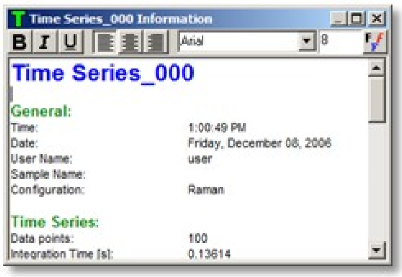
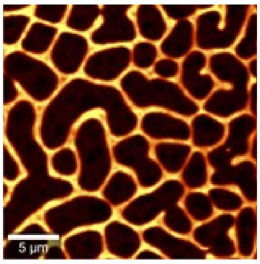
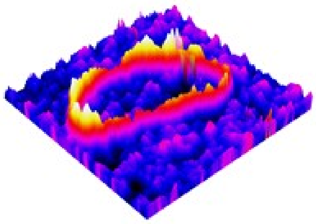
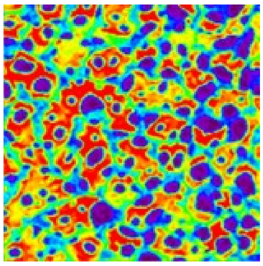


Image Viewer Overview







Description

The Image Viewer is able to visualize

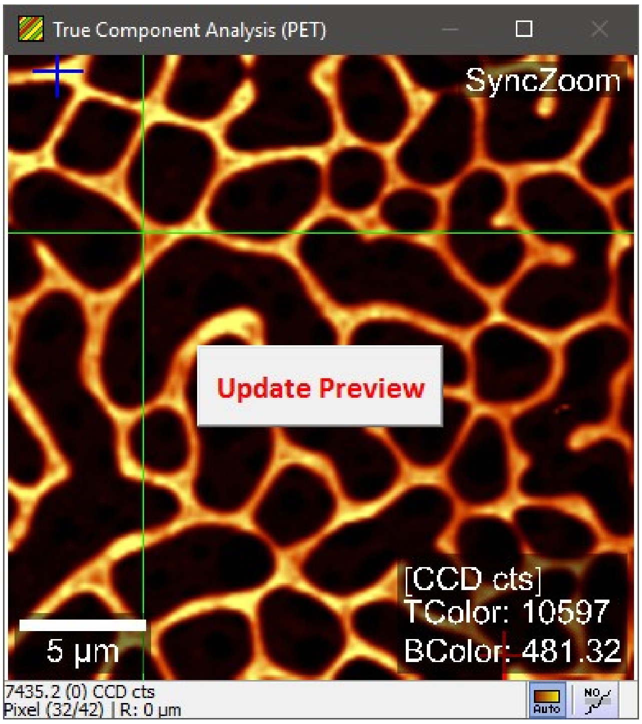
- Image Data Objects using a Color Profile Data Object to convert float values into color information.
- Bitmap Data Objects using the color data information in the bitmap.

A new Image Viewer can be created via the the Project Manager by simply double-clicking an image or bitmap object or by selecting one or multiple images and pressing enter.

Features

- Look at the general Image Viewer Appearance for a description on the image viewer window itself.
- Check out the Image Viewer Circle Menu to learn all the different Image Viewer Features:
  - Misc Visuals (Show/Hide Elements, Contour Plot, ...)
  - Draw Tools (Draw custom mask)
  - Actions (Data Analysis)
  - Color Scale (Usage of Color Table Scale, 3D-Z-Scale, Brightness Scale)
  - Camera (3D Mode, Camera Rotation/Tilt, Pixel-Zoom)
  - Export (Bitmap Export, Create Image Object, ..).
- Image Viewer Drag and Drop will show you some additional features which can be started by dropping other objects onto the viewer.

Image Viewer Appearance



SyncZoom:
This label is shown if synchronized Zoom mode is turned on (can be switched on at circle menu section Camera).

Update Preview (Button):
This Button can show up if the image is a preview of a calculation dialog and is no longer valid because of some parameter change. You can simply click on this button to calculate / update the preview image.

TColor / BColor:
This label is shown if additional information is turned on. It will show the minimum and maximum color scale values (can be switched on at circle menu Misc Visuals; only available if the color information is not a bitmap).

5 µm:
This is the color scale with label. Double-click on the scale to change its color or right-click on the scale to change more options.
Alternatively the Misc Visuals section from the circle menu can be used.
To change the unit from µm to another unit, open the context menu and change the spatial interpretation object.

Status Bar:
The first line of the status bar shows the floating point value of the image at the current cursor position.
In brackets you can see the difference value between the value at the current cursor position and the value of the previous left-mouse-clicked cursor position.
The second line shows the Pixel Position of the cursor and the spatial distance of the current cursor position to the previous left-mouse-clicked cursor position.

Automatic Color Scale (First Tool Button):
Click to execute an automatic color scale.
Click with the right mouse button to activate automatic color scale on image change.
A second Tool button for automatic color scale will show up during measurements which allows to automatically scale using only the values of the last changed line.

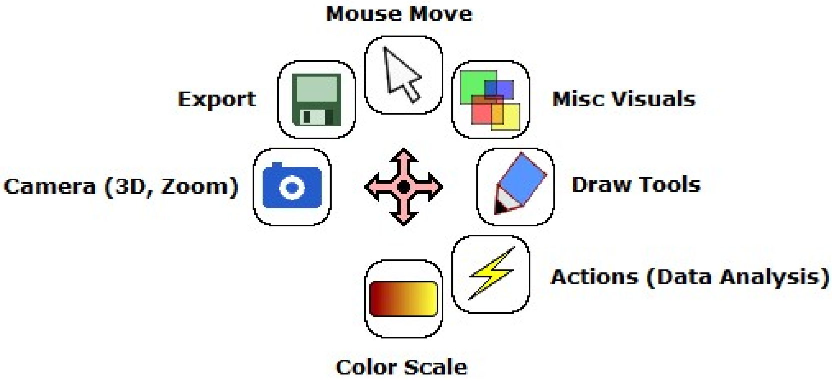
Line Subtraction (Second Tool Button):
Choose between one of the line subtraction modes:

- No Line Correction
- Line Correction by Average Subtraction
- Line Correction by Average Division
- Line Correction by Slope Subtraction.

Mathematical description see: Line Correction (Math)

Image Viewer Circle Menu

Use the circle menu by keeping the right mouse button pressed and moving the mouse for fast access of almost all features:



- Mouse Move (Change to Mouse Move Mode)
- Misc Visuals (Show/Hide Elements, Contour Plot, ...)
- Draw Tools (Draw custom mask)
- Actions (Data Analysis)
- Color Scale (Usage of Color Table Scale, 3D-Z-Scale, Brightness Scale)
- Camera (3D Mode, Camera Rotation/Tilt, Pixel-Zoom)
- Export (Bitmap Export, Create Image Object, ..).

Some features which are not available in the circle menu can be found in the context menu opening if clicking the right mouse button once.

Image Viewer Mouse Modes

You can change the image viewer mouse mode using the Image Viewer Circle Menu or the context menu (using a right mouse button click).

Mouse Move:
Change to the Mouse Move mode if have selected another mouse mode before and you do not want to use special mouse mode anymore.
This is the case for example after you have finished drawing with the draw tools. If you do not change the mouse mode, the selected draw tool is still active and you might accidentally change the mask in the image viewer.

Draw Tools:
see Image Viewer Draw Tools.

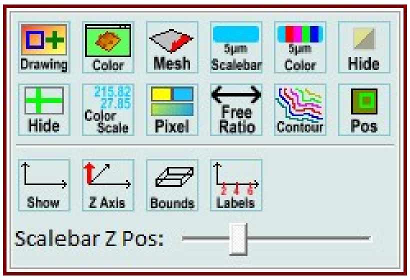
Marker Modes (Mark Region / Mark Line):
The Image Viewer automatically changes to the mark region or mark line mouse mode if some other software part listens to a spatial region or line (e.g. the cross section dialog).
It will automatically change back to mouse move mode if the other software part stops listening (or e.g. the listening dialog is closed).
Thus you don't have to change this mouse mode on your own (it's available via the right mouse button context menu).

Zoom:
see Image Viewer Camera.

Color Scale:
see Image Viewer Color Scale

Image Viewer Misc Visuals

You can open these features using the Image Viewer Circle Menu.



Drawing:
Opens the transformation drawing options. Here you can change the line drawing of transformations from other images / data

objects.

Color:
Changes the background color

Mesh:
Shows nice mesh borders in 3D mode. The marginal pixels are turned down to close the mesh at the borders.

Scale Bar:
Show or hides the scale bar.

Color:
Changes the scale bar color.

Hide (Mask):
Hides the mask temporarily (e.g. masks that are drawn by the user with the draw tools or are calculated from a dialog).

-

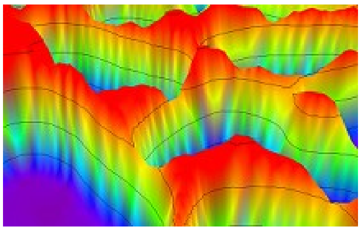
Hide (Crosshair):
Shows or hide the green cursor crosshair (useful if exporting an image).

Color Scale:
Shows the current color scale top and bottom values as overlay text on all image viewers.

Pixel:
Turns the pixel color interpolation on or off (e.g. if you would like to see pixel borders).

Free Ratio:
Turns the free ratio mode on or off. If turned on the image fits to the Viewer Window size without preserving the original ratio.

Contour:
Turns contour line drawing on or off. A dialog is shown to change the number and values of the contour lines.
In 2D-Mode the contour lines are calculated using the color image floating point values;
In 3D-Mode the contour lines are calculated using the 3D-Z image floating point values.



Pos:
Sends the position of the currently displayed image to all other viewers in order to see the region of this image in other viewers.

-

Show:
Shows or hides the coordinate system axes.

Z Axis:
Shows or hides the Z Axis, if coordinate system axes are shown.

Bounds:
Shows or hides the bounding box if the coordinate system axes are shown.

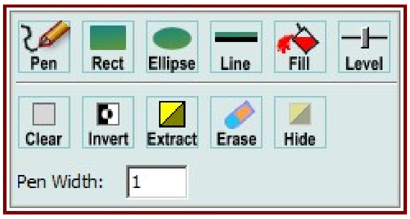
Labels:
Shows or hides tick labels and axes titles if the coordinate system axes are shown.

-

Scale Bar Z Pos:
Changes the Z-Position of the Scale Bar and other labels in 3D Display Mode.

Image Viewer Draw Tools

You can open these features using the [Image Viewer Circle Menu](#).



Mouse Draw Modes

Pen:
Draws a custom line or marks single pixels.

Rectangle:
Draws a filled rectangle. Keep the Control-Key pressed while drawing to draw a square.

Ellipse:
Draws a filled ellipse. Keep the Control-Key pressed while drawing to draw a circle.

Line:
Click to draw a horizontal line. Keep the Control-Key pressed while drawing to draw a vertical line.

Fill:
Flood fills an area.

Level:
Opens a slider window where you can define threshold for mask drawing:

Changing the threshold will set the whole image mask on pixels that are higher or equal than the threshold and clear the mask on pixels that are lower or equal than the threshold.
You can also invert the mask logic in order to set mask pixels that are lower than the threshold.

You can also use all tools to remove certain parts of the previously drawn area or line by keeping the shift key pressed and dragging the mouse.

Mask Tools

Clear:
Clears the current mask.

Invert:
inverts the current mask.

Extract:
extracts the current mask as a new image object to the current project.

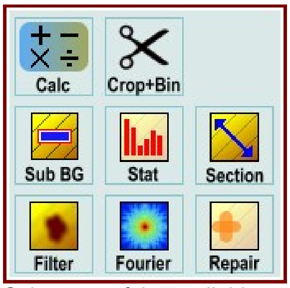
Erase:
turns the erase mode on or off. When turned on, all draw tools will erase the mask while drawing.

Hide:
hides the drawn mask (e.g. to have a better, quick look at the original image features).

Pen Width:
changes the pen with for the pen draw tool.

Image Viewer Actions

You can open these features using the Image Viewer Circle Menu.

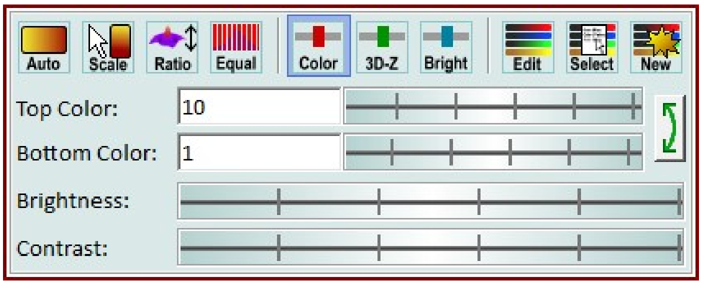


Select any of the available actions to use the current color image as an input Data Object for a data analysis tool.

See Data Analysis Overview.

Image Viewer Color Scale

You can open these features using the Image Viewer Circle Menu.



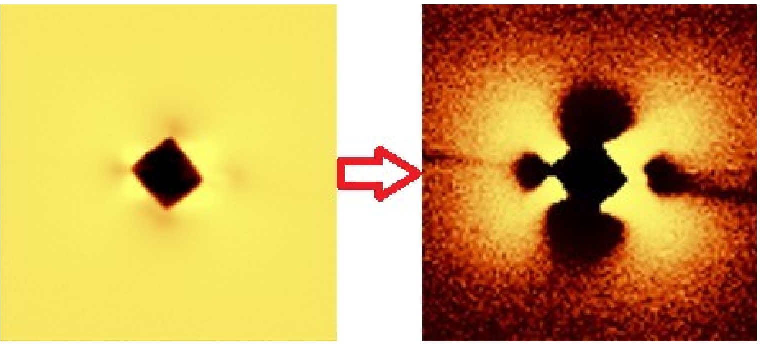
Automatic Color Scale:
Executes the automatic color scaling.

Mouse Color Scale:
Changes the mouse mode to the "scale color mouse mode".
Click somewhere in the image to set the image value at the current cursor position as the new color scale top value.
Hold down the shift-key while clicking to set the bottom color scale value instead.

Ratio:
Adjusts the 3D-Z scale to a correct XY/Z ratio. Works only with topography images.

Equal:
Equalize the color histogram. Used to show a high contrast for all dynamics of a floating point image. This might be useful if your image has two "plateaus" with each containing small value changes that could be interesting.

If checked, the color table colors are no longer assigned in a linear way using the top and bottom color scale values. Instead they are assigned in a non linear way by equalizing the histogram in order to get the same amount of "color changes" for the same amount of "floating point changes":



Color Scale:
Changes to Color Scale Mode. If selected, the edits and sliders will change the color scale.
This button is disabled if only one kind of scale can be changed.

3D-Z Scale:
Changes to 3D-Z Scale Mode. If selected, the edits and sliders will change the 3D-Z scale.
Only works if a floating point image is used as 3D-Z information image.

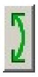
Brightness Scale:
Changes to Brightness Scale Mode. If selected, the edits and sliders will change the brightness scale.
Only works if a floating point image is used as brightness information image.

Edit Color Profile:
Opens the editor for currently used color profile object (see Color Profile Data).
Here you can choose another color table or change the color cycle, define top and bottom color to mark e.g. "extrema pixels".
All Image Viewers that use the same color profile object will also change their color drawing.

Select another Color Profile Object:
Opens a selector window to select another color profile object that you have created before using the following option.

Create a new Color Profile Object:
creates a new color profile object and assigns it to the current Image Viewer.
You can use the new color profile object in another Image Viewer by using the two features above.
If no additional Color Profile Object is created, all viewers always will use the same automatically created default color profile.

Top / Bottom edits + wheels:
here you can change the top and bottom color/3D-Z/brightness values.
The wheels can be moved infinitely; the mouse position is always moved back to the center when leaving the wheel area.

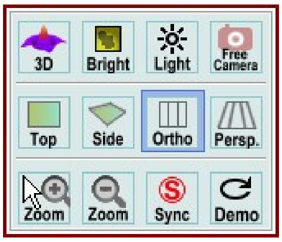
 **Swap Top and bottom Scale:**
swaps the top and bottom scale values.

Brightness (Wheel):
Changes the top and bottom values synchronously, this changes the brightness.

Contrast (Wheel):
Changes the top and bottom values in the opposite direction, this changes the contrast.

Image Viewer Camera

You can open these features using the Image Viewer Circle Menu.



3D Mode:
Turns on or off the 3D Display Mode.
Only works if a image data (not bitmap data) is used as 3D-Z information image.
You can assign another image to an Image Viewer to be used as the 3D-Z information image by drag & drop from the project manager and choosing the right option in the Image Viewer Drag and Drop menu. Otherwise the current image is used as color as well as 3D-Z information.
This mode also automatically enables the free camera mode, the camera side view and the perspective projection.

Use the left mouse button to tilt and rotate the image. Turn the wheel to zoom the camera. Hold down the Shift-Key and drag the image to pan.

Brightness Mode:
Turns on or off the Brightness Display Mode. Only works if a floating point image is used as a brightness information image.
You can assign another image to an Image Viewer to be used as the brightness information image by drag & drop from the Project Manager and choosing the right option in the Image Viewer Drag and Drop menu.
Brightness mode means that a brightness information image will define the brightness of a color, whereas the color image (+ color table) or a bitmap defines the color of a pixel.

Lighting:
Shows the Image Viewer Lighting dialog for rendering a nice 3D surface with light and reflections.

Free Camera:
Turns on or off the free camera mode.

If turned on, you can
- Tilt and rotate the image using the middle mouse button (press down the mouse wheel) and dragging the mouse cursor; or use the arrow keys to rotate and tilt
- Use the mouse wheel to do a free camera zoom.

If turned off, you can
- move the cursor with the arrow keys to exactly move through the pixels
- use the mouse wheel for a pixel zoom (camera distance is fixed)
- click the mouse wheel / middle button and drag the cursor to move the image around when zoomed in (pixel zoom).

Top View:
Changes to camera top view (automatically executed when turning off the 3D Mode).

Side View:
Changes to camera side view (automatically executed when turning on the 3D Mode).

Orthographic Projection:
Changes to orthographic camera projection (automatically executed when turning off the 3D Mode).

Perspective Projection
Changes to perspective camera projection (automatically executed when turning on the 3D Mode).

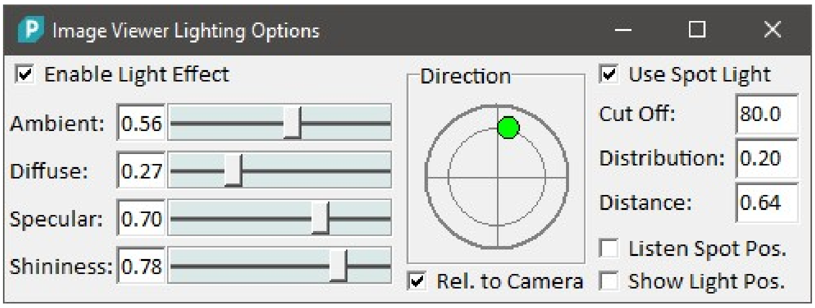
Mouse Zoom:
Turns on the Mouse Zoom Mode. If the mouse zoom mode is selected, you can click and drag a rectangle in the image and thus define an exact pixel zoom. Only the pixels of the selected range are displayed.
Don't forget to turn off this mouse mode by activating the mouse move mode.

Zoom Out:
Zooms out to see all image pixels (or in free camera mode will zoom to fit to the window).
If the synchronized zoom mode is turned on, all image viewers will zoom out to see all image pixels.

Synchronized Zoom:
Turns on or off the synchronized zoom mode; this mode is identical for all image viewers. When turned on, the pixel zoom will send the current spatial area to all other viewers that will in turn use the same pixel zoom.

Demonstration:
Lets the image rotate for demonstration purposes.

Image Viewer Lighting



Enable Light Effect
Turns on or off the light effect.

Ambient / Diffuse / Specular / Shininess
With those parameters you can affect the kind of "material", e.g. how much the surface reflects light.

Direction
Here you can click somewhere in the circle to define the light source position and direction of the light.

Rel. to Camera
If checked, the light position is relative to the camera/viewing position. If not checked, the light is relative to the sample/image.

Use Spot Light
If checked, a spot light source is used instead of an "all-over" plain light.

Cut Off
Lower values will do a hard cut at the light cone.

Distribution
Changes the angle of cone.

Distance
Changes the distance of the light source to the sample/image.

Listen Spot Pos.
If checked, you can click somewhere in the image to define the light spot position.

Show Light Pos.
If checked, shows the light position in the image viewer.

Example

Left: Without Lighting
Right: With Lighting

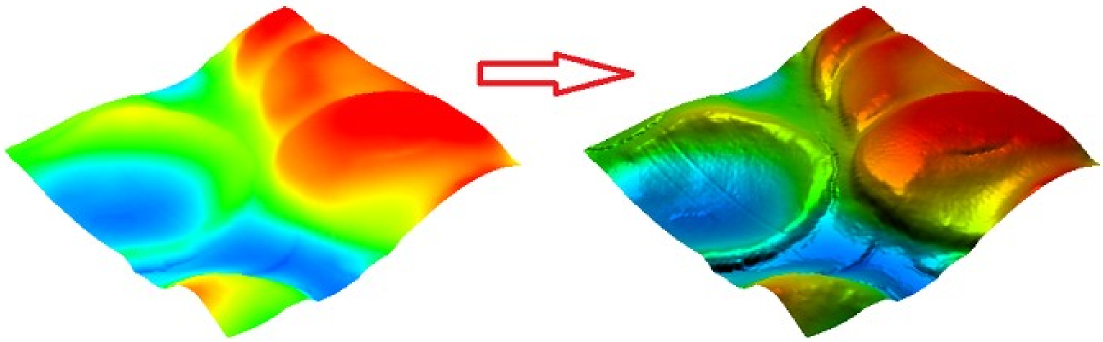
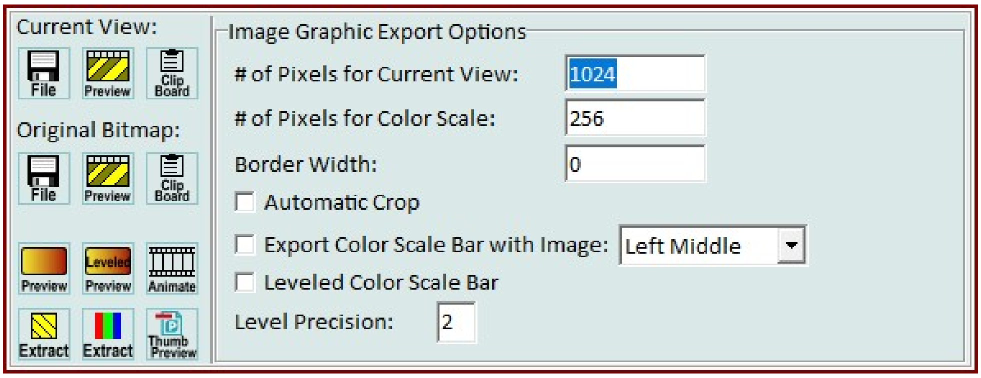


Image Viewer Export

You can open these features using the Image Viewer Circle Menu.



Export Bitmap to File:
Exports the current view to a file. You can choose between several image formats.

Export Bitmap to Preview:
Exports the current view to the built-in graphic editor. Here you can flip or rotate the bitmap and save it to a file or into the windows clipboard.

Export Bitmap to Clipboard:
Exports the current view as a bitmap into the clipboard. This allows you to paste the image into another graphic software (Shortcut: Ctrl+C)

Original Bitmap:
Exports the original bitmap in its original size without any scale bar or other overlay drawings instead of the current view of the image viewer.

Export Color Scale Bar to Preview:
Exports a the color scale bar to the graphic editor.

Export Leveled Color Scale Bar to Preview:
Exports a leveled color scale bar to the graphic editor (i.e. bottom value is set to 0).

Create and Export Animation:
Shows the Animation Editor for exporting a user defined animation.
The following parameters are animated:

- Rotation / Tilt / Camera Distance
- X / Y / Z Shift of the Image
- Background Color
- Color Scale and Z-Scale (if checked in the options)
- Pixel Zoom (if checked in the options)
- All light options
- Color Table index

Extract Image to Project:
Extracts the current floating point image as a new image object to the current project.

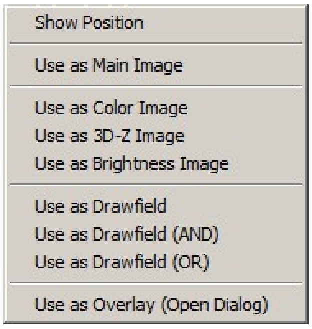
Extract View as Bitmap to Project:
exports the current view as a new bitmap object to the current project.

Set as WIP-File Thumbnail Preview in Windows Explorer:
sets the current view as the thumbnail preview for the WIP-File. You have to save the project afterwards to take effect. The windows file explorer may cache thumbnails so you might not immediately see the new thumbnail.

Image Graphic Export Options
see Image Viewer Options.

Image Viewer Drag and Drop

You can drag and drop other Data Objects (image/graph/bitmap objects) onto an image viewer in order to execute the following actions:



Show Position:
shows the position of the dropped object. You can drop any number of images, bitmaps and graph objects to see their position:
Images, Bitmaps and Image-Graph Objects are shown as a rectangle.
Line-Scan Graph Objects or Cross Section Graph Objects are shown as a line.
Single Spectrum Graph Objects are shown as a cross.
You can change the line width of drawings, see the Drawing Button in Image Viewer Misc Visuals circle menu.

Use as Main Image:
to use the dropped image as a new main image. If the dropped image has the same size than the current color image, the draw field mask is preserved, otherwise it is cleared.

Use as Color Image:
the dropped image is used as color information. This is useful if you opened a topography image displayed as a 3D image and then you would like to use a chemical image as a color texture / color information.
Only works if the dropped image has the same size and space transformation as the current color image.

Use as 3D-Z Image:
the dropped image is used as 3D-Z information. This is useful if you opened a chemical image and you would like to use a topography image as 3D-Z information for the 3D display mode.
Only works if the dropped image has the same size and space transformation as the current color image.

Use as Brightness Image:
the dropped image is used as brightness information. This is useful if you opened a chemical image and then you would like to use a mask or an error-mask image as brightness information to highlight masked pixels.
If the color image is a floating point image object, a rainbow color scale (containing colors only with maximum brightness) makes the most sense for the original image.
Only works if the dropped image has the same size and space transformation as the current color image.

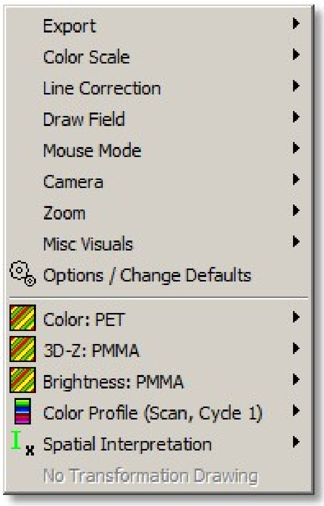
Shortcut: press the shift key on the keyboard while dropping.

Use as Draw field (and, or):
the dropped image is used as the draw field mask. You have to drop a mask image, otherwise you will most likely get a complete cleared or set mask.
Use and/or feature for a boolean and/or operation on the existing draw field mask.
Only works if the dropped image has the same size and space transformation as the current color image.

Shortcut: Press the control key on the keyboard while dropping.

Use as Overlay:
this action will open the Image Transform and Overlay dialog which can be used to draw an overlay and to change the spatial transformation of the dropped image/measurement.

Image Viewer Context Menu



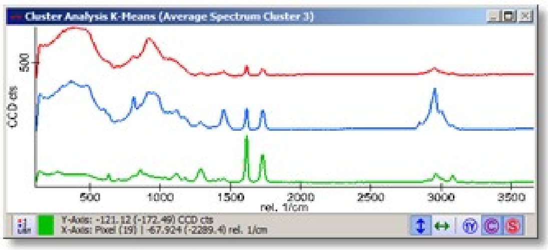
The context menu is an alternative way for accessing the features that you also can find in the circle menu. Just click and release the right mouse button anywhere in the viewer.

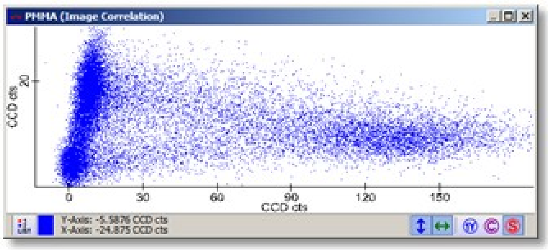
Options / Change Defaults:
This will open the program options for the image viewer.

At the **bottom of the context menu** you can find a list of data objects that are used by the viewer:

- the color image object that is displayed (also optionally the brightness and the 3D-Z information images)
- the color profile object in case of showing a floating point image as a color image
- the spatial interpretation, which you can use to switch between different spatial units
- Transformation Drawing, if you dropped other data objects to see their positions.

Graph Viewer Overview





Description

The Graph Viewer is able to visualize Graph Data Objects.

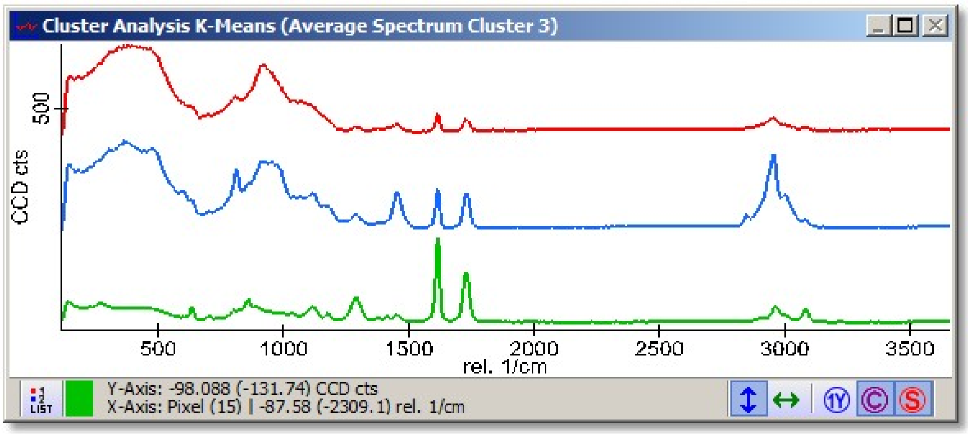
A new Graph Viewer can be created via the the Project Manager by simply double-clicking a Graph object, or by selecting one or multiple Graph objects and pressing enter.

Features

- Look at the general Graph Viewer Appearance for a description on the Graph Viewer window itself.
- Check out the Graph Viewer Circle Menu to learn all the different Graph Viewer Features.

- Graph Viewer Drag and Drop will show you some additional features that can be started by dropping other objects onto the viewer.

Graph Viewer Appearance



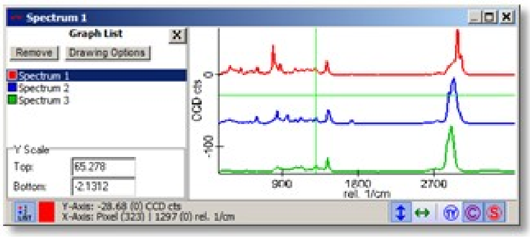
Title Bar

The text in the title bar shows the caption of the selected graph data object.

Status Bar

**Graph List Button and Selection Information:**
shows the color of the currently selected graph object. Click on the color to select the next graph object (in order to change its scale or drawing or to export it).

Click on the "List" Button of the icon to show the Graph Viewer List at the left side of the graph viewer.



Cursor Positions:
The first line of the status bar shows the Y-Axis Cursor Position and the Graph Object Value Unit. The value in brackets is the distance between the current cursor position and the cursor position of the last position where the left mouse button was pressed previously.

Zoom Modes

See Graph Viewer Zoom Modes

Coordinate Axis and Units

The X-Axis is always the same for all graph objects that are shown in the same viewer.
The Y-Axix shows the values for the currently selected graph object.
The unit can be changed by changing the interpretation data objects.

Graph Viewer Zoom Modes

Zoom Modes

For more Information, see Graph Viewer Scale and Zoom.

Zoom Out Y-Axis Scale:
Left-Click to zoom Out the Y-Axis Scale,
Right-Click to toggle the "Zoom Out Y-Axis On Change Mode".

Zoom Out X-Axis Scale:
Left-Click to zoom Out the X-Axis Scale,
Right-Click to toggle the "Zoom Out X-Axis On Change Mode".

Auto Zoom Out Y-Axis Only:
If checked, the automatic Y-Axis Zoom on change will only zoom out, not in.

Same Y-Axis Scale:
If checked, all graph data objects share the same Y-Axis Scale.

Cascade Graphs:
Cascades multiple graph objects using a cascade distance that can be changed in the Scale and Zoom Circle Menu.

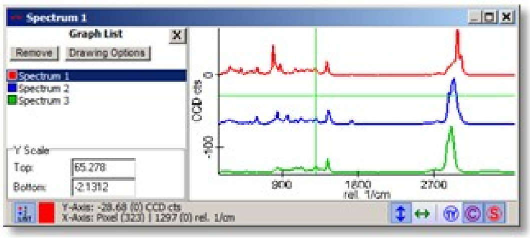
Synchronized Zoom
If checked, changing the Y-Axis via Mouse Wheel will zoom all graph objects in the viewer (only if graphs are not cascaded).

Fast Zoom Shortcuts

- Zoom fast into the current mouse/crosshair position by pressing the space key.
- You can zoom into a region fast by holding down the control key and marking a region using the mouse.
- You can use the mouse wheel to zoom the Y axis.
- Holding down the control key while turning the mouse wheel will zoom the X axis.
- Holding down the shift key while zooming will increase the zoom speed.
- Press X to zoom out the X axis (Y is automatically zoomed if the "Zoom Out Y-Axis on Change Mode" is turned on).
- Press Y to zoom out the Y axis.
- Press R to zoom out the Y axis with rayleigh peak.
- Press Control-A to toggle the "Auto Zoom Out Only" mode.

Graph Viewer List

Click on the "List" Button in the status bar to show the graph list at the left side of the graph viewer:

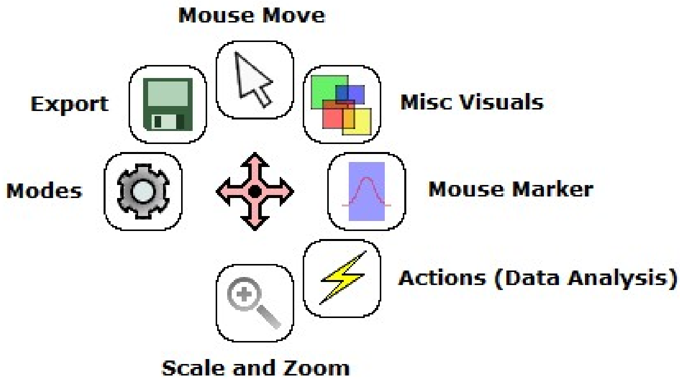


The Graph List shows all graph objects that are displayed by the graph viewer.

The following actions can be done here:
- You can just click on any graph to make it the selected graph (e.g. for scaling or changing the drawing options, or use the shortcut key Page-Up / Page-Down in the viewer without the list).
- You can delete a graph from the viewer (not from the project) by pressing the delete key in the Graph List or by pressing the "Remove" button above.
- A double-click will show the drawing options of the selected graph object.
- You can change the Y-scale for the selected graph.

Graph Viewer Circle Menu

Use the circle menu by keeping the right mouse button pressed and moving the mouse for fast access of almost all features:



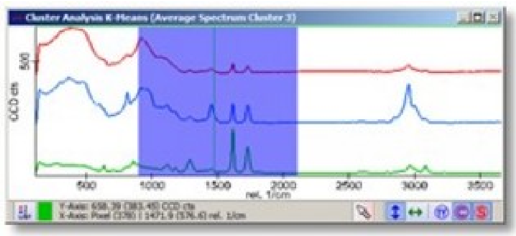
- Mouse Move (Change to Mouse Move Mode)
- Misc Visuals (Show/Hide Elements, Contour Plot, ...)
- Mouse Marker (Change to Mouse Marker Mode)
- Actions (Data Analysis)
- Scale and Zoom (Change the X- and Y-Axis scale, Cascade, Logarithmic Scale)
- Modes (Parametric Display, Listen Mode)
- Export (Bitmap Export, Create Graph Object, ..).

Graph Viewer Mouse Modes

You can change the Graph Viewer mouse mode using the Graph Viewer Circle Menu.

Mouse Move:
changes to the mouse move mode if you selected another mouse mode before and do not want to use the special mouse mode anymore.

Mouse Marker:
The mouse marker mode is used to manipulate masks or to send a region to other software parts.
The currently selected region is highlighted in the viewer:



This mode is automatically selected if another software part listens to a range so you can draw a range in a graph viewer. It will be automatically changed back to mouse move mode if that other software part stops to listen.

If you do an ASCII Export to an external program, only the current marked region is exported. If no region is selected, the complete graph/spectrum is exported.

Click and release the mouse at the same position to clear the region that was set by the mouse marker.

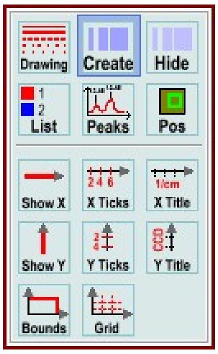
For further possibilities manipulating the mask see Graph Viewer Mask Manipulation.

Mouse Zoom:
See Graph Viewer Scale and Zoom.

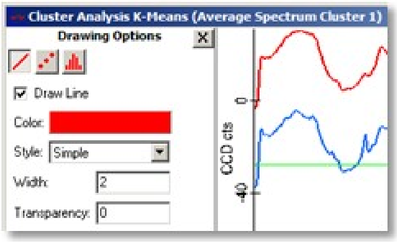
Mouse Follow Data:
See Graph Viewer Modes.

Graph Viewer Misc Visuals

You can open these features using the Graph Viewer Circle Menu.



Drawing:
Shows the graph drawing options at the left side of the viewer. Here you can change the color, line style etc. of each graph:



Create:
Switches to the mask creation mode. See Graph Viewer Mask Manipulation.
Changing the mouse mode to "Move" or clicking again on the Create Button will turn off the mask creation mode.

Hide:
Hides mask(s) temporarily. Only available on preview graph viewers that show a mask for manipulation or if the mask creation mode is turned on.

List:
Shows the Graph List of all graph objects that are displayed in the graph viewer.

Peaks:
Finds and labels peaks, see Graph Viewer Peak Labeling

Pos:
Sends the position of the currently selected spectrum to all other viewers in order to see the position of a single spectrum, line spectrum or image spectrum in an image viewer.

Show X:
Shows or hides the X Axis drawing.

X Ticks:
Shows or hides ticks and tick labels on the X Axis.

X Title:
Shows or hides the X Axis Title.

Show Y:
Shows or hides the Y Axis drawing.

Y Ticks:
Shows or hides ticks and tick labels on the Y Axis.

Y Title
Shows or hides the Y Axis Title.

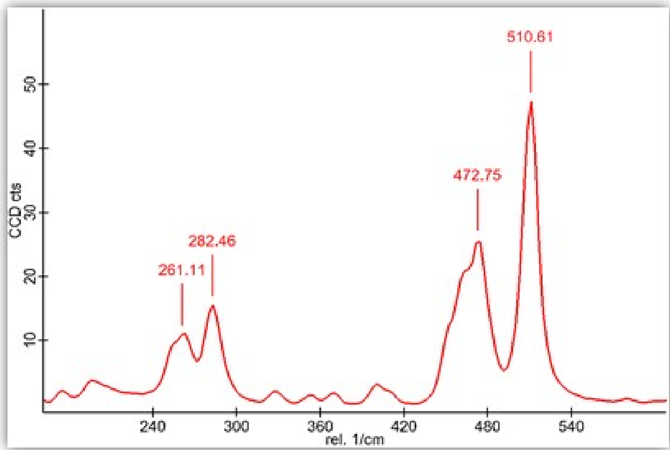
Bounds:
Shows or hides closing lines at the top and right bounds of the coordinate system.

Grid:
Shows or hides grid lines at the tick positions.

Graph Viewer Peak Labeling

The Graph Viewer allows to find and label peaks automatically; additionally the user can add or remove peaks manually. Peaks are saved in the project file.

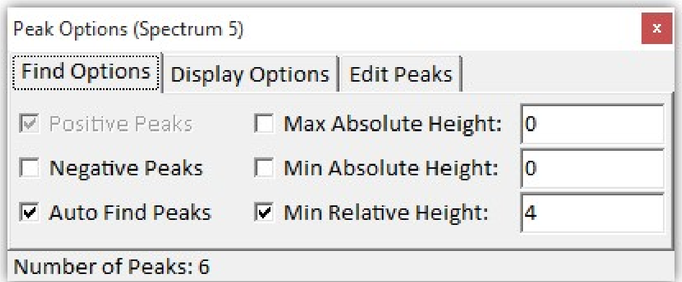
You can turn on or off the peak labeling using the Misc Visuals Circle Menu, the Context Menu or the Shortcut "F" ("Find peaks"):



User Interface

A peak find dialog will open if you enable the peak labeling feature; note that the labeling remains enabled if you close this dialog. You can reopen the dialog by selecting the "Show Peaks" feature again in the circle menu / context menu / via shortcut.

Find Options Tab



These options can be used to change the automatic peak find algorithm.

Positive Peaks (Check Box):
Enables the peak find calculation for positive peaks.

Negative Peaks (Check Box):
Enables the peak find calculation for negative peaks.

Auto Find Peaks (Check Box):
Enables or disables the automatic peak find algorithm. If you add or remove peaks manually, the automatic peak find algorithm will be disabled.

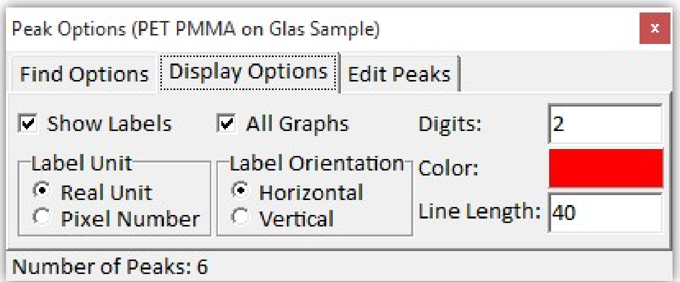
Max Absolute Height (Float Edit):
Peaks higher than this value will be ignored in the automatic peak find algorithm.

Min Absolute Height (Float Edit):
Peaks smaller than this value will be ignored in the automatic peak find algorithm.

Min Relative Height (Float Edit):
Peaks whose relative height is smaller than this value will be ignored in the automatic peak find algorithm.

Number of Peaks:
Shows the current number of peaks (including peaks added by the user).

Display Options Tab



Show Labels (Check Box):
Here you can switch between labels or vertical lines.

All Graphs (Check Box):
If checked, all graph objects in the current graph viewer are labeled.

Label Unit (Radio Group):
Defines, whether the real unit (e.g. "rel. 1/cm") or the pixel number should be used for labeling.

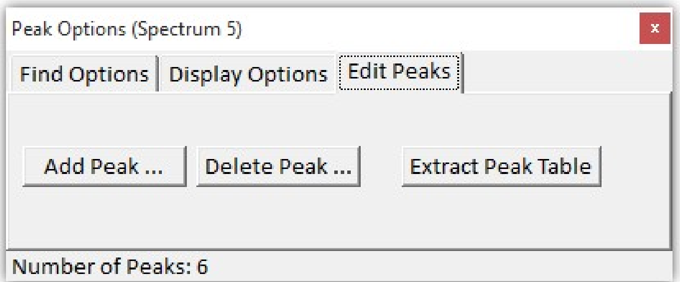
Label Orientation (Radio Group):
Defines the orientation of the labels.

Digits (Integer Edit):
Defines the precision of the peak label; note that the peak find has sub-pixel accuracy.

Color (Color Selector)
Defines the color of peak labels.

Line Length (Integer Edit)
Defines the length of the line that connects the peak to its label.

Edit Peaks Tab



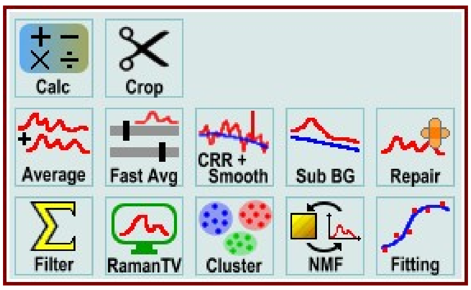
Add Peak (Button)
Opens a dialog where you can manually add a peak label at a desired X and Y Position.
Note that the automatic peak find algorithm will be disabled if you add or delete peaks.

Delete Peak (Button)
Opens a dialog where you can select one of the displayed peaks and remove it from the labeling list.
Note that the automatic peak find algorithm will be disabled if you add or delete peaks.

Extract Peak Table (Button)
This will extract all peaks with extended information as a table into a Text Data Object.

Graph Viewer Actions

You can open these features using the Graph Viewer Circle Menu.



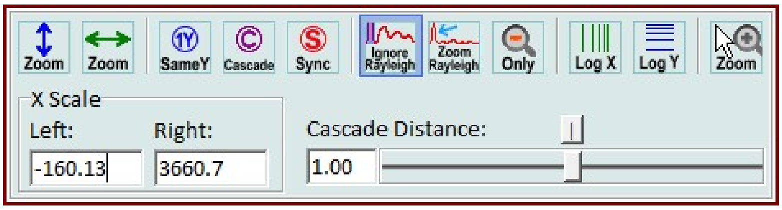
Press on any of the available actions to use the current selected graph as input data object for a data analysis tool.

See Data Analysis Overview.

Graph Viewer Scale and Zoom

You can open these features using the Graph Viewer Circle Menu.

In general the X-Axis is always identical for all displayed graph objects in the same viewer.
The Y-Axis can be different for all displayed graph objects in the same viewer. The values for the Y-scale of each single graph can be defined by using the Graph Viewer List. Additionally there are different actions that will change the Y-Axis Zoom behavior quickly (see below).



Zoom Out Y-Axis Scale:
Zooms out the Y-Axis scale to see the all Y-pixels of the currently selected graph object.
Click with the right mouse button toggle on or off the Auto-Zoom-Y-Mode. This will automatically execute the zoom out if the graph changes. Shortcut "Y".

Zoom Out X-Axis Scale:
Zooms out the X Axis scale to see the all X-pixels of all graph objects.
Click with the right mouse button to toggle on or off the Auto-Zoom-X-Mode. This will automatically execute the zoom out if the graph changes. Shortcut "X".

Same Y-Axis Scale:
If checked, all graph Data Objects share the same Y-Axis Scale. It is synchronized automatically upon changing the scale on any graph.
If the "Auto-Zoom-Y-Mode" is on: You can deactivate the Synchronized-Zoom and selected a desired graph (using the color area or by double-clicking the graph) in order to define which graph should be used for auto-zooming the Y-Scale. Shortcut "1".

Cascade Graphs:
Cascades multiple Graph Objects. Change the Cascade Distance to define the gap size between the graphs.
Note: if "Same Y-Axis Scale" is also active, you can zoom all graphs with the mouse wheel, but make sure that you position the mouse at the correct (selected) graph position. Shortcut "C".

Synchronized Zoom:
If checked, changing the Y-Axis via the mouse wheel will zoom all graph objects in the viewer.
This only works if multiple graphs are not cascaded. Shortcut "S".

Ignore Rayleigh:
If checked, any Zoom Out Y-Axis Scale Action will ignore the Rayleigh Area. Only works with spectral Graph Objects.

Zoom out Rayleigh Peak:
Zooms out the Rayleigh peak. This might be useful when calibrating on the Rayleigh peak. Shortcut "R".

Auto Zoom Out Y-Axis Only:
If checked, the automatic Y-Axis Zoom on change will only zoom out, not in.

Logarithmic X-Axis:
Turns on or off the logarithmic X-Axis scale. Shortcut "Control-L".

Logarithmic Y-Axis:
Turns on or off the logarithmic Y-Axis scale. Values smaller than 0 will be drawn at the very bottom of the window. Shortcut "L".

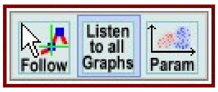
Mouse Zoom:
Changes the mouse mode to the "mouse zoom mode". Click and drag a rectangle in the graph viewer to zoom the selected Graph Object exactly to this area.
Instead of turning to mouse zoom mode, you can hold down the control key to zoom a rectangular region.

X-Scale Left/Right (Float Edits):
Defines the X-Axis scale for all graphs. You can also hold down the Control-Key on the keyboard while turning the mouse wheel to zoom the X-Axis.

Cascade Distance (Slider)
Here you can define a gap size if you are cascading multiple graph objects.
A value of 0.0 means no cascade, a value of 1.0 means full cascade. The small button on top of the slider can be used to set the value to 1.0.

Graph Viewer Modes

You can open these features using the Graph Viewer Circle Menu.



Mouse Follow Data:

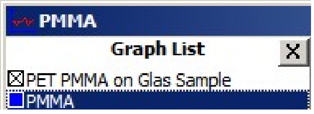
If checked, the cursor always follows the exact data points in X and Y direction.

Listen to all Graphs

If checked, all multidimensional graph objects will listen; i.e. if two image graph objects are shown in the same viewer and you click on another pixel in an image viewer, the graph viewer will show the corresponding graph/spectrum of this position for all the graph data objects.
You can turn this feature off to compare particular single spectra of multidimensional graph data objects.

Parametric Display

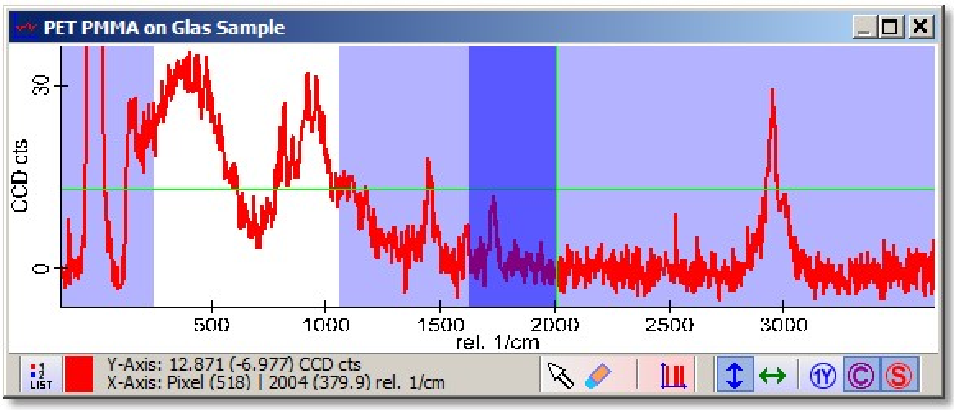
Turns on the parametric plot. The X-Axis is defined by the graph that is selected at the moment you activate the parametric display. So just deactivate the parametric display, select another graph and activate it again to change the X-Axis-Graph.
In the Graph Viewer List the X-Axis-Graph used in the parametric display is marked by a small cross:



Graph Viewer Mask Manipulation

Some Drop Action Dialogs / Data Analysis Actions exhibit graph viewers that show a mask.With graph masks you can define, which pixels should be used for the calculation.

You can manipulate those masks directly in the preview graph viewer:



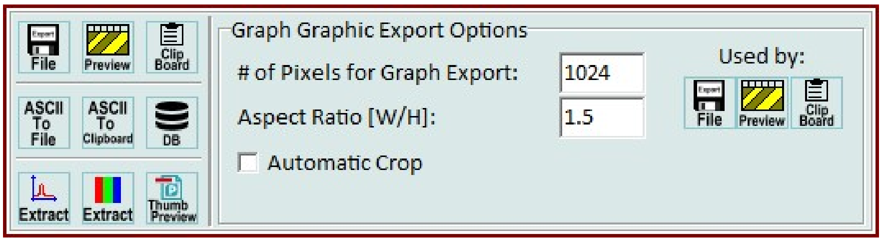
Usage

- If not already selected: select the mouse marker tool in the graph viewer.
  The mouse marker tool is automatically selected in graph viewers that show and allow manipulation of a mask.
- Just click down the left mouse button at a certain position and drag an area.
- If you release the left mouse button, the selected region of this mask is set.
- If the shift key is pressed while you release the left mouse button, the selected region is cleared.
-  You can also toggle the Eraser mode (visible in the status bar of the graph viewer) to clear the mask without having to press the shift button.
-  Press the extract button to extract the current mask as a new mask data object into the current project in order to reuse the mask.

Though this is the fastest way to change a mask, you can also use the Mask Manipulation Tools of a belonging drop action dialog in order to change the mask. There you can exactly define which pixels should be masked and its also possible to export a mask to the project for later usage.

Graph Viewer Export

You can open these features using the Graph Viewer Circle Menu.



Graph Graphic Export Options
Here you can change the size of exported bitmaps
See Graph Viewer Options

Export Bitmap to File:
Exports the current view to a file. You can choose between several image formats.

Export Bitmap to Preview:
Exports the current view to the built-in graphic editor. Here you can flip or rotate the bitmap and save it to a file or clipboard.

Export Bitmap to Clipboard:
Exports the current view as a bitmap into the clipboard. This allows you to paste the bitmap into another graphic software.

Export ASCII To File:
Exports the current graph in ASCII Format to a file.
For all ASCII exports, the format is: <Interpreted X-Axis Value> <Tab> <Y-Axis Value>

Export ASCII To Clipboard:
Exports the current graph in ASCII Format to the clipboard.

Export to Database Application
Exports all spectral data objects (using the selected region, if any set) to a database application which can be defined in the Database Export Options.
Also see Database Search in WITec Project.
Note 1: The export only works if the graph has a spectral X-Transformation and the interpretation unit of the X-Axis is "rel. 1/cm"
Note 2: If a region is marked in the graph viewer only the marked region is exported. Clear the marked region by switching to the mark region mouse mode and click somewhere in the window.

Extract Graph to Project:
Extracts the current displayed single graph as a new graph object to the current project.

Extract View as Bitmap to Project
Exports the current view as a new bitmap object to the current project.

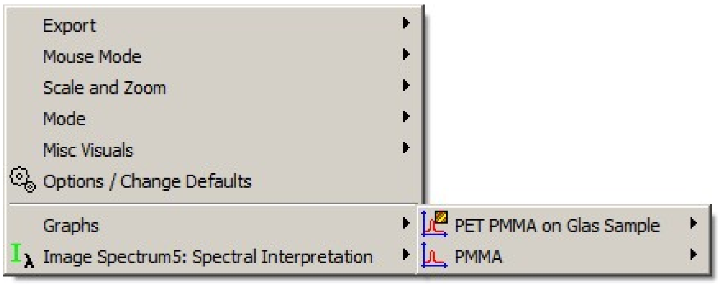
Set as WIP-File Thumbnail Preview in Windows Explorer:
Sets the current view as the thumbnail preview for the WIP-File. You have to save the project afterwards to take effect. The windows file explorer may cache thumbnails so you might not immediately see the new thumbnail.

Graph Viewer Drag and Drop

You can drag and drop the following items on a graph viewer:

- Graph Objects (to display and compare multiple graph objects in the same viewer):
  Only works if the dropped object uses the same x axis unit kind
- Graph Mask Objects (to reuse a previously saved mask):
  Only works if the graph viewer is a preview containing a mask for manipulation (see Graph Viewer Mask Manipulation).
  If multiple masks are shown by the viewer, the mask below the mouse position is overwritten when dropping a mask.

Graph Viewer Context Menu



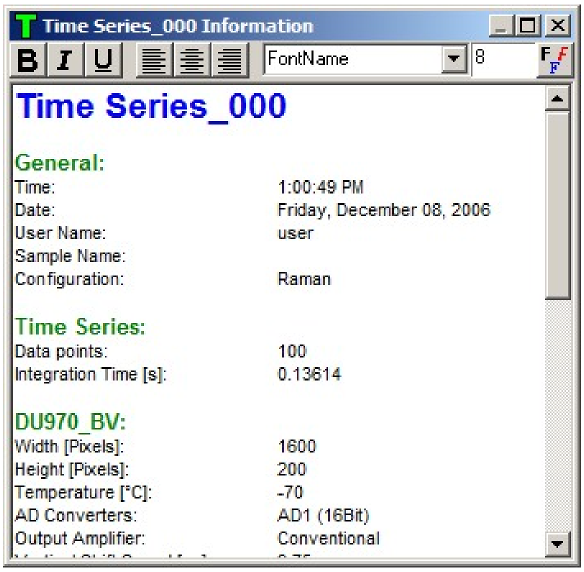
The context menu is an alternative way for accessing the features that you also can find in the circle menu. Just click and release the right mouse button anywhere in the viewer.

Options / Change Defaults
This will open the program options for the graph viewer.

At the bottom of the context menu you can find a list of data objects that are used by the viewer:

- graphs that are displayed (sub menu)
- the X-Axis Interpretation, which you can use to switch between different units (e.g. rel. 1/cm or eV).

Text Viewer



The Text Viewer can show text data objects that contain text in rich text format (RTF).

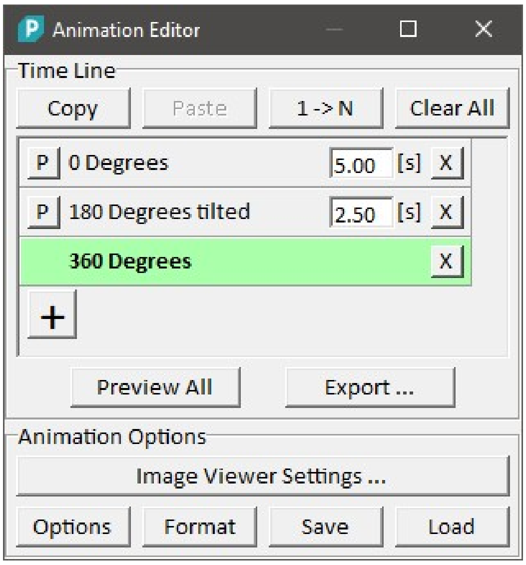
Just double-click a text object to create a Text Viewer. If the text object is already shown in a text viewer, no new viewer is created but the existing text viewer will come on top of all windows.

You can type, format, copy and paste text in the text viewer.

It's possible to **export** one or multiple text objects into a .txt (ASCII) or .rtf (Rich Text Format) file, see Export Overview.

Animation Editor

The animation editor is used to create user defined animations by defining any number of steps.
The editor is used by the Image Viewer and the Image Transform and Overlay Dialog.



Copy:
Copies the selected step to the "local clipboard".

Paste:
Pastes the copied step from the clipboard after the selected step.

1 -> N:
Copies the first step to the end.
Angles are measured continuously (e.g. -200° or +540°). This can result in a complete rotation or even more back to e.g. 45° when using this button, To prevent this, select the first step in the list and open the Image Viewer Settings. Enter e.g. 360 and click on Custom Rotate to add one full rotation to the first step as new step.

Clear All:
Clears all steps.

Preview Step ("P" Button):
Shows the preview for the step.

Step Name ("0 Degrees" Label / Edit):
This is the step name.
You can select a step or edit the step name by clicking on the text.

Interval Time ("5.00 [s]" Edit):
Changes the interval time for the step.

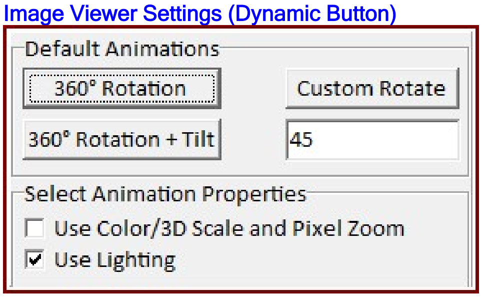
Delete ("X" Button):
Deletes the step.

Add New Step ("+" Button):
Adds a new step.

Preview All (Button)
Shows a preview animation for all steps.

Export (Button)
Exports the animation using the current Image Export Options.
The aspect ratio and resolution of the exported data is defined by the window size.

Image Viewer Settings (Dynamic Button)

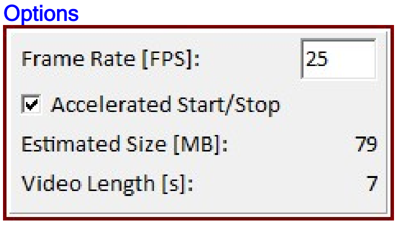


Depending on which software component uses the animation editor, it shows options for the special component:

- Default Animations: one or more default animation, overwrites the current steps.
- Custom Rotate: Adds a new step with a rotation defined by the value below in °.
- Use Color/3D Scale and Pixel Zoom: Also changes of the Color or z scale are recorded.

- Use Lighting: Also in changes of the Lighting are recorded

Options



Shows animation options:

- Frame Rate: defines the frame rate for AVI videos
- Accelerated Start/Stop: if checked, the first and last step are accelerated and not linear.
- Estimated Size: Shows the estimated size of the file(s). Not valid for compressed AVI files.
- Video Length: Shows the video length / sum of all step intervals.

Format

Opens the Image Export Options to define the export format and open settings.

Save

Saves the current animation to the hard drive.

Load

Loads an animation from the hard drive.

Data Analysis Overview

This chapter shows all important software features for analyzing your data.

- Drop Actions Window
  contains Technical Documentation of all Drop Action Dialogs.

- Raman Analysis
  shows a list of all important analysis features used for a Raman Image Scan analysis.

- Database Search in WITec Project
  shows an overview of using a database search in WITec Project.

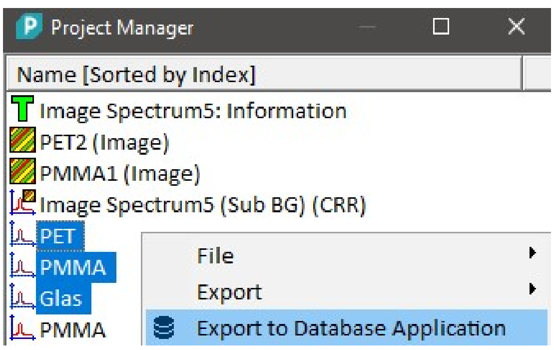
Database Search in WITec Project

It's possible to use a Spectrum Database to search for unknown components.
For this WITec developed the search software WITec TrueMatch. It's also possible to use the ACDLabs Software.
You can create your own databases or use the commercial database ST Japan.

There are several ways to get spectra into the WITec TrueMatch Database Software or ACDLabs.
Before you use one of them, make sure you have configured the Database Export Options.

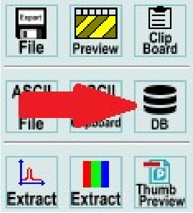
Project Manager

You can select multiple single spectrum data objects in the Project Manager and use the Context Menu "Export To Database Application":



Graph Viewer

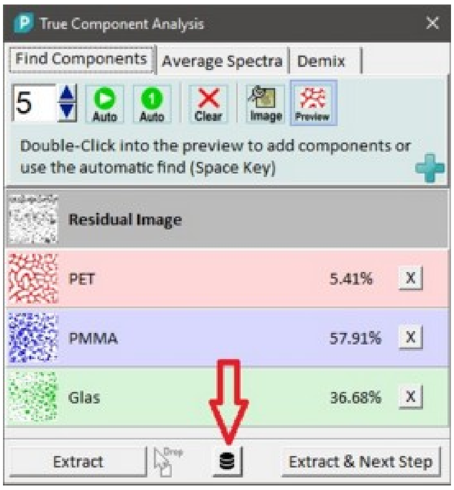
All visible spectra in the Graph Viewer can be sent to the TrueMatch Software using Circle Menu or Context Menu "Export -> Export to Database Application" (Shortcut E):



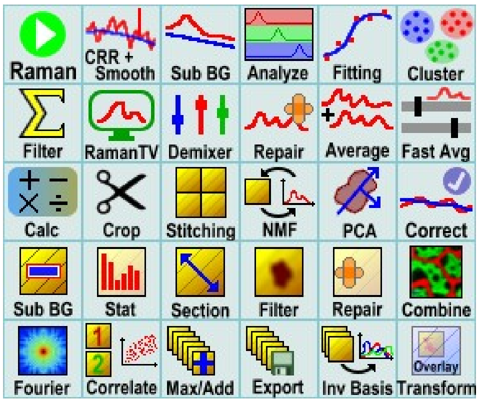
If a certain region is marked using the Graph Viewer Mouse Marker, only the selected region is sent to the TrueMatch Software.

True Component Analysis

You can directly put your analysis result spectra into the TrueMatch Software using the Database Button in the True Component Analysis Dialog:



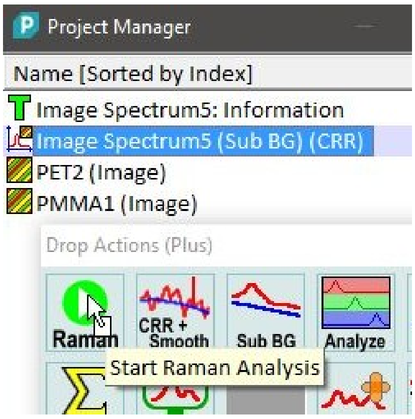
Drop Actions Window



Click on one of the Drop Action buttons to see the corresponding help page.

The Drop Actions window is the portal for all data analysis features of WITec Project.

To use the Drop Action features you have to drag one or several selected Data Objects from the Project Manager and drop them onto one of the Drop Action buttons:



Depending on the chosen Drop Action this will either start a calculation or open a dialog together with a preview window. The latter allows the effect of changing the parameters to be observed before starting the calculation on all data.

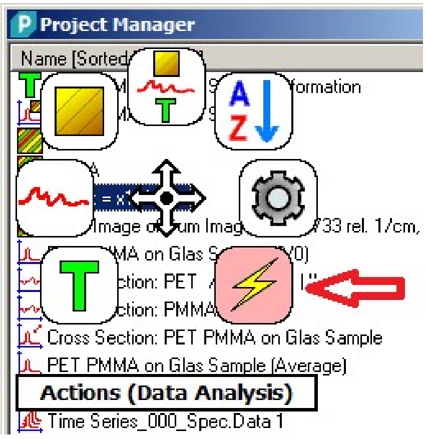
The "Extract" button(s) in each of the Drop Action dialog windows will calculate the result and create new Data Objects in the current Project.

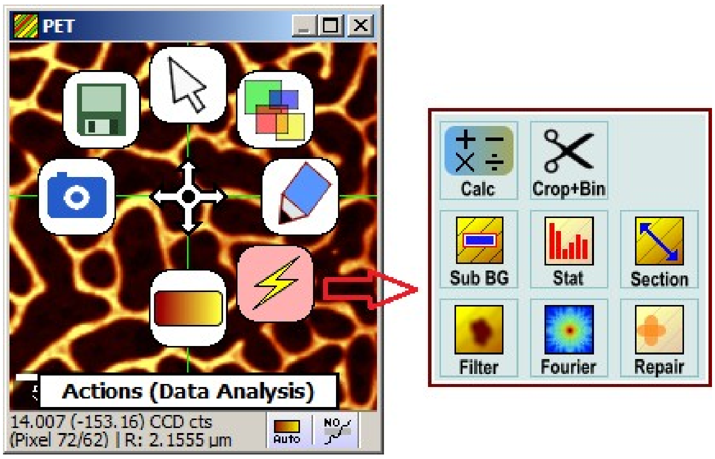
You can show or hide the Drop Actions window using the main menu "View > Drop Actions Window".
If the window is hidden, it will automatically pop up temporarily near the mouse position upon dragging items from the Project Manager.

A good way for starting a Raman analysis is the "Start Raman Analysis" button, which will start the first analysis step.

Another way of starting data analysis

Alternatively, you can directly open the action circle menu in the Project Manager or Image- or Graph-Viewer and click on one of the Action buttons:





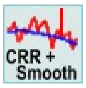
Raman Analysis

If you have measured a Raman Image, you can just start your analysis by dropping your dataset on the Start Raman Analysis Drop

Action. The "Extract & Next Step" Buttons in the dialogs will guide you through the different steps of the analysis.

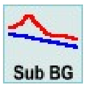
Start Raman Analysis

This will open the first dialog for the analysis, the Cosmic Ray Removal Drop Action:



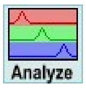
Cosmic Ray Removal

After removing the cosmic rays, you can go on with the Background Subtraction:



Background Subtraction

Now the data is prepared for further analysis. The True Component Analysis can be used in the next step. It helps finding all the components, creates nice images and spectra for each component:



True Component Analysis

The result component images can be presented very nicely using a smoothing algorithm, if desired:

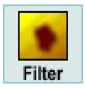


Image Smoothing

Multiple component images can be combined in a single, multicolored bitmap using the image combination dialog:

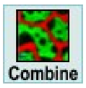
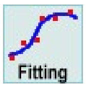


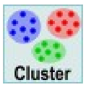
Image Combination

If your measurement has peak shifts due to certain effects, you can use the Advanced Fitting Tool to fit your peaks automatically:

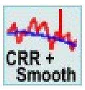


Advanced Fitting Tool

The Cluster Analysis helps finding out differences in spectra and how many components are in your measurement:



Cluster Analysis



Graph Smoothing and Cosmic Ray Removal Dialog

Description

With this dialog it is possible to apply several spectral smoothing filters on spectra or to do a cosmic ray removal, which is the first step of the spectra preprocessing.

Input and Results

Input:
one or multiple Graph Objects (single spectra, line or image Graph Objects).

Results:
a smoothed or cosmic ray removed graph Data Object.

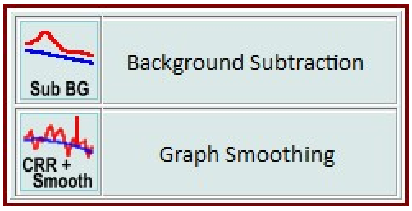
User Interface

- Savitzky-Golay Tab
- Median Tab
- Average Tab

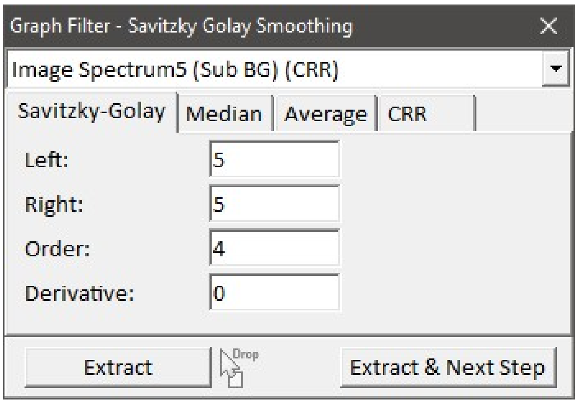
- CRR Tab
- Preview Window

Extract (Button & Drop Zone)
Press the "Extract" button in order to start the currently selected smoothing or cosmic ray removal algorithm on all spectra of the input graph object.
You can also drag and drop multiple graph objects from the Project Manager onto this button in order to do a batch processing using the same algorithm and settings.

Extract & Next Step (Button)
Wizard Feature: you can choose whether you would like to do a background subtraction or further graph smoothing algorithms with the result of the current calculation:



Savitzky-Golay Tab
If the "Savitzky-Golay" Tab is selected, the graph is smoothed using the Savitzky-Golay Filtering algorithm.



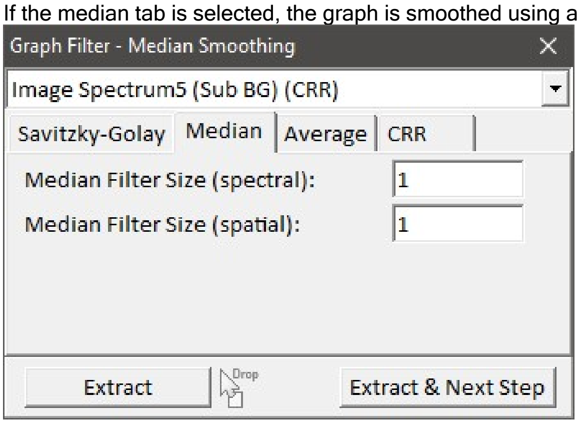
Left (Integer Edit):
defines the window size of the smoothing algorithm (left from the current pixel)
The total window size is Left + Right + 1.

Right (Integer Edit):
defines the window size of the smoothing algorithm (right from the current pixel)
The total window size is Left + Right + 1.

Order (Integer Edit):
the order of the polynomial which is fitted to the smoothing window.

Derivative (Integer Edit):
defines the order of derivative of the filter. A value of 0 means no derivation, i.e. "only" a smoothing is done.
If a value of 1 is entered the calculated result will be the first derivative; the yielded data can be used e.g. not to be being sensitive to fluorescence when doing a basis analysis.

Median Tab
If the median tab is selected, the graph is smoothed using a median filter algorithm.



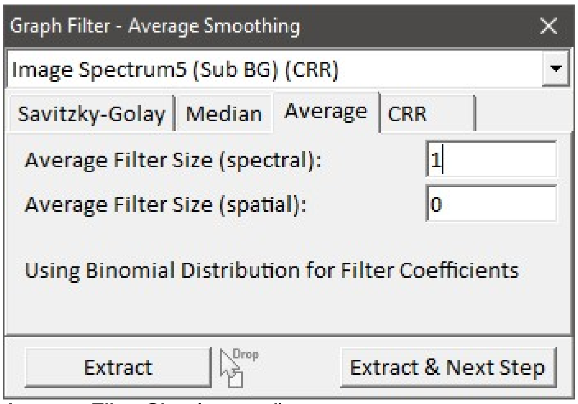
Median Filter Size (spectral):
the spectral filter size for the median filter. The total spectral window size is 2*<Filter Size> + 1.

Median Filter Size (spatial):
the spatial filter size for the median filter. If larger than zero, the spectra of neighbored scan pixels are used for smoothing.

The total window size is <Filter Size * 2 + 1>^2 multiplied by the total spectral window size.

Average Tab

If the average tab is selected, the graph is smoothed using a average filter algorithm that uses binomial distributed filter coefficients.

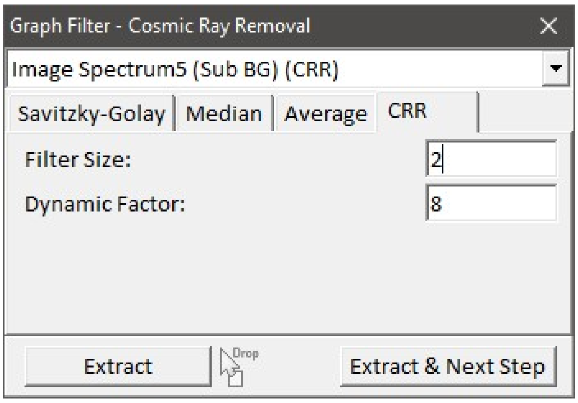


Average Filter Size (spectral):
the spectral filter size for the average filter. The total spectral window size is 2*<Filter Size> + 1.

Average Filter Size (spatial):
the spatial filter size for the average filter. If larger than zero, the spectra of neighbored scan pixels are used for smoothing.
The total window size is <Filter Size * 2 + 1>^2 multiplied by the total spectral window size.

CRR Tab

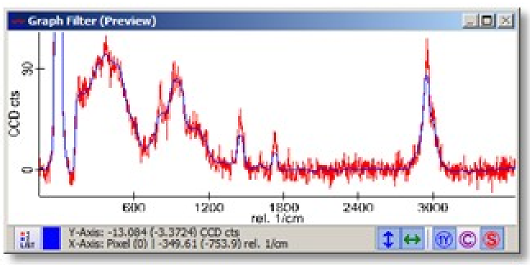
If the CRR tab is selected, cosmic rays will be removed from the graph using an cosmic ray detection algorithm.



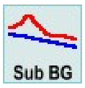
Filter Size:
the filter size of the cosmic ray detection algorithm. The total window size is 2*<Filter Size> + 1.

Dynamic Factor:
this factor changes the sensitivity of the cosmic ray detection algorithm (a smaller value means a higher sensitivity).

Preview Window



The preview graph viewer window shows the original graph object as a red graph and the result preview as a blue graph.



Graph Background Subtraction Dialog

Description

With this dialog a background can be subtracted from one or multiple spectra using various algorithms.
If used on a multi-spectral data set, all spectra can be corrected at once using the same mask and algorithm.

Input and Results

Input:
One graph object that can be a single spectrum or a multiple spectra object (e.g. Image Graph).

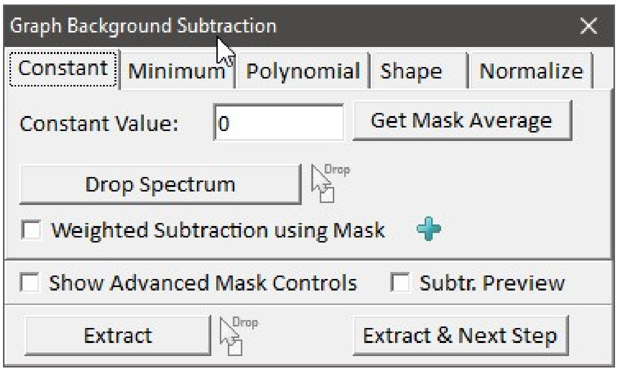
Results:
A copy of the input graph object, background subtracted.
Suffix: (Sub BG)

User Interface

- Constant Tab
- Minimum Tab
- Polynomial Tab
- Shape Tab
- Normalize Tab
- Advanced Mask Controls
- Preview Window

Constant Tab and General UI

If the "Constant" tab is selected, the background is subtracted using a static constant user definable value and/or using a single spectrum which is subtracted from all input spectra.



Constant Value (Float Edit)
The constant value will be subtracted from all pixels and all spectra.

Get Mask Average (Button)
Press this button to set the constant value to the average value of all pixels that are currently set in the mask using the current preview spectrum.

Drop Spectrum (Button & Drop Zone)
You can drop a single spectrum onto this button in order to subtract this spectrum from all your input spectra. Click the button if you do not want to use the single spectrum for subtraction anymore.
The Constant Value will be set to zero if you drop a single spectrum; however, but you can enter a constant offset afterwards for an additional constant value subtraction.

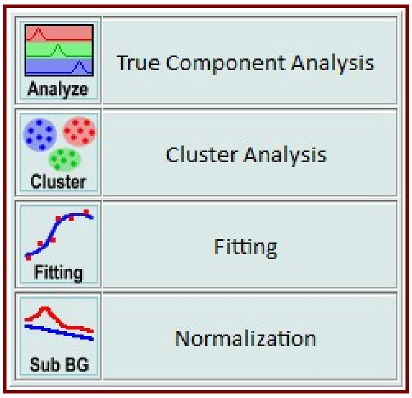
Weighted Subtraction using Mask (Check Box)
If checked, you can change the mask in order to define which spectral area should be used for calculating a weighting factor for subtracting a dropped single spectrum. This is a plus feature.

Subtr. Preview (Checkbox)
If checked, the blue preview graph shows the subtracted spectrum preview instead of the line, that will be subtracted.

Extract (Button & Drop Zone)
performs the background subtraction for all spectra of the input graph data object and adds the result to the current project.
You can drag and drop multiple other graph Data Objects onto this button for batch processing.

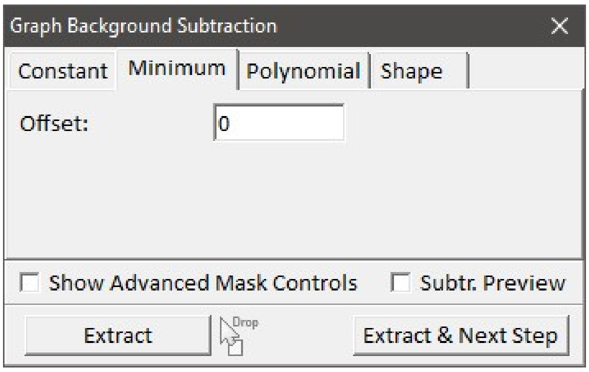
Extract & Next Step (Button)

Wizard Feature: With this Button, you can choose whether you would like to use the result of this dialog and do a true component analysis, a cluster analysis, peak fitting or a normalization



Minimum Tab

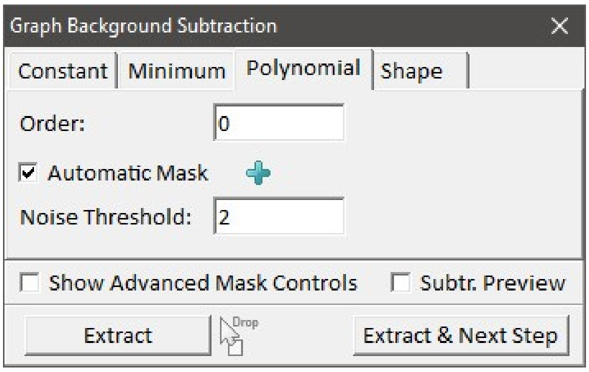
If the "Minimum" tab is selected, the background is subtracted using a horizontal line at the minimum value of all spectral pixels in the marked area.



Offset (Float Edit):
Adds an offset to the found minimum value.

Polynomial Tab

If the "Polynomial" tab is selected, the background is subtracted by fitting a n-order polynomial to the masked spectrum.
If this background subtraction mode is used, all Raman peak areas should be removed from the mask - unless you use the automatic mask mode.

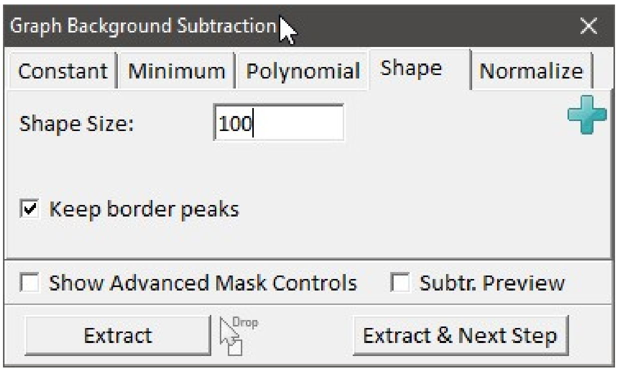


Order (Integer Edit):
The order of the polynomial for fitting the background. An order of 0 will subtract a horizontal line, an order of 1 will subtract a slope, e.c.

Automatic Mask (Check Box):
If checked, the algorithm tries to ignore peaks by automatically use spectral noise pixels only. Thus you can also set the mask at pixels where you have Raman information.
This is a WITec Project Plus feature.

Noise Threshold (Float Edit):
The noise threshold for the automatic polynomial mode. You can shift the background level horizontally by changing this parameter.
It is only available, if the "Automatic Mask" mode is enabled.

Shape Tab
If the "Shape" tab is selected, the background is subtracted using a rounded shape which is approached to the spectrum from below pixel by pixel of the spectrum. The shape method is very effective for subtracting fluorescence areas and it is quite easy to use.
It is a WITec Project Plus feature.

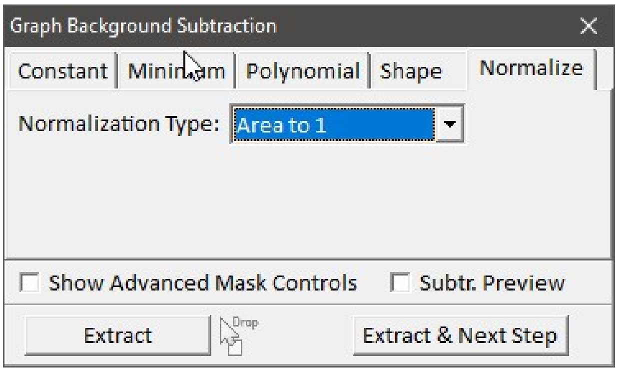


Shape Size:
The size of the rounded shape. A smaller size will subtract more details from the spectrum, whereas a larger size will subtract more rough shapes.

Keep border peaks:
If not checked, then peaks at near the border pixels are subtracted.

Mask:
Use the blue mask for a linear interpolation of pixels.

Normalize Tab
If the "Normalize" tab is selected, the spectrum will be normalized to a desired value.

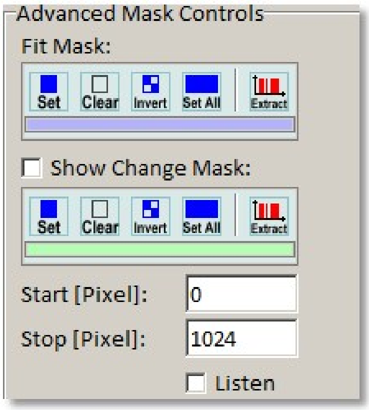


Normalization Type:
Area to 1 - The area within the mask will be 1
Area Absolute to 1 - The area within the mask will be 1, using an absolute value for negative values
Max Peak to 1 - The maximum spectrum value within the mask will be normalized to 1
Max Peak to 100 - The maximum spectrum value within the mask will be normalized to 100

Mask:
Use the blue mask to define which part(s) of the spectrum should be used for normalization.

Advanced Mask Controls

Show Advanced Mask Edits (Check Box):
If checked, the advanced mask edits are shown. These edits are optional, you can change the masks directly in the preview graph viewer.

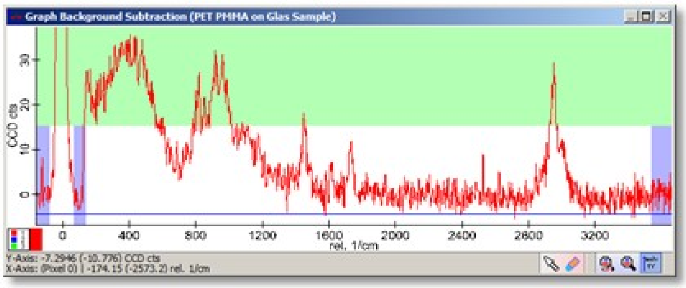


Fit Mask (Mask Tool Bar):
With those tool buttons you can modify the blue fit mask (using the Start / Stop [Pixel] Edits).

Show Change Mask (Check Box):
if checked, there is an additional, green mask in the graph preview window that can be manipulated. With the tool buttons below you can modify the change mask (using the Start / Stop [Pixel] Edits).
Clearing pixels in the change mask will flatten the result spectrum at this position using the value of the last masked pixel. This could be useful e.g. if a polynomial fit has very extreme values at the borders of a spectrum.

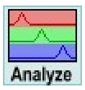
Start / Stop [Pixel], Listen (Edits, Check Box):
see Mask Manipulation Tools.

Preview Window



The Preview Window shows the original graph object in red as well as a blue preview curve that will be subtracted from the original.

If a multi-spectral graph object (line spectrum, image spectrum) is used, you can click on any pixel in an image to see the preview of the selected spectrum.



True Component Analysis Dialog

Description

The True Component Analysis Dialog is the successor of the Basis Analysis Dialog. It creates intensity distribution images that show the distribution of different components. In the WITec Project Plus Version, the dialog finds components automatically, creates average component spectra and supports demixing of spectra.

Input and Results

Input:

- One spectral Raman image data set OR
  One spectral line graph data set (e.g. spectra along a line) and
- <n> Component Spectra (can be added via drag drop or using the find component feature of the dialog)

Results:

- One image for each component spectra showing the intensity distribution for this spectrum
  or

One single spectrum for each of the single spectra if a line graph data set is used.

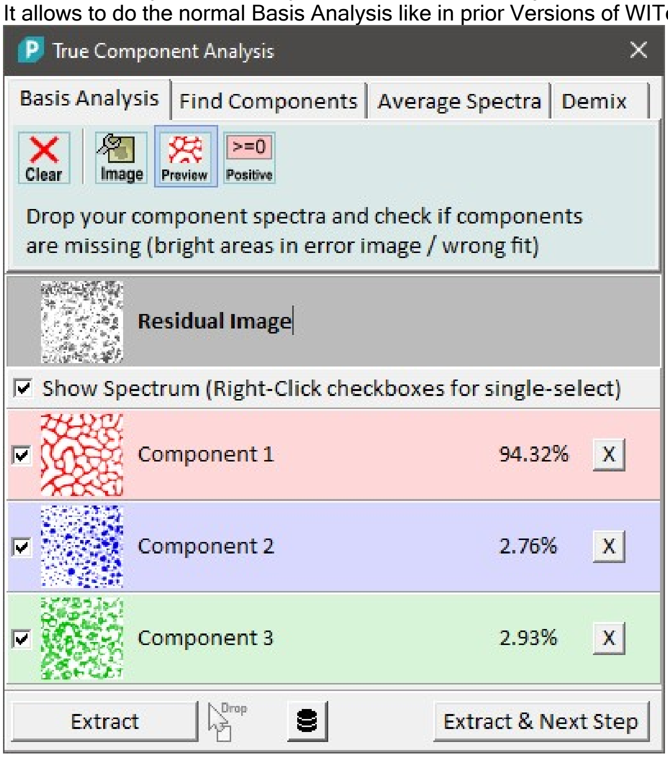
- Average Component Spectra if added using the find component feature.

User Interface

- Basis Analysis Tab
- Find Components Tab
- Average Tab
- Demix Tab

Basis Analysis Tab and General UI

The Basis Analysis Tab is only visible, if the WITec Project PLUS Version is not active.
It allows to do the normal Basis Analysis like in prior Versions of WITec Project.



Clear (Tool Button)
Press clear to delete all component spectra.

Image (Tool Button)
Shows options for changing the preview thumbnail size.

Preview (Tool Button)
Turns the preview calculation on or off. If turned on (default), the basis analysis is calculated for the whole image graph data object and shows a preview image for the currently selected component or the residual image.
For very large datasets, this feature is turned off by default and can be turned on by the user.

Positive (Tool Button)
If checked, negative weighting factors will be set to zero. This way you can e.g. check whether you have mixed spectra.

Residual Image (First List Entry)
Shows a preview thumbnail for the residual components. You can click on this entry to select the residual image as a large preview in the image viewer. In this image bright areas show you which components are missing so you can find and add them to your list of components.
In the demix mode, this image shows bright areas on components that might be mixed so you can demix it easily.

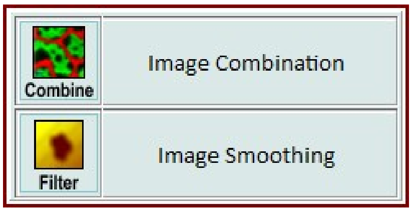
Show Spectrum (Check Box)
Here you can show or hide all components from the preview graph window.

Component 1, 2, ... (Further List Entries)
The check boxes can be used to show or hide each individual component spectrum in the preview graph window.
Shows a preview thumbnail of the intensity image for this component.
You can edit the name just by clicking on the label "Component 1".
The percentage label shows you how much of each component is mixed to describe the currently selected spectrum.
The X button simply lets you delete the component from your list.

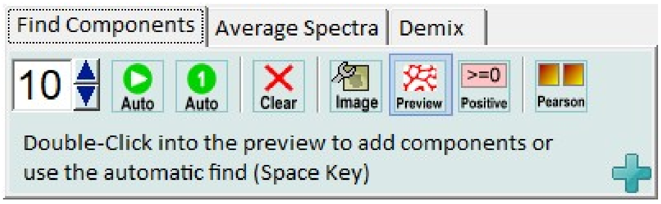
Extract (Button)
Extracts the intensity distribution images and average component spectra (if created by the dialog) in your project.
You can drop multiple image graph data objects on this button for batch processing.

Export to Database Application (Button)
Exports all component spectra to the database application, e.g. to WITec TrueMatch or ACDLabs

Extract & Next Step (Button)
Wizard Feature: you can choose whether you would like to use the result images of this dialog as an image combination or do some image smoothing:



Find Components Tab



This is a WITec Project Plus Feature!

Number Edit and Up/Down Buttons
Sets the number of spectra for the automatic component finder. Just select a number of components and press "Auto".

Auto (Tool Button)
Starts the automatic component finder. Automatically finds and adds a desired number of spectra.

Auto 1 (Tool Button)
Automatically adds one component using the current residual image.

Clear (Tool Button)
Deletes all your component spectra.

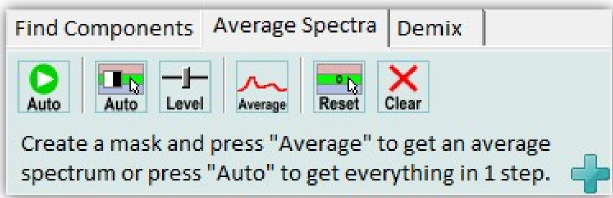
Image (Tool Button)
Shows Options for adding and finding components, see Advanced Options.

Preview (Tool Button)
Starts the automatic component finder.

Positive (Tool Button)
If checked, negative weighting factors will be set to zero. This way you can e.g. check whether you have mixed spectra.

Pearson (Tool Button)
Exports all component images using the Pearson correlation coefficient. Uses the spectral mask for calculation.

Average Spectra Tab



This is a WITec Project Plus Feature!

Auto (First Tool Button)
This will calculate the average spectrum for all your components.

Auto (Second Tool Button)
Automatically calculates an image mask for the currently selected component.
This mask can be edited or directly used for calculating an average spectrum (just press the Average Tool Button).

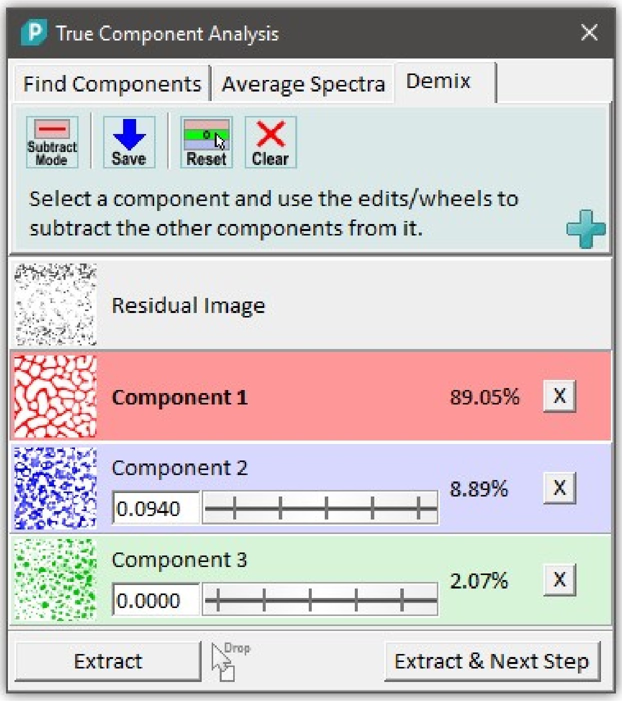
Level
This opens the threshold mask tool of the image viewer in order to define which pixels should be set in the image mask.
This mask can be edited or directly used for calculating an average spectrum (just press the Average Tool Button).

Average
This will calculate the average spectrum for the selected component using the current image mask.
You can use the Automatic Mask or level/threshold tool to define the mask or use the custom image viewer mask tools to define your own mask.

Reset
Resets the average operation of the currently selected spectrum.

Clear
Resets all average operations of all components.

Demix Tab



This is a WITec Project Plus Feature!

Subtract Mode (Tool Button)
If checked, the selected component can be subtracted from all the other components by changing the weighting factors.
If not checked, the selected component will be changed by subtracting the other components using the weighting factors.

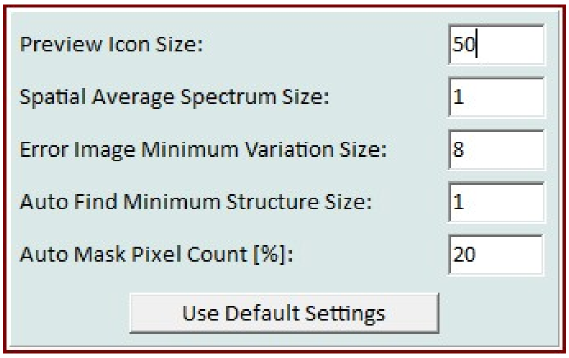
Save (Tool Button)
Saves the current demix in order to subtract a demixed spectrum from the other spectra.

Reset (Tool Button)
Resets the demix of the currently selected component (sets all weighting factors to zero). This will not reset saved demixes.

Clear (Tool Button)
Resets all demixes.

Weighting Factor (Number Edit and Wheel Control)
You can simply turn the wheels or edit the number to define a weighting factor for subtracting the spectra from each other.

Advanced Options



Preview Icon Size
This will change the size of your preview icons / thumbnails in your component list.

Spatial Average Spectrum Size:
If a spectrum is added using the double-click or the auto find algorithm, your component spectra will be an average of the nearby pixels. This parameter defines the spatial average size of this spectrum.

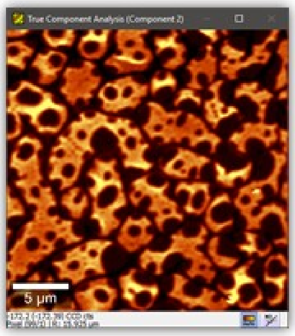
Error Image Minimum Variation Size:
A parameter defining how noise is treated when calculating the error image. A higher value avoids noise.

Auto Find Minimum Structure Size:
The structure size of an automatically found spectrum must be larger than this value.

Auto Mask Pixel Count:
In the Average Tab, you can automatically calculate an image mask for the selected component. This parameter gives you the chance to only select the most "important" pixels, avoiding to select pixels on edges of a structure leading to mixed spectra.

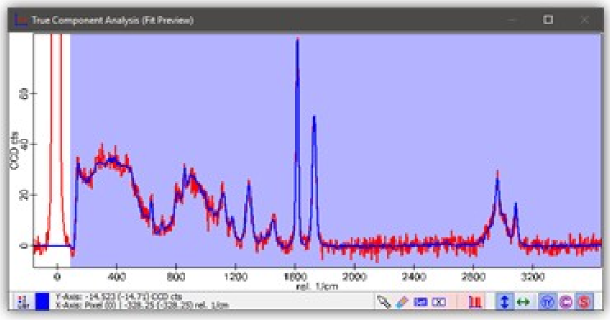
Preview Windows

Residual Image / Intensity Image



This image preview window shows the residual image or one of the component distribution images.
In the WITec Project PLUS Version, you can double click into this image to add a selected spectrum as a new component. The residual image will show you the missing components.

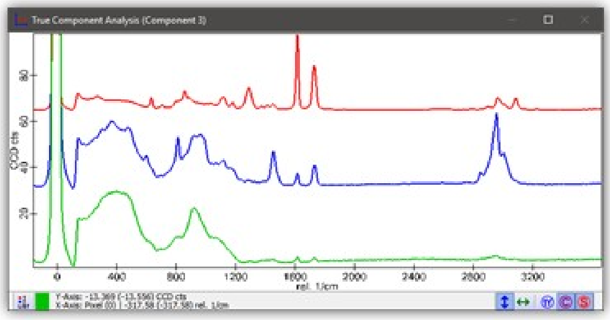
Fit Preview and Mask



The fit graph preview window shows the original spectrum in red and the fit preview in blue. This preview is the linear combination of the all component spectra that fits the original spectrum the best.
Just click somewhere in the preview image to see the selected spectrum and the fit curve using your components.

Use the mask to define which spectral area should be considered for fitting your component spectra combination.

Component Spectra



This graph preview window shows the component spectra which were dropped by the user or added using the dialog.

Basis Analysis Dialog

Description

Deprecated. In WITec Suite 5.0 and newer, the Basis Analysis Dialog was replaced by the True Component Analysis Dialog.

The Basis Analysis Dialog creates intensity distribution images that show the distribution of different components.

Input and Results

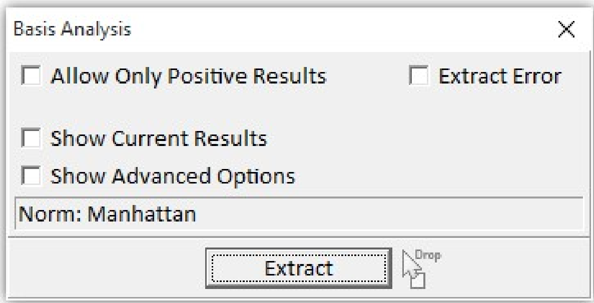
Input:

- <n> single spectra (normally each containing a pure component spectrum)
  and
- one spectral Raman image data set OR
  one spectral line graph data set (e.g. spectra along a line)

Results:

- One weighting factor image for each of the <n> single spectra showing the intensity distribution for this spectrum
  or
- One single spectrum for each of the single spectra if a line graph data set is used.

User Interface



Allow Only Positive Results (Check Box):
if checked, the fitting method is constrained, allowing only positive results. Otherwise, results may contain negative values.
You can use this feature to find out if you are missing basis components or if you have mixed spectra:

- Fit works with checkbox unchecked:
  You have found all basis components.
- Fit works with checkbox unchecked, but fit doesn't work with checkbox checked:

You have mixed spectra

- Fit works with checked and unchecked checkbox:
  Everything is ok: all basis components found and no mixed spectra

Extract Error (Check Box):
if checked, the Basis Analysis Error Image will be extracted. The error image shows higher intensities for spectra where the fit did not work properly. This can help you to find components not regarded by the current set of basis spectra.

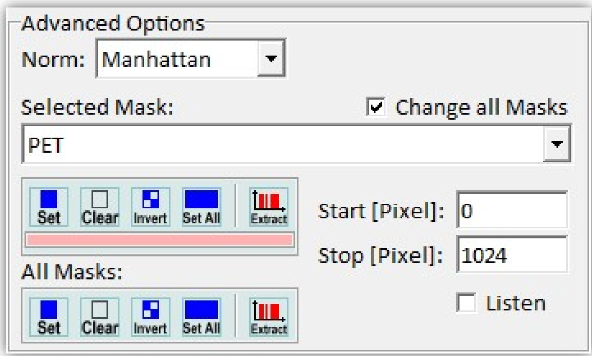
Show Current Results (Check Box):
shows the weighting factors for the current preview spectrum in the bottom list view (white area).
You can edit the name of each basis spectrum which will used in the result data objects.

Show Advanced Options (Check Box):
shows advanced options and the mask tool bars for changing the mask via edits or listen modes.

Norm (Status Information):
shows the current norm mode; can be changed in the advanced options.

Extract (Button and Drop Zone):
calculates the basis analysis fit for all pixels and creates the result data objects.
You can drag and drop other image graph (or line graph) data objects onto the "Extract" button for batch processing.

Advanced Options



Norm (Combo Box):
changes the normalization mode:

- None
- Manhattan
- Euclidean.

Change all Masks with Marker (Check Box):
if checked, all masks of all basis spectra are modified simultaneously if you add or clear a mask area of one of the masks in the mask preview window using the marker. Otherwise only the mask which is under the mouse position is changed.

Selected Mask (Combo Box and Mask Tool Bar):
You can select one of the input basis spectra in order to decide which basis spectrum mask will be changed by using the graph mask edits and mask tool buttons.
With the Mask Tool Bar you can change the mask of the selected basis spectrum. The color below the tool buttons shows the color of the chosen mask in the basis spectrum mask preview window.
These edits are optional; in many cases it is easier to change the masks directly in the preview graph viewer.

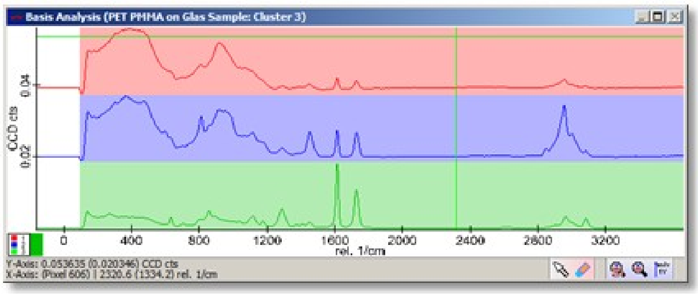
All Masks (Mask Tool Bar):
change all basis spectrum masks simultaneously (also using the Edits and Listen Modes)
Also these edits are optional; in many cases it is easier to change the masks directly in the preview graph viewer.

Start / Stop [Pixel], Listen (Edits, Check Box):
see Mask Manipulation Tools.

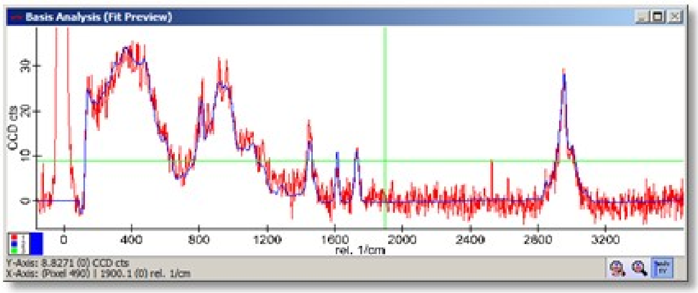
Preview Windows

Basis Spectrum Masks

This graph preview window shows the input single spectra which will be used as basis spectra. You can change the masks of all spectra simultaneously or the mask of each basis spectrum separately to define which spectral pixels should be considered for the fit. **At least clear the Rayleigh area should be removed from all masks!**

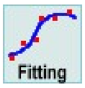


Fit Preview



The fit graph preview window shows the original spectrum in red and the fit preview in blue. This preview is the linear combination of the complete set of basis spectra that fits the original spectrum the best.

If a multi-spectral graph object (line spectrum, image spectrum) is used, you can click on any pixel in a corresponding image to see the preview of the selected spectrum.



Advanced Fitting Tool Dialog

Description

With the Advanced Fitting Tool it is possible to do simple as well as more advanced curve fitting. The tool enables peak fitting as well as other curves like exponential or polynomial curves or even a user defined functions.

Input and Results

Input:
One graph object (single spectra or hyper spectral data object).

Results:

- For input single graph objects: a text object containing all fit parameters.
- For input line graph objects: one spectrum for each fit parameter.
- For input image graph object: one image for each fit parameter.

How do I ... ?

Save my fit function parameters to use it again later:

1. Change your function parameters in the Fit Parameters Tab.
2. Open the Fit Function Tab and press "Add" above the Fit Function List. This will add the currently selected function and all its current parameters to the category "User".
3. Select the newly added function in the "User" category. Now you can change its name as desired.

Use my own fitting function formula:

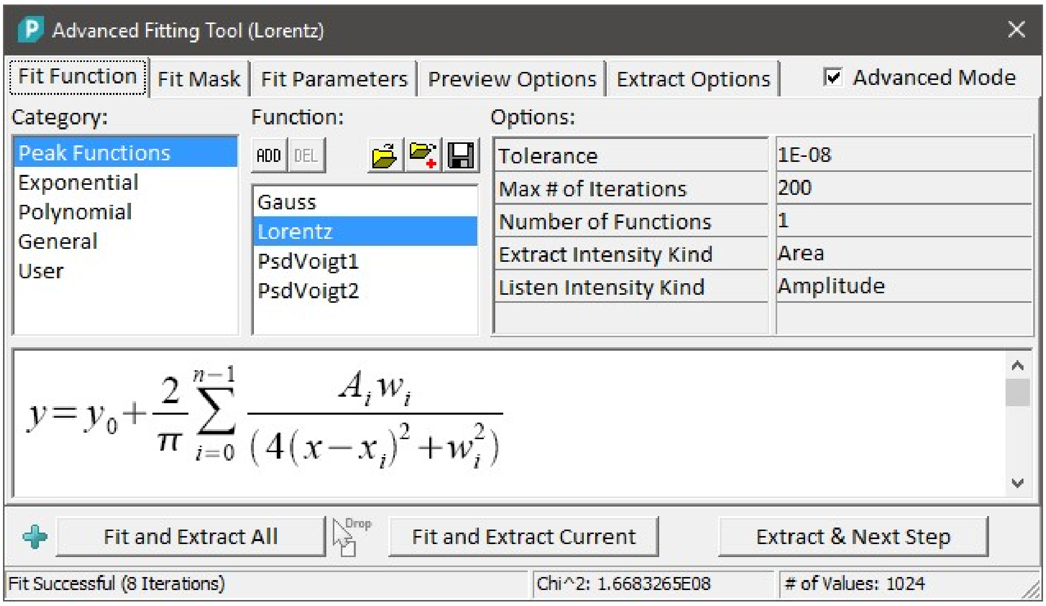
1. Open the Fit Function Tab and select the category "General". Select the fitting function "User Defined".
2. Change the number of fit parameters.
3. You can define each fit parameters' name and unit by setting the parameter number first (Parameter #) and then change the rest of the parameters.

User Interface

- Fit Function Tab
- Fit Mask Tab
- Fit Parameters Tab
- Preview Options Tab
- Extract Options Tab

- Preview Window
- Fit Function Options

Fit Function Tab



Category (List Box):
Select a fit function category here. The "Function" list will be updated upon selecting another category.

Function (List Box):
Select a fit function here.

Add (Tool Button):
Adds the currently selected function and all its current settings and parameters as a user fit function. An additional category "User" will be created where the added functions can be found.
All functions added by a user will be saved automatically when closing the dialog ("per user" setting).

Del (Tool Button):
Removes a user defined function from the user function list.

Open (Tool Button):
Opens a WITec User Fit Functions file and replaces the current user fit functions.

Append (Tool Button):
Opens a WITec User Fit Functions file and adds the loaded fit functions to the current user defined fit functions.

Save (Tool Button):
Saves the current user fit function list into a file.

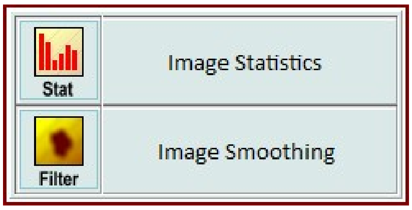
Options (Parameter List):
Some standard fit algorithm parameters can be changed here (like tolerance and number of iterations). Each fit function may also have its own parameters like extraction kind for some parameters or the number of curves e.g. for multiple peak fitting.
See Fit Function Options.

Description (Graphic Box):
Shows the fitting formula and all its parameters. You can move the graphic by clicking and moving it or by using the scroll bars.

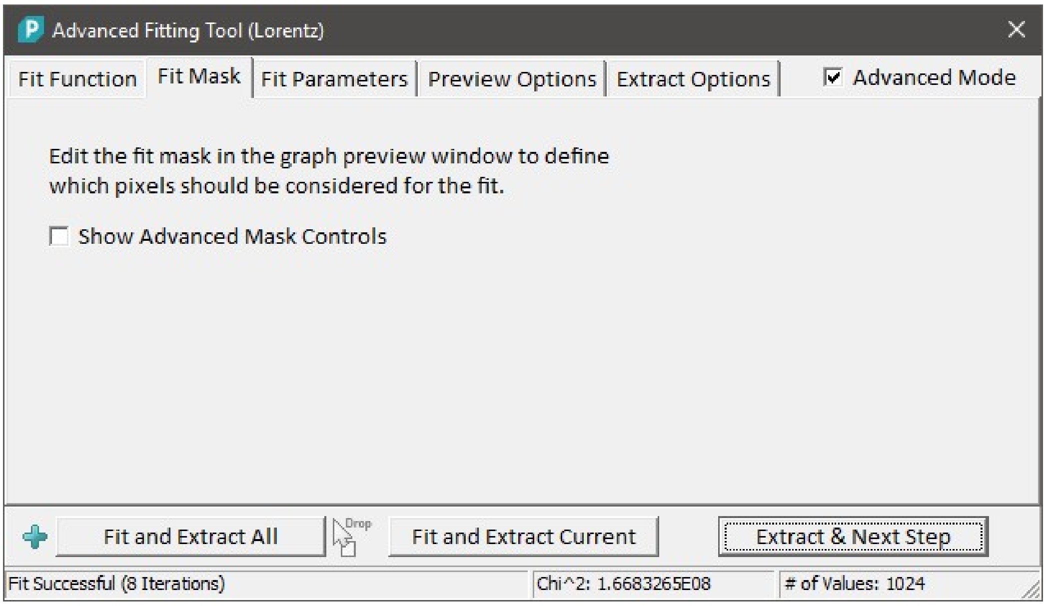
Fit and Extract All (Button, Drop Zone):
Starts the fitting calculation for all spectra in the current hyper spectral data set. You can also drop (multiple) data objects from the project manager onto this button in order to do batch processing. This is a WITec Project Plus feature.

Fit and Extract Current (Button):
Starts the fitting calculation for the currently selected spectrum and extracts the results.

Extract & Next Step (Button):
Wizard Feature: you can choose whether you would like to use the result images of this dialog in the image statistics dialog or do some image smoothing:



Fit Mask Tab

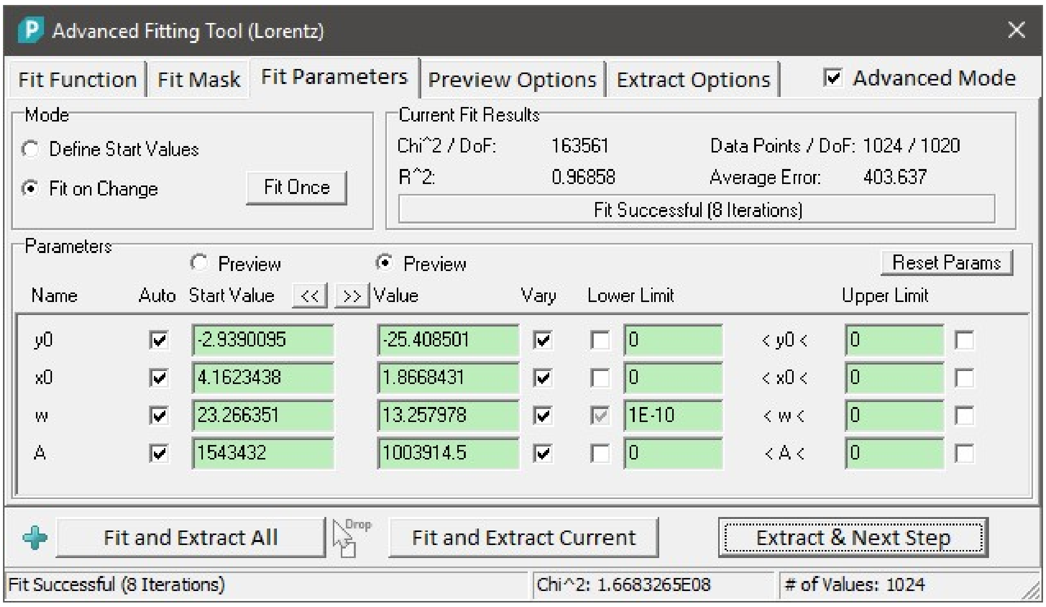


You can change the fit mask in order to define which pixels should be considered for the fitting algorithm. These edits are optional, you can also change the masks directly in the preview graph viewer.

Advanced Mode

If the advanced mode is turned on, there is access to all fit parameters and preview/extract options.
This is necessary if you e.g. do a multiple peak fit or a user defined fit function in order to define start values for all fit parameters.

Fit Parameters Tab



Mode

Define Start Values (Radio Button):
Select this mode in order to define the start values of the fit. This will show a fit function using the start values as a blue preview curve in the preview graph viewer in order to facilitate the finding of good start values.

Also select this mode if you would like to change any parameter or limit without doing an automatic fit: The values in the "Start Value" column (or "Value" column resp.) are preserved.

Fit on Change (Radio Button):
Select this mode if the fit should automatically be calculated if any parameter or limit is changed, or even if another spectrum is selected by clicking to another position in e.g. an image.
This is the default mode.

Fit Once (Button):
Click this button to execute the fit algorithm once.

Current Fit Results

Indicates whether the last fit was successful or not and shows typical fit result information.

Parameters

Show all the fit function parameters. Note that all green edits can be double-clicked in order enable the listening to a mouse action done in a viewer window.

Reset Params (Button):
Resets all parameters, values, start values, limits and all check boxes to their default values.

Name (Label Column):
Shows the name for each function parameter. Drag over the label with the mouse in order to get a more detailed information.

Auto (Check Box Column):
If checked, the start value for the function parameter will be calculated automatically when doing a fit.
If using multiple peak functions or user defined functions, this feature is not possible.

Start Value (Float Edit Column):
Shows the start values for all parameters.

Preview (Start Value Column Radio Button):
If this Radio Button is checked, the blue graph in the preview graph viewer will show the current fit function using parameters from the start value column (automatically estimated or defined by the user).

Value (Float Edit Column):
Shows all parameters of the current fit result.

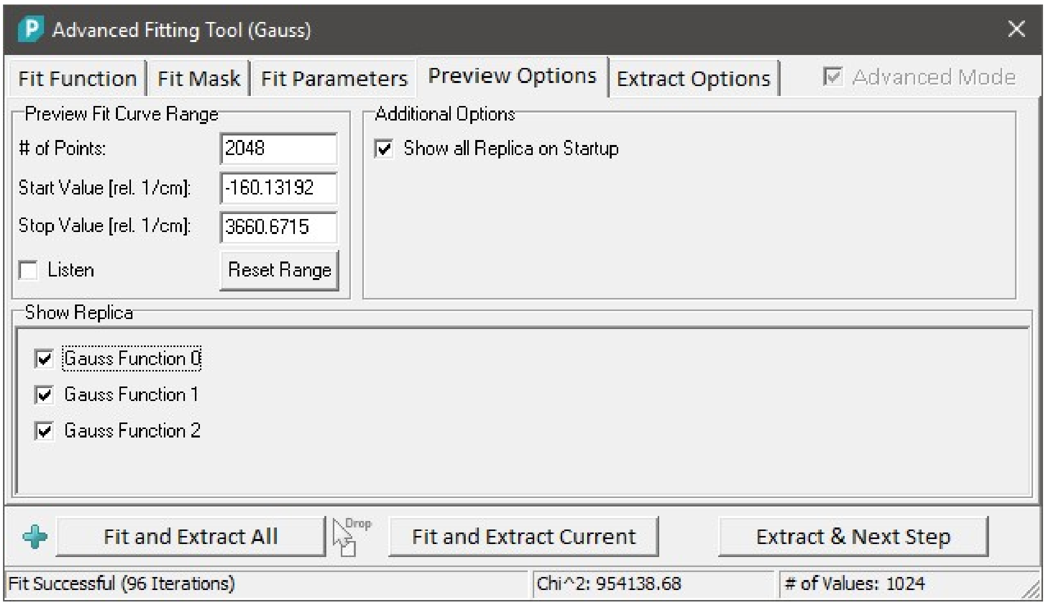
Preview (Value Column Radio Button):
If this Radio Button is checked, the blue graph in the preview graph viewer will show the current fit function using parameters from the value column (typically the current fit result).

Vary (Check Box Column):
If checked, the parameter (value column) is used for fitted and therefore changed by a fit process - Don't vary a parameter if you want it to be static (e.g. a known peak position).

Lower Limit (Check Box and Float Edit Column):
Enables defining a lower limit for each parameter. The limit will only be used if the check box is checked.

Upper Limit (Check Box and Float Edit Column)
Enables defining an upper limit for each parameter. The limit will only be used if the check box is checked.

Preview Options Tab



Preview Fit Curve Range

# of Points (Integer Edit):
Sets the number of supporting points for the fit preview curve (it usually should be around twice the number of spectral pixels of your input graph).

Start/Stop Value (Float Edits):
Set a range that should be shown as a preview fit curve.
With this feature, you can hide "unwanted" areas (e.g. if a curve like polynomial has extreme values).

Listen (Check Box):
It can be listened to a range from graph viewer (using the mark region mouse mode) in order to set the range.

Reset Range (Button):
Resets the range to the complete input spectral range.

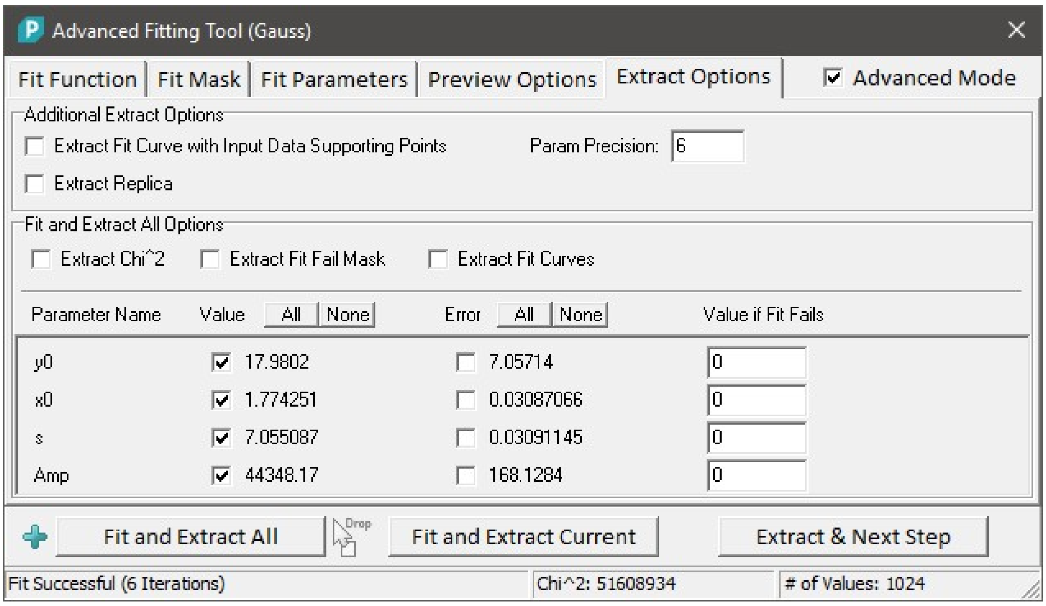
Additional Options

Show all Replica on Startup (Check Box)
If checked, the replica of a multiple peak curve will be shown as green graphs in the preview graph window.

Show Replica (Check Box List)

You can toggle the visibility of each single replica curve of a multiple peak fitting function in the preview graph window.

Extract Options Tab



Additional Extract Options

Extract Fit Curve with Input Data Supporting Points (Check Box):
If checked, the extracted fit curve uses the exact supporting points and the same x-transformation as the input data object. This enables to use the extracted fit curve together with the spectral objects in other drop action dialogs (e.g. Calculator).

Extract Replica (Check Box):
If checked, each replica fit curve is extracted separately when executing the extract action.

Param Precision (Integer Edit):
Defines the precision of floating point numbers in text objects when using the "Fit and Extract Current" Button.

Fit and Extract All Options

Extract Chi^2 (Check Box):
If checked, the Chi^2 (which describes the fit error) is extracted together with the fit results.

Extract Fit Fail Mask (Check Box):
If checked, a fit fail mask is extracted together with the fit results. All pixels that could **not** be fitted (due to an fitting error) are set to 1 in this mask.

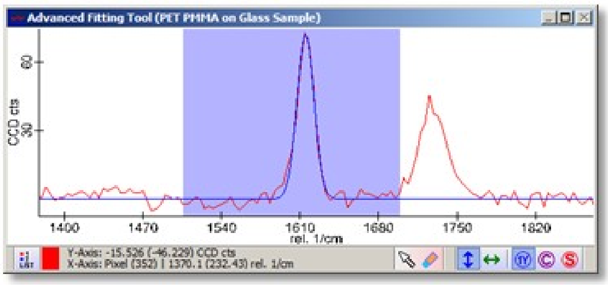
Extract Fit Curves (Check Box):
If checked, the fit curves are extracted together with the fit results.

Value (Check Box Column):
You can select whose function parameter's fit result should be extracted as a result data object.

Error (Check Box Column):
You can select whose function parameter's fit error should be extracted as a result data object.

Value if Fit Fails (Float Edit Column):
Enter a value that should be used as the parameter's fit result if the fit fails.

Preview Window



The graph preview window shows the original graph as a red graph and the fit preview as a blue curve.
In Advanced Mode it's possible to show the start value column as a preview curve. In this case, the blue curve shows the fit function using start values.

Fit Function Options

Options for peak fitting

Options:

Tolerance	1E-08
Max # of Iterations	200
Number of Functions	1
Extract Peak Width Kind	Standard Deviation
Extract Intensity Kind	Amplitude
Extract Sort Kind	No Sort

Tolerance:
If this error threshold is reached, the fit algorithm stops.

Max # Number of Iterations:
If the the number of fit iterations specified in this edit is reached the fit algorithm also stops - even if the Tolerance error is not reached yet.

Number of Functions:
Some peak fit functions (Gauss, Lorentz) allow multiple peak fitting; the number of functions can be changed here.

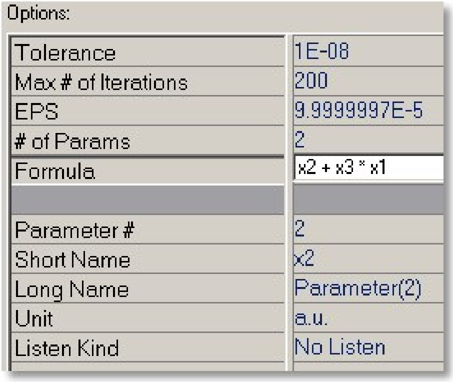
Extract Peak Width Kind:

Some peak functions allow different peak width kinds (like "Standard Deviation" or "FWHM"). Only the extracted results contain these width kinds.

Extract Peak Intensity Kind:
Some peak functions allow the different peak intensity kinds "Area" and "Amplitude". Only the extracted results contain these intensity kinds.

Extract Sort Kind:
The Gauss fit function allows to sort the extracted results when using multiple peak fitting, e.g. by peak center/position. That means that the first result has the lowest peak position, the second result has the second lowest peak position and so on.

Options for user defined fit functions



# of Params:
Defines the number of variables for the fit function.

Formula:
Enter your fit formula here (see Formula Editor):

$$
\begin{aligned}
n &= \textit{Number of Parameters} \\
x_1 &= x\ (\textit{Independent Variable}) \\
x_i &= P_{i-1}\ (2 \le i \le n+1)
\end{aligned}
$$

So for example x2 + x3 * x1 is a simple line with x2 being the offset (Parameter Number 2) and x3 being the slope (Parameter Number 3).

Parameter Number:
Enter a parameter index/number in order to define a short/long name, a unit and a listen kind for the parameter.
E.g. parameter number 2 is the first parameter, named x2 in the formula.

Short Name:
The short name for a parameter. Should only be a few characters.

Long Name
A detailed name for a parameter.

Unit:
The parameter unit. You can use the following variables:

- $x represents the X-Axis unit of the input graph.
- $y represents the Y-Axis unit of the input graph.

Listen Kind:
The listen kind of this parameter. E.g. if the parameter represents the peak position, the listen kind "X-Axis" can be used in order to find good start values using the listen mechanism in the Fit Parameters Tab.
The following listen kinds are available:

- X-Axis (listens to an absolute X-Axis position).
- Y-Axis (listens to an absolute Y-Axis position).
- X-Diff (listens to the difference of a clicked and moved cursor position in the X-Axis).
- Y-Diff (listens to the difference of a clicked and moved cursor position in the Y-Axis).
- X-Diff Absolute (same as X-Diff but always positive values).
- Y-Diff Absolute (same as Y-Diff but always positive values).
- Area (listens to the calculated area from the clicked and moved cursor position in the X-Axis).

Cluster Analysis Dialog

Description

The Cluster Analysis Dialog automatically finds similar spectra in an image spectrum data object and creates the corresponding cluster average spectra as well as the cluster distribution maps.

Input and Results

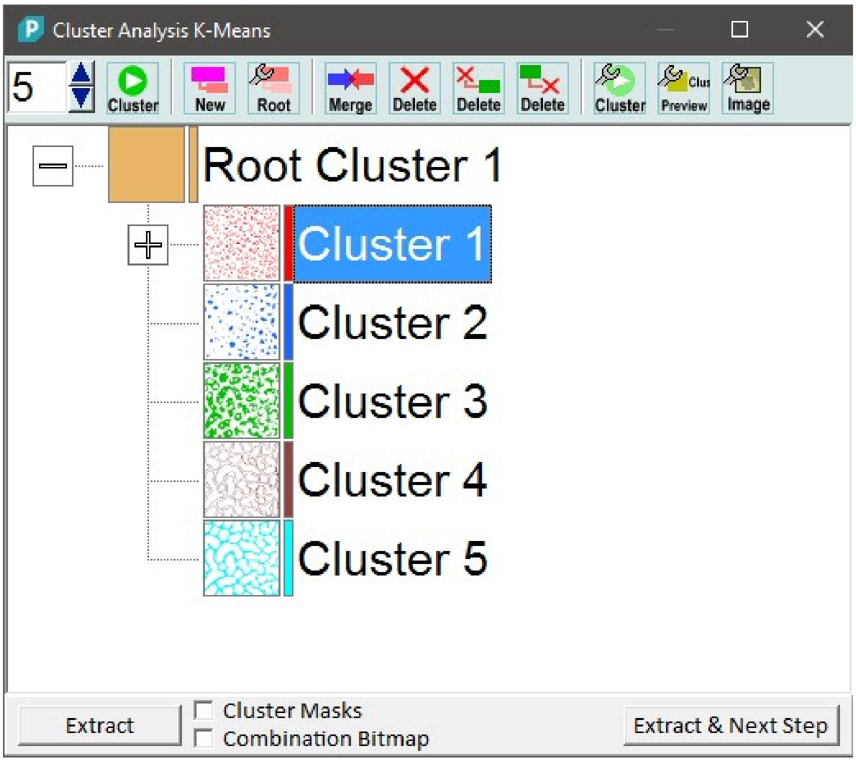
Input:
One hyper spectral data object.

Results:
- Cluster Average Spectra
- Cluster Distribution Masks
  or
  Relative Cluster affiliation
  (when using intensity images, the result image shows the "distance" from each spectrum/pixel to its cluster center)
- Cluster Color Combination Bitmaps

User Interface

- Main Window
- Context Menu
- Root Cluster Options
- Cluster Algorithm Options
- Preview Options
- Intensity Image Options
- Preview Windows

Main Window



Number of Clusters (Integer Edit / Up/Down Buttons):
Sets the number of clusters to be used for the following cluster analysis.

Cluster (Start Cluster Analysis):

Starts the Cluster Analysis using the cluster node that is currently selected.
If no root cluster was created before, a new root cluster is created and clustered automatically (using the current root cluster creation options).

New (Create New Root Cluster):
Creates new root cluster using the current root cluster creation options.

Root (Show Root Cluster Options):
Shows the Root Cluster Options.

Merge (Merge Selected Clusters):
Merges the selected clusters into a new cluster using an OR Operation (i.e. the new merge cluster contains all pixels of all merged clusters).

Delete (Delete Selected Clusters):
Deletes all selected clusters recursively.

Delete (Delete and keep Children):
Deletes the selected cluster and keeps the sub-clusters ("**children**"), moving them to the tree level of their deleted original cluster ("**parent**").

Delete (Delete only all Children):
Deletes all children of the selected cluster while preserving the existence of the selected parent cluster.

Cluster (Show Cluster Algorithm Options):
Shows the Cluster Algorithm Options.

Preview (Show Preview Options):
Shows the Preview Options.

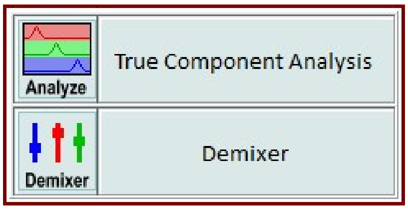
Image (Show Intensity Image Options):
Shows the Intensity Image Options.

Extract (Button):
Extracts the average spectra of all selected clusters.

Cluster Masks (Checkbox):
If checked, the cluster masks / distribution images are additionally extracted upon pressing the extract button.

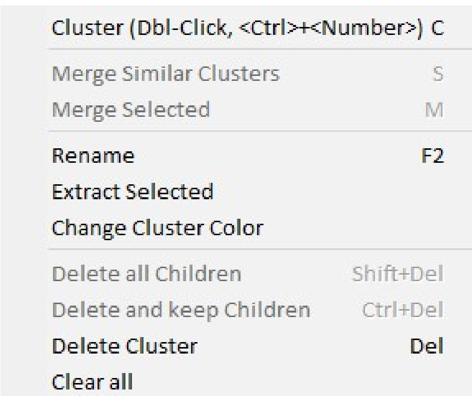
Combination Bitmap (Checkbox):
If checked, the current combination preview bitmap is additionally extracted upon pressing the extract button.

Extract & Next Step (Button):
Wizard feature: you can use the cluster result spectra for the true component analysis or for demixing:



Context Menu

You can right-click on a cluster result to open the context menu:



Cluster
This will execute the cluster analysis on the currently selected root cluster / cluster result / sub cluster.

Merge Similar Clusters

Merges two sub clusters, that are most similar to each other. Only works on a cluster that has sub cluster results.

Merge Selected
Merges all selected clusters into one bigger cluster and adds the selected clusters as sub clusters.

Rename
Renames the selected cluster. The name is used in extracted data objects.

Extract Selected
Extracts the selected clusters into the project (Average Spectrum + Cluster Distribution Map).

Change Cluster Color
Changes the color for a cluster (Cluster Distribution Map and Average Spectrum).

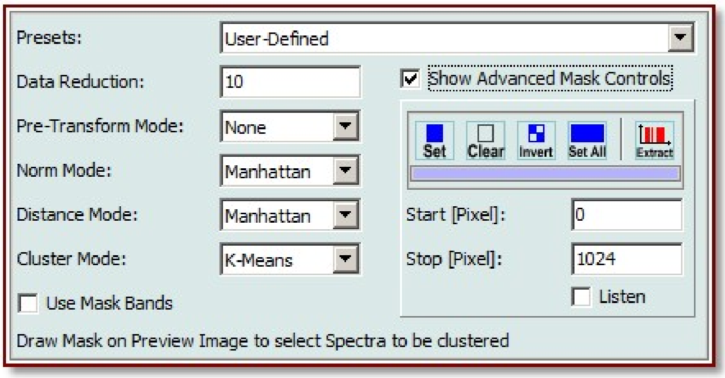
Delete all Children
Deletes all children / sub clusters of the selected parent cluster but keeps the parent cluster.

Delete and keep Children
Deletes the selected cluster and moves the sub clusters one level up.

Delete Cluster
Deletes the selected cluster and all sub clusters.

Clear all
Deletes everything, all root clusters with sub clusters.

Root Cluster Options



Presets (Combo Box):
One of the pre-defined root cluster options can be chosen:
- K-Means: Raman Spectra w/o Background
- K-Means: Raman Spectra with Background
- Fuzzy: Raman Spectra w/o Background

Data Reduction (Integer Edit):
Data Reduction means that the given number of pixels of a spectrum are averaged and used as one property for the cluster analysis algorithm instead of all single pixels.

Pre-Transform Mode (Combo Box):
Transforms the input spectra before using them in the cluster analysis:
- None (No Pre Transformation)
- Derivative
- SG (6, 6, 4, 1) (Uses a Savitzky-Golay smoothed Derivative of the data)

Norm Mode (Combo Box):
Normalizes the input spectra before using them in the cluster analysis:
- None
- Manhattan
- Euclidean

See also Spectrum Normalization (Math).

Distance Mode (Combo Box):
Defines a distance mode for calculating the similarity/distance of spectra:
- Manhattan
- Euclidean

See also Spectrum Normalization (Math).

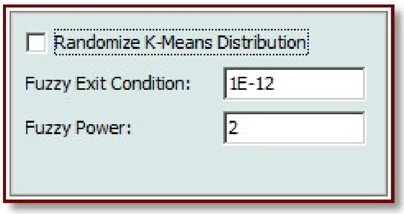
Cluster Mode (Combo Box):
Defines the cluster mode:
- K-Means (Creates Boolean Cluster Maps, Sub-Clustering is allowed, see also Cluster Analysis K-Means (Math).

- Fuzzy (Creates Intensity Cluster Images, Sub-Clustering is not allowed.

Use Mask Bands (Check Box):
If checked each single mask band in the preview window is used as one property for the cluster analysis algorithm (instead of the single pixels in the spectra).

Advanced Mask Controls (Edits and Tool Buttons):
You can change the cluster mask in order to define which pixels should be considered for the cluster analysis algorithm. These edits are optional, you can change the masks directly in the preview graph viewer.

Cluster Algorithm Options

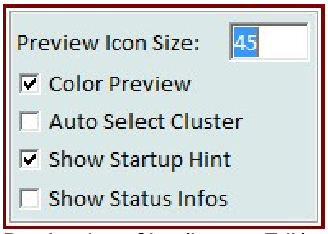


Randomize K-Means Distribution (Check Box):
If checked, the K-Means Start-Iteration begins with a real random cluster distribution.
If not checked, the pixels are sequentially sorted into the clusters (modulo number of clusters: 1, 2, 3, 1, 2, 3, ...). The latter will lead to the same results for the same root cluster options and mask.

Fuzzy Exit Condition (Float Edit):
Defines an exit condition for the iterative fuzzy cluster algorithm.

Fuzzy Power (Float Edit):
Affects the fuzzy cluster algorithm results.

Preview Options



Preview Icon Size (Integer Edit):
Defines the icon size of the cluster tree preview thumbnails.

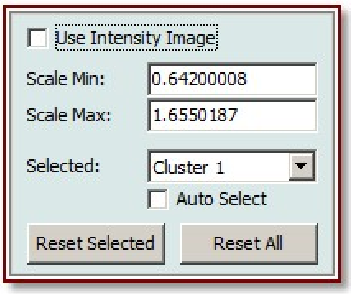
Color Preview (Check Box):
If checked, the cluster tree preview thumbnails use their cluster color.
If not checked, a standard black-yellow color-scheme is used.

Auto Select Cluster (Check Box):
If checked, a cluster node is automatically selected if the mouse cursor clicks and moves in an image viewer.
Note that if you have multiple root clusters, only the sub-clusters or siblings (clusters on the same level) of the currently selected cluster are selected.

Show Startup Hint (Check Box):
If checked, the Cluster Analysis Dialog shows a small startup hint / wizard.

Show Status Infos (Check Box):
If checked, some status infos about the current root cluster / selected cluster are shown in a status bar at the bottom.

Intensity Image Options



Use Intensity Image (Check Box):
If checked, the K-Means Cluster preview images - and also extracted images - don't show boolean cluster distribution maps but intensity images showing the "distance" of the spectra to their cluster average spectra (see "Distance Mode" in Root cluster Options). I.e. the brighter a single pixel in the intensity image is, the higher is the similarity of the selected spectrum to its average cluster spectrum.
This enables to find structures within the same cluster which could be a hint for another component.

Scale Min/Max (Float Edit):
It's possible to select more than 1 cluster in the cluster tree view, showing them together in the preview image viewer. You can change the intensity scale of each of those selected clusters separately.

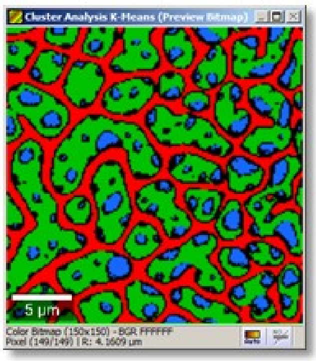
Selected (Combo Box):
The Scale Min/Max Edits act on the selected cluster from this window.

Auto Select (Check Box):
If checked, the selected cluster from this window is changed by clicking in an image.

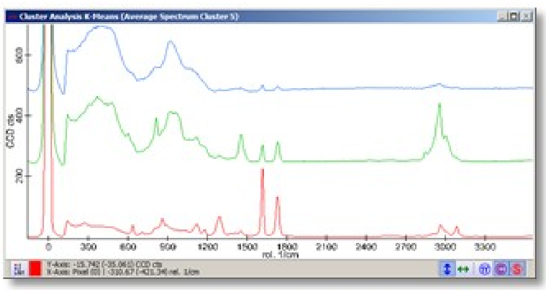
Reset Selected (Button):
Resets the scale of the selected cluster from this window.

Reset All (Button):
Resets all scales of all selected cluster of the cluster tree.

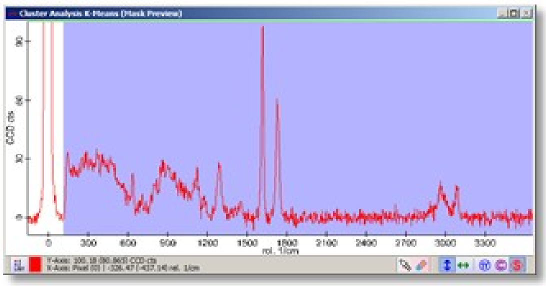
Preview Windows



The preview image viewer shows the selected cluster distribution maps.



The first preview graph viewer shows the average spectra for all selected clusters.



The second preview graph viewer shows the original spectrum and the cluster mask.
Before you start the cluster analysis, you can change the cluster mask here in order to define which part of the spectra (or mask bands) should be used for the cluster analysis.

Filter Viewer

Description

The Filter Viewer creates images from image-graph objects (or graph objects from line-graph objects or single result values from single spectra) using defined filters, e.g. a sum filter.

Input and Results

Input:
Use can use any graph object with this dialog.

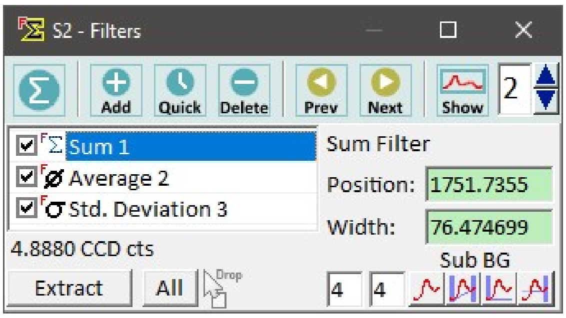
Results:
The result is depending on the dimensionality of the input graph object.
The Filter Viewer creates the following results for each defined filter:

- image objects for image graph input data objects
- single graph objects for line graph input data objects
- text object containing result as text for single graph input data objects,

Special Features

- Some measurements (especially multi-spectral measurements) will create a Filter Viewer upon starting a measurement.
- In contrast to other Drop Actions or Data Analysis Features it is possible to use the Filter Viewer during the measurement.
- The Filter Viewer together with the contained filters is saved with the project. Preview Windows as well as the input graph preview is not saved but can be reopened after loading (see Saving a Project).

User Interface

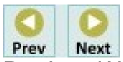


Create Sum Filter (Button):
This creates a new sum filter.

Create Filters (Button):
You can simply create a new filter by pressing "Create Filters" and selecting one of the available filters.
See Filter List for a short description for each filter and its purpose.

Quick Filters (Button):
If you would like to save your filters to the hard drive and reload them later on, you can use the "Quick Filters" menu.
You can save **selected filters** using the context menu in the white Filter List Box. **All filters** can saved using the quick filters button.
Filter that are saved in the Quick Filter directory are automatically shown in the Quick Filter Menu.
You can open the directory and organize your quick filters using subdirectories which are shown as sub menus in the quick filter menu.

Delete (Button):
Deletes all selected filters.



Previous / Next (Buttons):
Switches to the next or previous possible graph object in the project manager to use it as the new input graph object.
Shortcut: Page-Up or Page-Down in a preview image viewer (showing the results of a filter).

Show Input Graph (Check Button):
Shows or hides the graph viewer window showing the (averaged) input graph.

Spatial Average Size (Integer Edit):
Defines the average filter size of scanned spectra, that will be averaged and shown as a preview in the graph viewer mentioned above.

Extract (Button):
This will create new data objects for the selected filters.

All (Button):
This will create new data objects for all your filters.

Filter List Box:
Shows all filters

- Click on the "Filter Name" column heading to select or deselect all filters.
- Click on the "Show" check boxes to toggle the filter preview (affects all selected filters).
- Double-click on any filter to show the preview only for this filter (shortcut: return key).
- Filter parameter changes will affect all selected filters.
- Click on the "Start" or "Stop" column header to turn on/off the listen mechanism.

"4.8880 CCD Cts." (Label)
Shows the result of the selected filter for single spectrum input graph objects.

Position (Float Edit):
Defines the position of the selected filter(s).
Double-click to listen to a position from any graph viewer window; if listening is enabled the edit is colored red. The listening is disabled again by double-clicking once more.

Width (Float Edit)
Defines the width of the selected filter(s). The filter range will be from <Position - Width/2> to <Position + Width/2>.
Double-click to listen to a position from any graph viewer window; if listening is enabled the edit is colored red. The listening is disabled again by double-clicking once more.

Background Subtraction (Edits and Buttons)
Changes the background subtraction used with the current filter:

- The left and right edit field will define the number of pixels on the left and right of the filter area that is used as an average value for the background subtraction.
- A value of 0 for both edits indicates no background subtraction.
- If both edits are not 0, a slope that is connected from the average of the left side pixels and the average of the right side pixels is subtracted
-  Click on the tool buttons for defining:
  - no Background Subtraction
  - 4 and 4 (both sides, subtracts a slope)
  - 4 and 0 (left side, subtracts a line)
  - 0 and 4 (right side, subtracts a line).

See Filter Viewer (Math)

Drop Zones / Batch Processing

The both following options are possible if the dropped graph has the same dimensionality and x-transformation kind:

- drag & drop a graph object onto the form caption bar to set a new input graph object
- drag & drop one or more graph objects onto the "Extract" or "Extract All" button to do batch processing.

Filter List

Purpose of different Filters of the Filter Viewer

For a mathematical description of all filters, see Filter Viewer (Math)

Sum
Calculates the overall intensity of the selected range.
Is typically used to make structures visible, that are described by a (Raman) peak.
Can also be used to suggest the overall number of electrons/photons.

Average
Can be used e.g. to show the background (if the filter is set to a range where there is no raman signal).

Average minus Minimum
The minimum of the selected range is subtracted from the average.
Can be used e.g. to do some kind of "background subtraction" if a Raman peak is on a fluorescence offset.

Standard Deviation
Shows the changes within a range.
Can be used to determine the amount of noise or to show variations in the spectral range.

Center of Mass (Weighted Position)
Calculates the peak position (roughly). Use peak fitting tools for more accurate peak position fitting.

Peak Width
Calculates the peak width (roughly). Use peak fitting tools for more accurate peak width fitting.

Maximum
Calculates the maximum of the range. Shows the position of the maximum intensity in the result image.
Can also be used e.g. to find a specific cosmic ray that couldn't be removed by the Cosmic Ray Removal tool. For this, calculate the total average of all spectra in an spectral image, then do the maximum filter on the area of the "small cosmic ray peak" that could be visible in this total average spectrum. The result image then could show the position of the cosmic ray.

Raman TV Dialog

Description

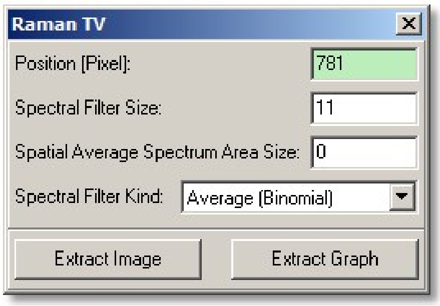
This dialog creates images very quickly from image spectrum data objects using different filters; it ts also possible to see a local average spectrum for a selected image pixel. This combination allows a very easy and fast overview on your complete Raman image measurement.

Input and Results

Input:
One image spectrum data object.

Results:
An image calculated using a selected spectral position or the local average graph for a selected image position.

User Interface



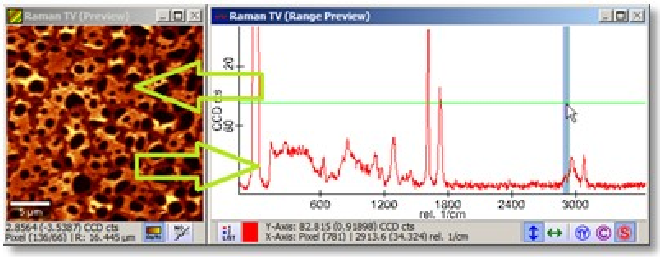
Position (Integer Edit):
The current spectral pixel position for image creation.

Spectral Filter Size (Integer Edit):
The spectral filter size for image calculation. The total window size is 2*<filter size> + 1.

Spatial Average Spectrum Area Size (Integer Edit):
The spatial window size for the local average graph calculation. The total window size is (2*<filter size> + 1)^2.

Spectral Filter Kind (Combo Box):
Chose one of those filters:
- Average (Binomial): averages the spectral pixel window using binomial distributed weighting factors.
- Average (Box): averages the spectral pixel window without weighting factors.
- Sum: calculates the sum of the spectral pixel window.
- Standard Deviation: calculates the standard deviation of the spectral pixel window.
- Average - Minimum: subtracts the minimum from the average of the spectral pixel window.

Preview Windows



The preview image viewer shows the image which is calculated from the current selected spectral position.
The preview graph viewer shows the local average spectrum of the current selected image position.

Graph Demixer Dialog

Description

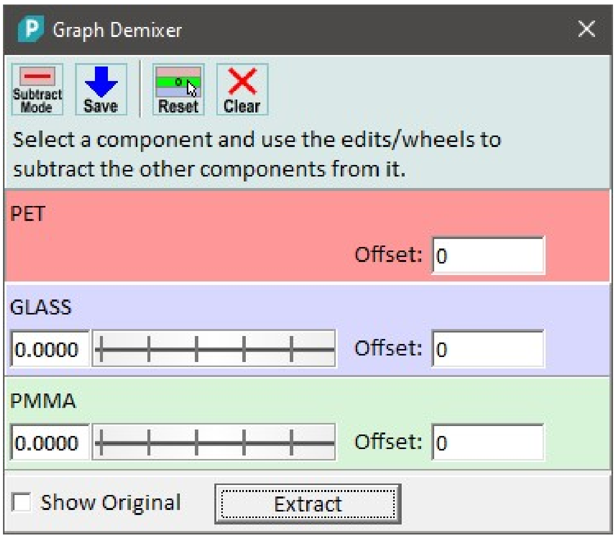
The Graph Demixer Dialog allows to subtract several single spectra from each other in order to create pure component spectra from mixed spectra (very often you have average spectra that are mixed).

Input and Results

Input:
<n> single spectra data objects (at least 2)

Results:
<n> single spectra (demixed)

User Interface



Subtract Mode (Tool Button)
If checked, the selected component can be subtracted from all the other components by changing the weighting factors.
If not checked, the selected component will be changed by subtracting the other components using the weighting factors.

Save (Tool Button)
Saves the current demix in order to subtract a demixed spectrum from the other spectra.

Reset (Tool Button)
Resets the demix of the currently selected component (sets all weighting factors to zero). This will not reset saved demixes.

Clear (Tool Button)
Resets all demixes.

Show Original
If checked, the preview graph viewer window will show the original (dropped) graph objects.

Extract:
Extracts the demixed spectra.

Preview Windows

The preview graph window shows the current mix graphs.
Zooming the baseline makes it easier to find good weighting factors.

Graph Repair Dialog

Description

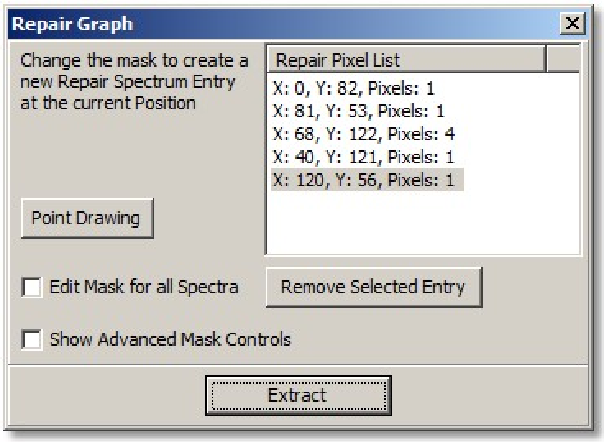
The Graph Repair Dialog can be used to repair a selection of pixels like cosmic rays, hot or dark pixels of the CCD camera or other defects using simple interpolation.

Input and Results

Input:
One graph data object.

Results:
One repaired graph data object.

User Interface



Repair Pixel List (List Box):
If you change the mask for a selected spectrum (select a spectrum by clicking e.g. into an image), this part of the spectrum automatically is added to the repair pixel list, the pixel coordinates as well as the number of pixels that were repaired are listed. Click on any repair pixel to show the r in the preview. Additionally, the repair mask for this pixel will be shown.

Remove Selected Entry (Button):
Deletes the Repair Pixel item that is selected in the Repair Pixel List above.

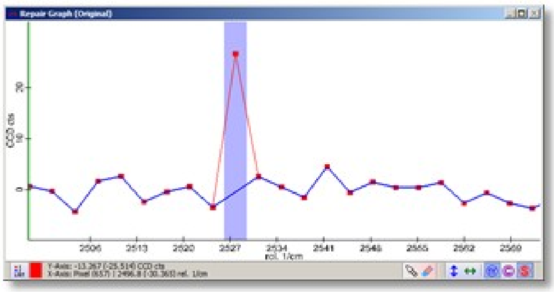
Point Drawing (Button):
Toggles the point drawing of the original graph in the preview graph window.

Edit Mask for all Spectra (Check Box):
If checked, you can define global repair mask which will be applied to all spectra in a hyper spectral data set.
Uncheck if you would like to repair a single pixel again.

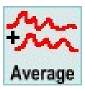
Show Advanced Mask Controls (Check Box):
Shows the mask controls for mask export or for changing the mask via listen mechanism.
You can also directly change the repair mask in the preview graph window.

Extract (Button):
Creates a new graph data object containing the repaired / interpolated pixels.

Preview Windows



The preview graph window shows the original spectral data object as a red graph and the preview repaired graph as a blue graph.



Average Spectrum

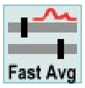
Description

Average Spectrum calculates the average spectrum of a multidimensional graph data object (optionally using weighting factors).
To average a couple of single spectra data objects the Calculator Dialog has to be used.

Input and Results

Input:
- You can use any kind of multidimensional graph object with this dialog.
  Additionally, you can **combine** this graph **with one or multiple images** that have a corresponding size. The additional objects can be used to define weighting factors for each spectrum that shall be averaged. Thus you can use Image Masks to average only those pixels that are set in the mask (weight = 1.0 or 0.0).
- You can use any number of single spectrum data objects to create the average of all those spectra.
- You can use multiple multidimensional graph objects for batch processing.

Results:
Depending on the number <n> of additional weighting factor objects, the result data object is one or <n> average graph objects.
If no additional weighting factor object is used, only one single graph is created: the total average of all spectra in the dropped data object.



Advanced Graph Average Dialog

Description

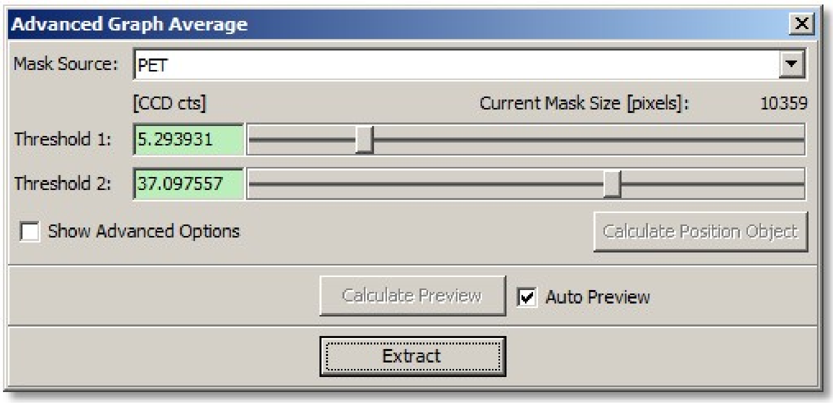
With this dialog image masks can be created using thresholds and calculate an average spectrum for the resulting mask in real time.

Input and Results

Input:
- Image Graph and optionally corresponding images (of no images are used, an image can be created using a sum filter mask) OR
- Line Graph (e.g. from a line scan) and a corresponding single spectrum (which is e.g. the result of the Filter of the line graph)

Results:
One average spectrum for each mask object.

User Interface



Mask Source (Combo Box):
you can toggle to each of the dropped images in order to use it to create a mask using thresholds.

Threshold 1/2 (Float Edits and Sliders):
these are the two thresholds that will define the image mask. An image pixel is marked, if the pixel value is within the range of the two thresholds.

Calculate Position Object (Button):
calculates a new image object using the sum of all pixels in the graph preview mask. This image can be used to define a mask using thresholds. The button is only enabled if the "Mask Source" is set to "User Position Object".

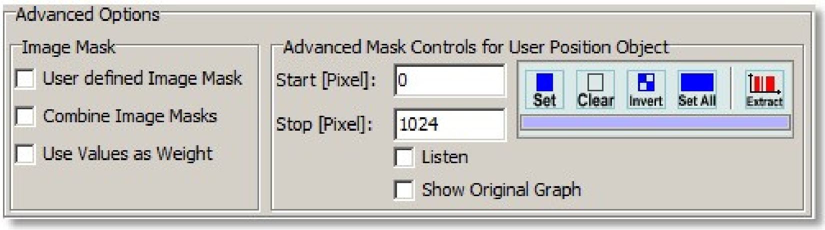
Calculate Preview (Button):
calculates the preview average spectrum once if "Auto Preview" is enabled.

Auto Preview (Check Box):

turns on or off the automatic preview average spectrum calculation.
For very large data sets, this is turned off automatically and you have to press the "Calculate Preview" Button in order to see a preview average spectrum.

Extract (Button):
extracts the average spectra, one for each mask/additional image.

Show Advanced Options (Check Box):
shows advanced options:



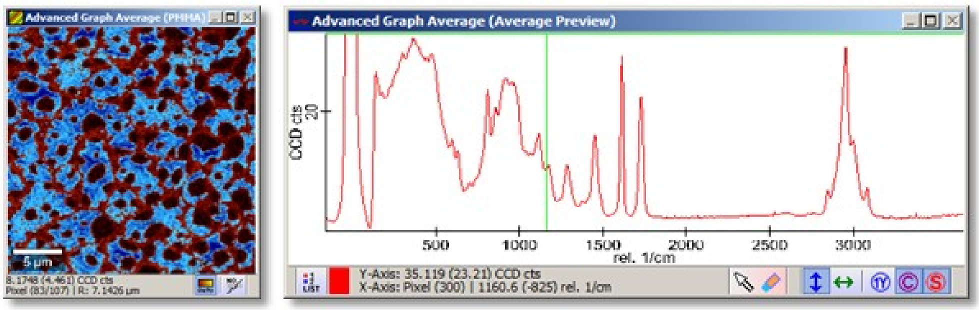
User Defined Image Mask (Check Box):
if checked, the Threshold Edits/Sliders are disabled. Will be automatically checked, if the user changes the image mask in the image viewer preview window with the image viewer draw tools.
This behavior will prevent the user from accidentally destroying the user defined mask.
If the check box is unchecked by the user, the Thresholds are used in order to overwrite the current mask.

Combine Image Masks (Check Box):
if checked, all masks from all additional images will be combined using an AND-operation.

Use Values as Weight (Check Box):
if checked, the image mask will be ignored; instead, the image values itself define weighting factors for each spectrum in the averaging process.

Advanced Mask Controls for User Position Object:
These edits are optional.
You can define a mask in the graph preview window in order to create a user position object (sum image).
This is interesting if you don't have any images and dropped only a graph object onto this dialog.
Check the "Show Original Graph" Check Box in order to see a valid spectrum for defining the mask.

Preview Windows



The Image Viewer shows the current selected image and its mask.
The Graph Viewer shows the average spectrum preview calculated with the current image mask.
It is also possible to define a spectral mask in the graph viewer in order to create a user defined position object (e.g. sum image) for mask creation.

Calculator Dialog

Description

The calculator can be used to convert or combine values of image or graph objects by typing a custom formula.
Each single floating point value of an image or a (multidimensional) graph object is converted using this formula.

Input and Results

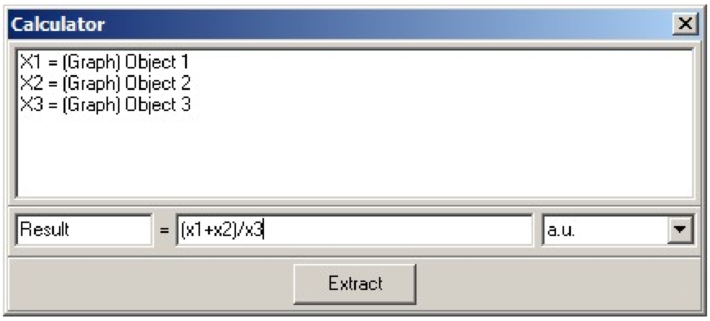
Input:
You can eihter use a single graph or image object with this dialog or combine multiple input data objects to create a new data object.

The following combinations are allowed:

- Multiple Image (and Image Graph data) objects that have the same size and space transformation
- Multiple Graph data objects that have the same spectral size and x transformation
- Multiple Line Graph objects and optionally corresponding single graph objects that

Results:
Depending on the dimensionality of the input data, the result data object is an image, a single graph, a line graph or an image graph. If graph objects with a different dimensionality are dropped, the result will be a graph with the dimensionality of the largest-dimensioned input graph.

User Interface



Object List View:
This list shows the input data objects. Each object defines a variable (x1, x2, ...). These variables can be used in the formula.

Result (String Edit):
Enter the caption/name for the new data object (the formula string will be appended to this caption).

"(x1+x2)/x3" (String Edit):
The desired formula can be entered here (see Formula Editor for possible operators, functions and examples).

"a.u." (String Edit + Preselection):
Enter the desired unit of the result or select one of the predefined names (a.u. = arbitrary unit).

Extract (Button):
Pressing that button will start the calculation / conversion.

Preview Windows

If there are only image data objects used, there is a preview Image Viewer window showing the result image.
If there is at least one graph object in the input data list, there is a preview Graph Viewer showing the result graph.
In case of a multidimensional input graph (e.g. an Image Graph), the Dialog listens to the respective cursor and shows the corresponding preview graph.

Formula Editor

The Formula Editor (formula parser) converts an algebraic expression (text) into a stack of operations which can be understood by the computer. This formula parser can process several mathematical operators and functions (see below).

The order of execution depends on the priority of the operator. Although the formula parser uses floating point numbers, some operators need boolean or integer values to operate. In this case, the float value is converted prior to operation. A float to integer conversion truncates the decimal places.

A float to boolean conversion is given by:

$$\mathrm{Boolean}(x) = \begin{cases} \text{true} & \text{for} \quad x <> 0 \\ \text{false} & \text{for} \quad x = 0 \end{cases}$$

The result is converted back into a floating point number. A boolean value of true is converted to 1.0, a boolean value of false is converted to 0.0.

All functions have at least 10 significant digits after the decimal point other than the besselj1() and the airysqr() function, which deal with only 7 significant digits after the decimal point.

Depending on the usage, the formula parser accepts a fixed number N of input variables. These variables are addressed by X1, X2 ... Xn.

Example Formulas

x1+500	Result is the original value plus 500
x1>250	Result is 1, if the original value is larger than 250; result is 0 if it is smaller
x1+x2	Result is the sum of x1 and x2
x1*(x2>250)	Result is the original value of x1, if x2 is larger than 250, otherwise zero

Operators

Priority	Operator	Description
1	|	Or (Boolean)
2	&	And (Boolean)
3	!	Not Equal (Boolean)
4	=	Equal (Boolean)
5	>	Larger (Boolean)
6	<	Smaller (Boolean)
7	-	Minus (Float)
7	+	Plus (Float)
8	%	Modulo (Integer)
9	*	Times (Float)
9	/	Over (Float)
10	- (algebraic sign)	Change Sign (Float)
11	^	Power (Float)
12	( )	Bracket (Float)

Functions

Function	Description
sin()	Sine (Radian)
asin()	Arc Sine (Radian)
cos()	Cosine (Radian)
acos()	Arc Cosine (Radian)
tan()	Tangent (Radian)
atan()	Arc Tangent (Radian)
cotan()	Cotangent (Radian)
sinh()	Hyperbolic Sine
asinh()	Hyperbolic Arc Sine
cosh()	Hyperbolic Cosine
acosh()	Hyperbolic Arc Cosine
tanh()	Hyperbolic Tangent
atanh()	Hyperbolic Arc Tangent
loge()	Natural Logarithm
log10()	Logarithm of Base 10
log2()	Logarithm of Base 2
exp()	Exponential
abs()	Absolute
sqrt()	Square Root
sinc()	sin(x)/x (Radian)
sincsqr()	(sin(x)/x) ^ 2
heavyside()	0 for x < 0 | 0.5 for x = 0 | 1 for x > 0
sign()	-1 for x < 0 | 0 for x = 0 | 1 for x > 0
besselj1()	J1(x) bessel function of first kind
airysqr()	((2J1(x)) / x) ^ 2

pi()	Mathematical constant PI (use "pi(0)")

Used by:

- Calculator Dialog
- Advanced Fitting Tool Dialog

Data Cropping and Reduction Dialog

Description

With the Data Cropping and Reduction dialog it is possible to cut away parts of the data and to reduce the number of pixels / the resolution.

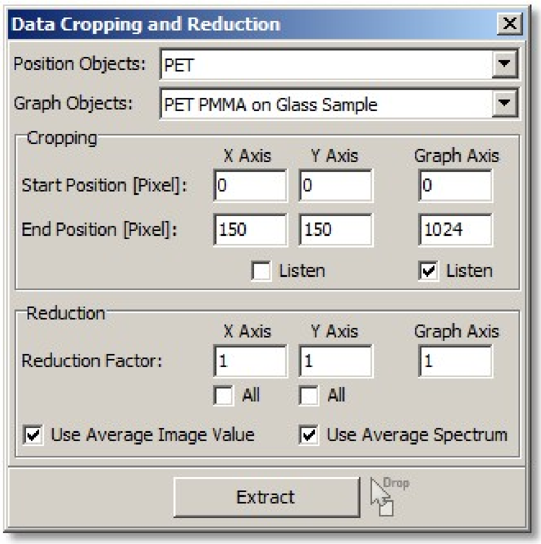
Input and Results

Input:

- one image spectrum data object and any number of belonging images or
- one line spectrum data object and any number of belonging graph objects or
- one or a number of images that have the same spatial transformation or
- one or a number of single spectrum data objects that were created from the same Raman image scan, e.g. average spectra

Results:
Cropped and/or reduced data objects.

User Interface



Position Objects (Combo Box):
Shows the input data objects that either

- define a spatial position for images/image spectrum objects or
- define other units like a time line for time series.

The selected object is shown in the preview windows.

Graph Objects (Combo Box):
Shows input data objects like an image spectrum, line spectrum or single spectrum object (if it's not defining a space or other position). Is used to switch the preview if multiple objects are dropped.

Cropping

Start/Stop Position X/Y Axis (Integer Edits):
Can be used to crop images or image spectrum objects.

Start/Stop Position X/Y Axis Listen (Check Box)
If checked, a rectangle in an image viewer can be simply marked in order to crop image or image spectrum data objects.

Start/Stop Position Graph Axis (Integer Edits):
Can be used to crop a part of the spectral axis.

Start/Stop Position Graph Axis Listen (Check Box):
If checked an area in an graph viewer can be simply marked in order to crop spectral objects.

Reduction

Reduction Factor X/Y Axis (Integer Edits):
Can be used to change the number of pixels respectively the resolution of images or image spectra data objects.
Example:
A factor of 1 means no reduction. A factor of 2 means the result contains only half the number of pixels by using every second pixel of the original data in the result. A factor of 3 means the result contains only a third of all original pixels using every third pixel of the original data in the result.
If the "Use Average Image Value" (for the spatial axes) or "Use Average Spectrum" (for the spectral axis) check box is selected, the data is reduced using the average value/spectra of 2, 3, 4, .. pixels, see below.

Reduction Factor Graph Axis (Integer Edit):
Can be used to change the number of pixels / resolution of spectral data objects.

Reduction X Axis All (Check Box):
Does a data reduction for the complete X Axis. The result is a line graph object (vertical line).

Reduction Y Axis All (Check Box):
Does a data reduction for the complete Y Axis. The result is a line graph object (horizontal line).

Use Average Image Value (Check Box):
If checked, the data reduction is done using the average of all reduced pixels. E.g. if reduction factor for one axis is 2, the result pixel is the average of 2 neighbored original pixels.
If not checked, the reduced original pixels are just skipped and not used in the result.

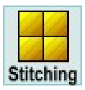
Use Average Spectrum (Check Box):
If checked, the result spectrum for reduced image spectrum data objects is an average spectrum calculated from the reduced neighbor image pixels. E.g. if reduction factor for one axis is 2, the result spectrum is the average of two spectra from two neighbored pixels.
If not checked, only a single spectrum is used and reduced original spectra are just skipped and not used in the result.

Extract (Button and Drop Zone):
Calculates and extracts the cropped/reduced data. You can do batch processing by dropping a number of data objects on this button.
Note that batch processing only works, if the dropped data objects have the same dimensionality as the data objects in the dialog.
Graph batch processing only works if only one graph object is currently in the dialog.

Preview Windows

Depending on the input data objects, there are preview image and/or preview graph viewers.
One window always shows the original size and one window shows the preview which is cropped or reduced.

For example if you drop
- only spectral graph data objects you will see two graph viewers (original and preview of spectral / graph axis)
- at least one image or bitmap object you will also see two image viewers (original and preview of spatial axes)
- a hyper spectral line graph (e.g. time series) and a belonging single graph (e.g. time line) you will see 4 graph viewers (original and preview of spectral axis, original and preview of time line axis).



Graph and Image Data Stitching Dialog

Description

The Graph and Image Data Stitching Dialog allows showing multiple images side by side / as tiles in one bigger image.
It is also possible to stitch multiple spectral image data objects into one bigger graph data object. That can be useful if e.g. 3D data consisting of several stacked image scans shall be analyzed using multi-variate algorithms like Cluster Analysis.

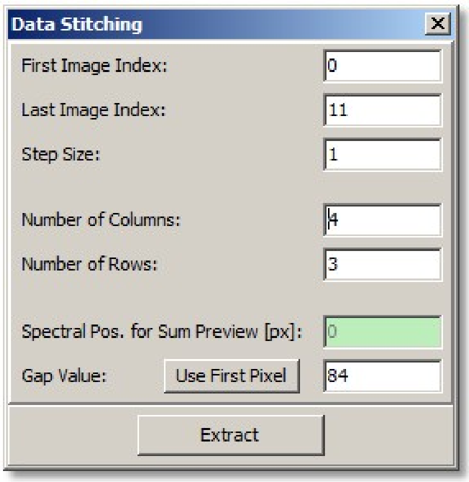
Input and Results

Input:
- any number of image data objects or
- any number of bitmap data objects or
- any number of image spectrum data objects.

All objects must have the same pixel size.

Results:
one bigger/stitched image or image spectrum data object.

User Interface



First Image Index (Integer Edit):
Define the first image here.
If doing depth stacks it's often the case that the first and last images don't show Raman signal, so you can hide them in the stitching image.

Last Image Index (Integer Edit):
Define the last image here.

Step Size (Integer Edit):
You can skip images with the step size; e.g. if you want to show larger differences in a high-resolution depth stack.

Number of Columns (Integer Edit):
defines the number of columns for the stitching image.

Number of Rows (Integer Edit):
defines the number of rows for the stitching image.

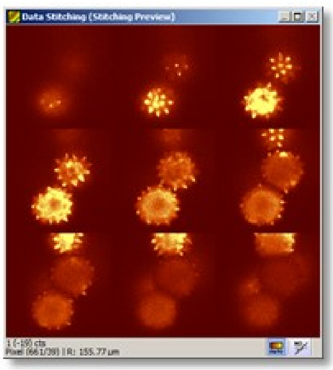
Spectral Pos. for Sum Preview (Float Edit):
When stitching image spectrum data objects the preview shows a sum image of a certain spectral position.
Change the position or double-click to turn on the listen mode in order to see another preview image.

Gap Value (Integer Edit):
If the number of images doesn't fit the number of tiles (rows * columns), there is an empty gap.
The gap value will be used in those empty areas.

Use First Pixel (Button):
If you have image gaps it can be useful to have a gap value which is similar to the image data. This button uses the first image pixel value as a gap value.
If a gap value is chosen that is not optimal there can be problems with the image viewer auto scale and it might be difficult to see enough details in the stitched image.

Extract (Button):
creates the new stitching data object and adds it to the current project.

Preview Windows



The preview image viewer shows the stitched image - possibly with smaller resolution than the real result (in order to have a better preview performance).
If image spectrum data objects are stitched, the preview image viewer shows a sum image for the selected spectral position.

Non Negative Matrix Factorization Dialog

Description

The Non-Negative Matrix Factorization is a multivariate analysis which creates intensity distribution images and their belonging spectra at the same time. For this it uses the fact that both images and spectra must have positive values in order to be a meaningful result. The calculation is an iterative process which consists of three parts:

1. Optimization of the distribution images
2. Optimization of the basis spectra
3. Optimization of the offset

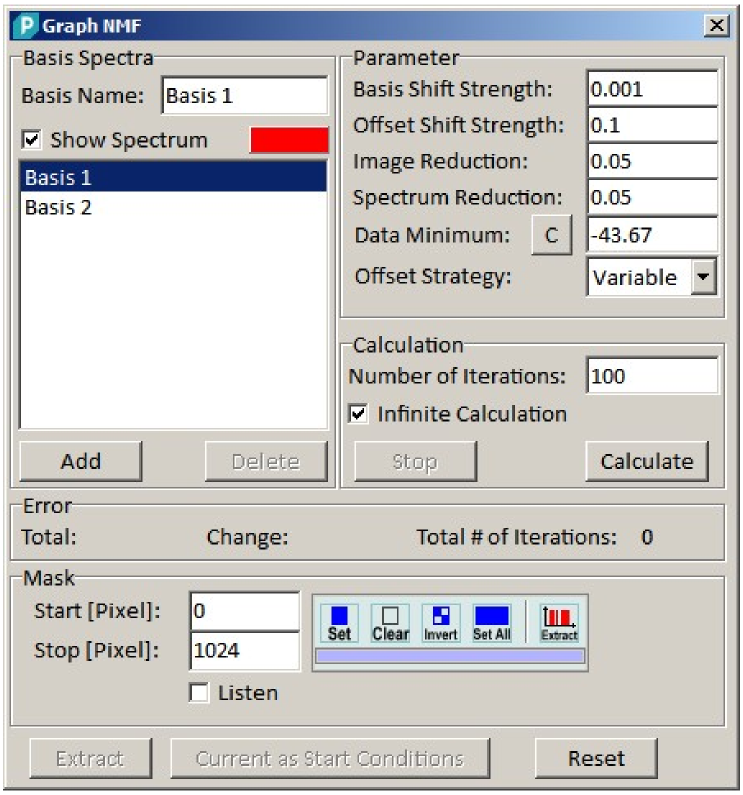
The first iteration starts from random. This dialog is part of the WITec Project Plus package.

Input and Results

Input:
One spectral Raman image data set

Results:
One image and spectrum for each component

User Interface



Basis Spectra Group

In this group the number of basis spectra that are needed to describe the dataset can be defined.

Add (Button)
Adds a new basis spectrum to the describing model.

Delete (Button)
Deletes the selected basis spectrum from the model.
The minimum number of basis spectra is two.

List Box
The list box shows the names of all basis spectra. To switch between the different components, click on one entry of the list box. The belonging information (Name, Show Spectrum and Graph Color) will change and in addition the image preview window will show the distribution map.

Basis Name (Edit Box)
The name of the selected component will be shown in the edit box. Before extracting the data you can change the name of the component. The name will be used as caption for the data object.

Show Spectrum (Check Box)
Unchecking the check box will exclude the basis spectrum from the spectrum preview

Color Box
Here you can define the color for the spectrum.

Parameter Group

The parameters in this group will change the behavior of the algorithm.

Basis Shift Strength
Many solutions with only positive values are possible. In order to get unique and meaningful results it is necessary to push the basis spectra towards the data.
This value is the area which is added to the normalized basis spectrum before an iteration starts.

Offset Shift Strength
Many solutions with only positive values are possible. In order to get unique and meaningful results it is necessary to push the basis spectra towards the data.
This value is an offset which is added to the offset spectrum before an iteration starts.

Image Reduction
Applying the algorithm on hyper spectral datasets is very time-consuming. Besides the image mask the number of pixel which will be used for calculation can be reduced by this factor.
Pixel from the mask are randomly added until all distributions have at least this portion of their total intensity.
At each iteration the selected pixels will change. Set this parameter close to 1, if all basis spectra are found.

Spectrum Reduction
Applying the algorithm on hyper spectral datasets is very time-consuming. Besides the spectral mask the number of spectral pixels which will be used for calculation can be reduced by this factor.
Pixels from the spectral mask are randomly added until all basis spectra have at least this portion of their total intensity.
At each iteration the selected pixels will change. Set this parameter close to 1, if all basis spectra are found.

Data Minimum
For the calculation all values of the dataset must be positive. Therefore an offset is added to the data before calculation. After starting the dialog the absolute minimum value of the data set is searched and copied to the edit box. Due to some preprocessing it can happen that the minimum value is too low (e.g. the background subtraction step did a miscalculation). In this case adapt this value slightly below the noise of the baseline.

Offset Strategy
Two different strategy for offset calculations can be chosen.

- choose "Const" if the offset is a horizontal flat line.
- choose "Variable" if one component always has the same intensity (e.g. Raman spectrum of the substrate)

Calculation Group

Number of Iterations
Defines the number of iterations that will be used.

Infinite Calculation
If this check box is enabled, the calculation runs until the user presses the stop button

Stop (Button)
Stops the the NMF calculation.

Calculate (Button)
Starts the NMF calculation. During the calculation the preview windows are updated regularly.

Error Group

During the calculation these values are updated.

Total
Average error between fit and dataset. If the value decreases the fits gets better.

Change
Difference between the last and the current average error. If this value is positive the fit gets better. If this value fluctuates between positive and negative, increase the value of Image Reduction and Spectrum Reduction.

Total # of iterations
Show the number of iterations.
You can simply turn the wheels or edit the number to define a weighting factor for subtracting the spectra from each other.

Mask Group

This group shows the standard Mask Manipulation Tools.

Buttons

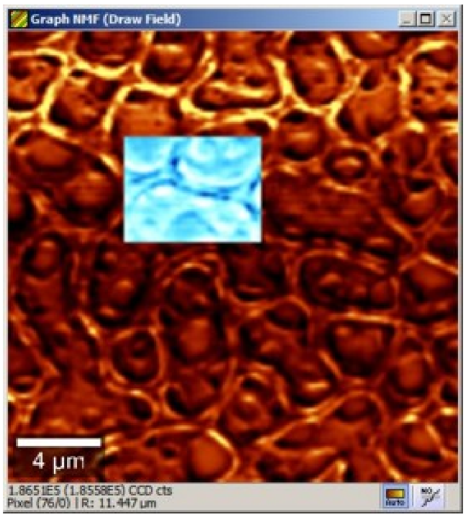
Extract (Button)
Extracts the basis spectra and distribution images.

Current as Start Conditions (Button)
To find the basis spectra only few spectra of the data set are needed. But in this case only the distribution map of the selected pixels are valid. In order to calculate the distribution map of all pixels press this button. After this it is possible to extend the image mask and start the calculation again. The distribution maps are now used as start condition for the algorithm.

Reset
Resets all basis spectra and distribution maps to random. This can be used if a new basis spectrum was added and the calculation ran before and change the basis spectra and distribution maps.

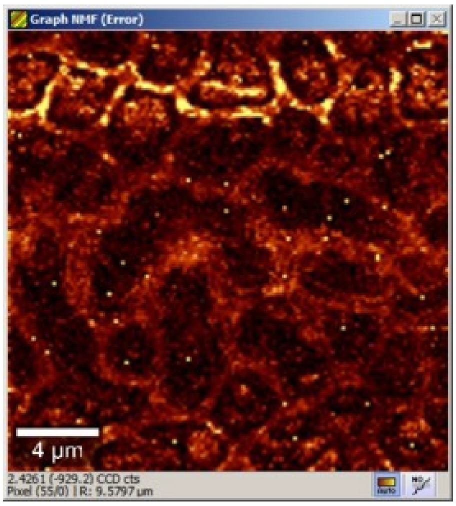
Preview Windows

Graph NMF (Draw Field)



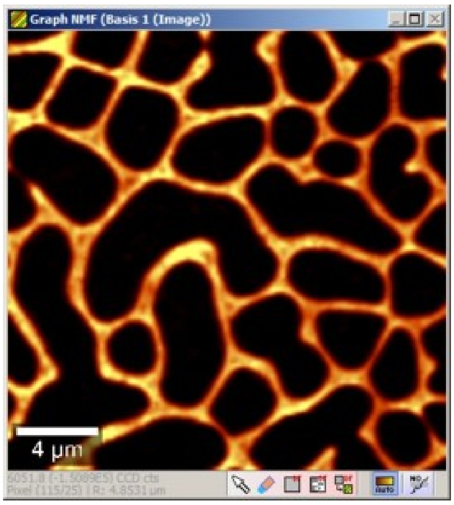
The image data shows the total sum of the spectrum. Use the draw field of this image preview window to select the pixels that should be used for the calculation.

Graph NMF (Error)



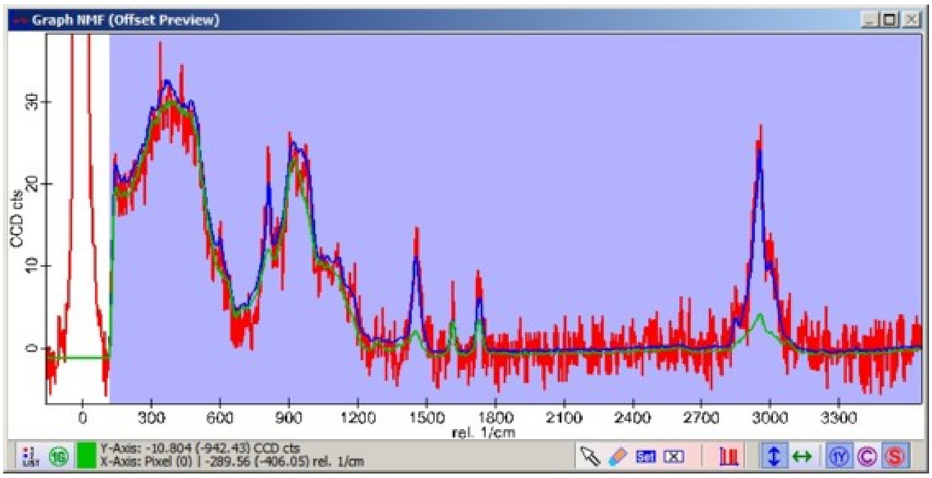
Show the average error between fit and data. A high value might be a hint that a additional basis spectrum is needed.

Graph NMF (Distribution Map)



Shows the distribution map of the currently selected basis spectrum.

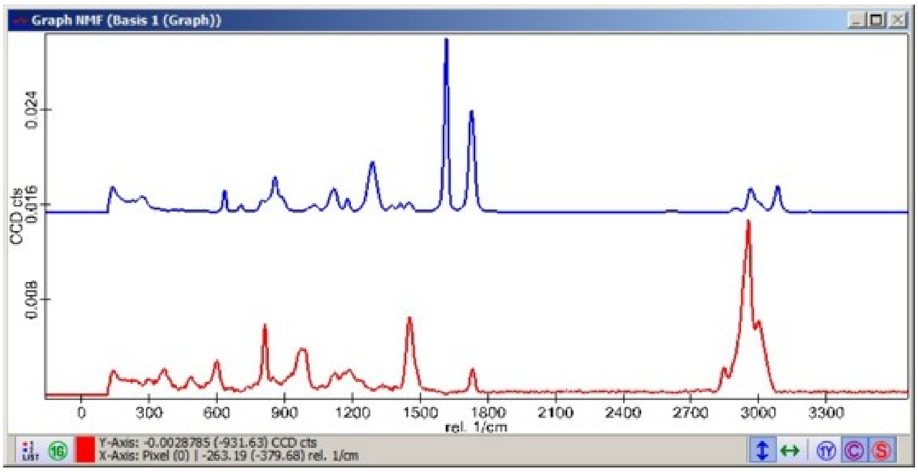
Fit Preview and Mask



The fit graph preview window shows the original spectrum in red, the fit preview in blue and the offset in green.
Just click somewhere in the preview image to see the selected spectrum.

Use the mask to define which spectral area should be considered for NMF calculation.

Basis Spectra



This graph preview window shows the normalized basis spectra.

Principal Component Analysis Dialog

Description

The Principal Component Analysis dialog does a principal component calculation and allows to extract its results.

Input and Results

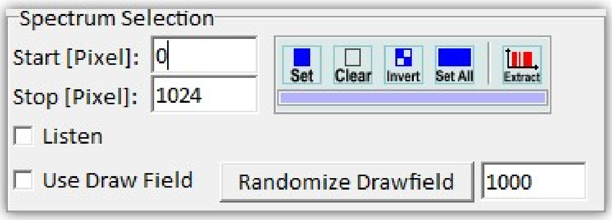
Input:

- One spectral Raman image data set
  or
- One spectral line graph data set (e.g. spectra along a line)

Results:
see "Extract Data" below.

User Interface

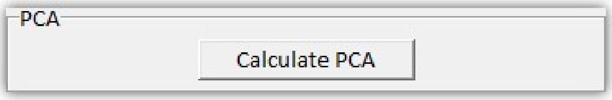
Spectrum Selection



Here you can select

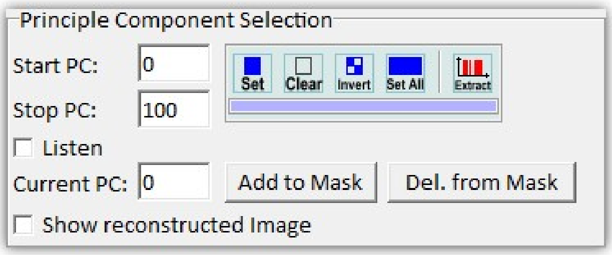
- which spectral range should take part in the PCA, see Mask Manipulation Tools
- which spectra should take part in the principal component calculation:
  If "**Use Draw Field**" is checked, the current mask on the the preview image viewer is used to select the spectra.
  If you click on "**Randomize Drawfield**", then the desired number of pixels are randomly selected.

Calculate PCA



Starts the PCA Calculation.

Principle Component Selection



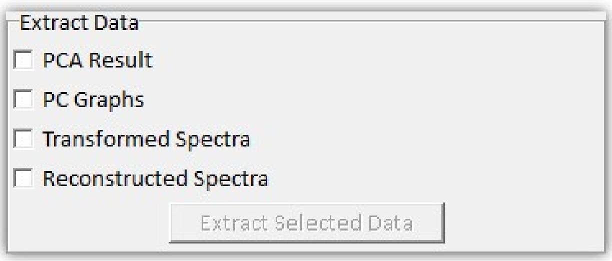
Here you can add or remove principal components using the graph mask of the "Eigenvalues" preview, see Mask Manipulation Tools.
The selected principal components are used to calculate a reconstructed spectrum preview.
Only the selected principal components are used when extracting data.

Show Reconstructed Image
If checked, a reconstructed image will be shown in the preview.
The value "Current PC" defines which component will be reconstructed

Add to Mask / Del. from Mask
Adds or removes the principle component of the "Current PC" value.

Extract Data

Here you can choose with result should be exported, if you press the button "Extract Selected Data".



PCA Result
Three graph objects are added to the project:

- The Eigenvalues
- The corresponding Eigenvectors
- The average spectrum (offset spectrum)

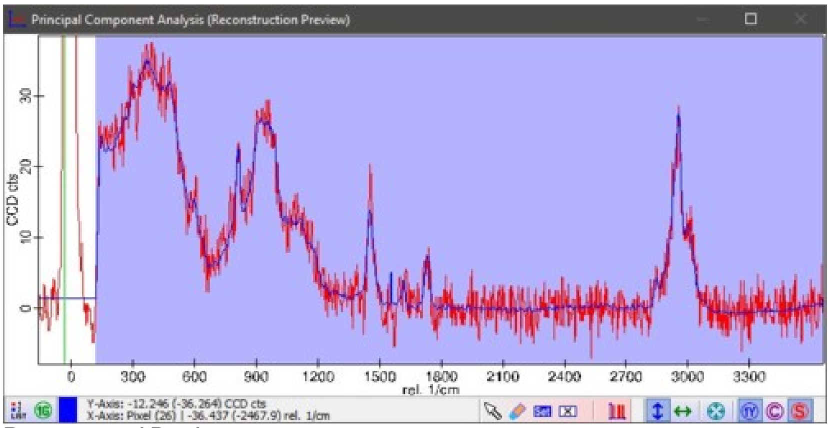
By clicking into the graph of the Eigenvalues it is possible to navigate through the Eigenvectors.

PC Graphs
The Eigenvector of each selected/marked principle component is extracted as a single graph object.

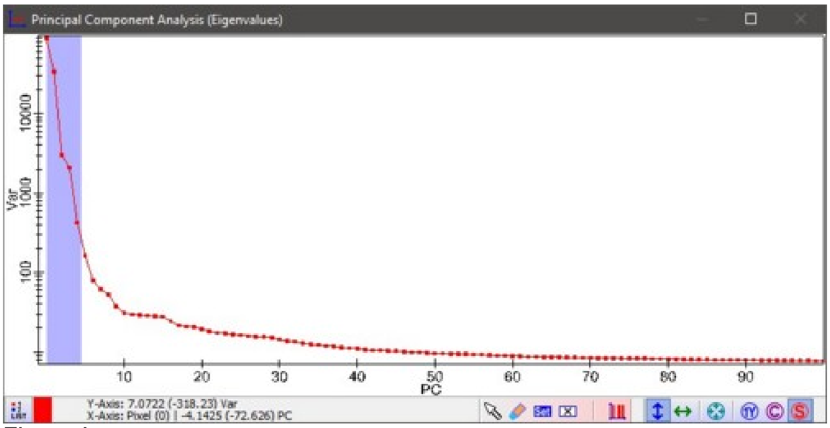
Transformed Spectra
The selected Eigenvectors define a new coordinate system. Each original spectrum can be represented in the new coordinate system. For each selected Eigenvector a new coordinate is calculated.
These transformed coordinates are stored into a graph object.

Reconstructed Spectra
It is also possible to do a back transformation of the transformed spectra. The output is equal to the blue spectrum of the Reconstructed Preview window.

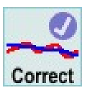
Preview Windows



Reconstructed Preview
Shows the original data in red and the reconstructed preview spectrum in blue.
The reconstructed spectrum is calculated using the principal component selection (mask in Eigenvalues preview).
You can manipulate the mask to define which spectral range should take part in the principle component calculation.



Eigenvalues
Shows the sorted Eigenvalues.
You can manipulate the mask to define which principle components should be used for the reconstruction preview and for extracting the data.



Graph Intensity Correction Dialog

Description

In some cases the signal response detected by a CCD is not equal for all pixels. This imperfection can be seen especially if a Raman spectrum contains high fluorescent background.
An optical etaloning effect inside CCD detectors and the optical filters which are used to reduce the Rayleigh light can cause this

problem.
In order to remove this imperfection, this dialog uses a fluorescence measurement in order to determine a correction curve.

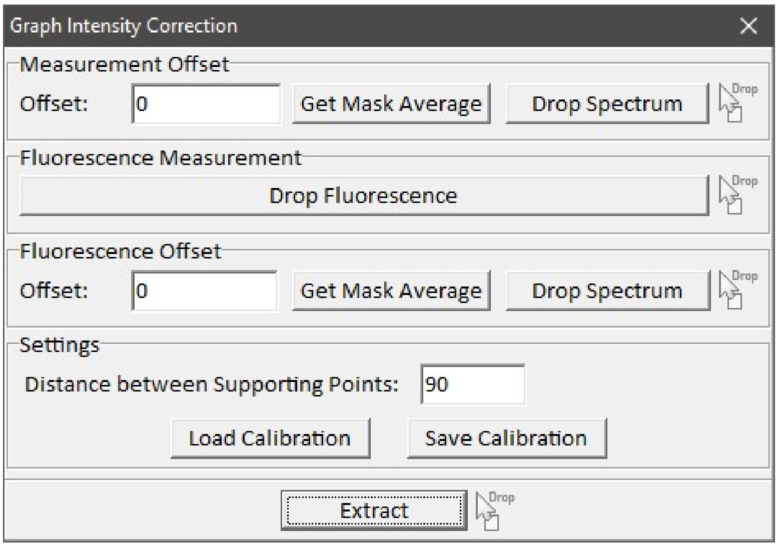
Please read Using Graph Intensity Correction for detailed information about how to use the dialog.

Input and Results

Input:
One graph object that can be a single spectrum or a multiple spectra object (e.g. Image Graph).
This is the object that will be corrected.

Results:
One graph object with the same dimensionality

User Interface



Measurement Offset - Offset (Edit)
Here you can define the offset manually, which will be subtracted before calculation.

Measurement Offset - Get Mask Average (Button)
If you press this button, the current spectrum and the selected mask (blue) is used to calculate an average. This average value is entered into the offset edit.

Measurement Offset - Drop Spectrum (Button)
If a dark spectrum is measured (single spectrum or series), you can drop it here in order to use it.
If you press this button, the offset is deleted.

Fluorescence Measurement - Drop Spectrum (Button)
Drop the fluorescence spectra here. An average is calculated and displayed inside a preview window.

Fluorescence Offset - Offset (Edit)
Here you can define the offset for the fluorescence spectra manually, which will be subtracted before calculation.

Fluorescence Offset - Get Mask Average (Button)
If you press this button, the average fluorescence spectrum and the selected mask (blue) is use to calculate an average. This average value is entered into the offset edit.

Fluorescence Offset - Drop Spectrum (Button)
If a dark spectrum is measured (single spectrum or series), you can drop it here in order to use it.
If you press this button, the offset is deleted.

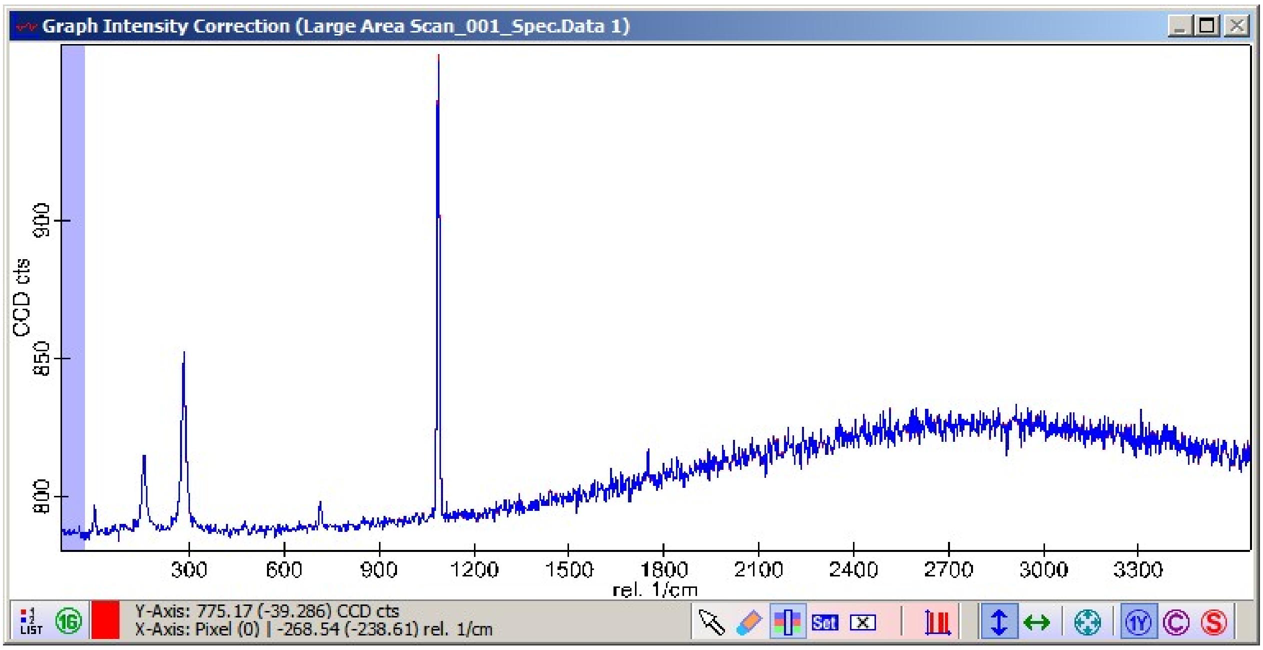
Settings - Distance between Supporting Points (Edit)
A smooth spline function is calculated from the average fluorescence spectra. The distance between the spline supporting points can be set with this edit.

Settings - Load / Save Calibration (Buttons)
Here you can save and load your calibrations to/from the hard drive. You can reuse it for all future measurements that are acquired under exactly the same conditions than the fluorescence spectra (same laser, same spectral position, same CCD settings).

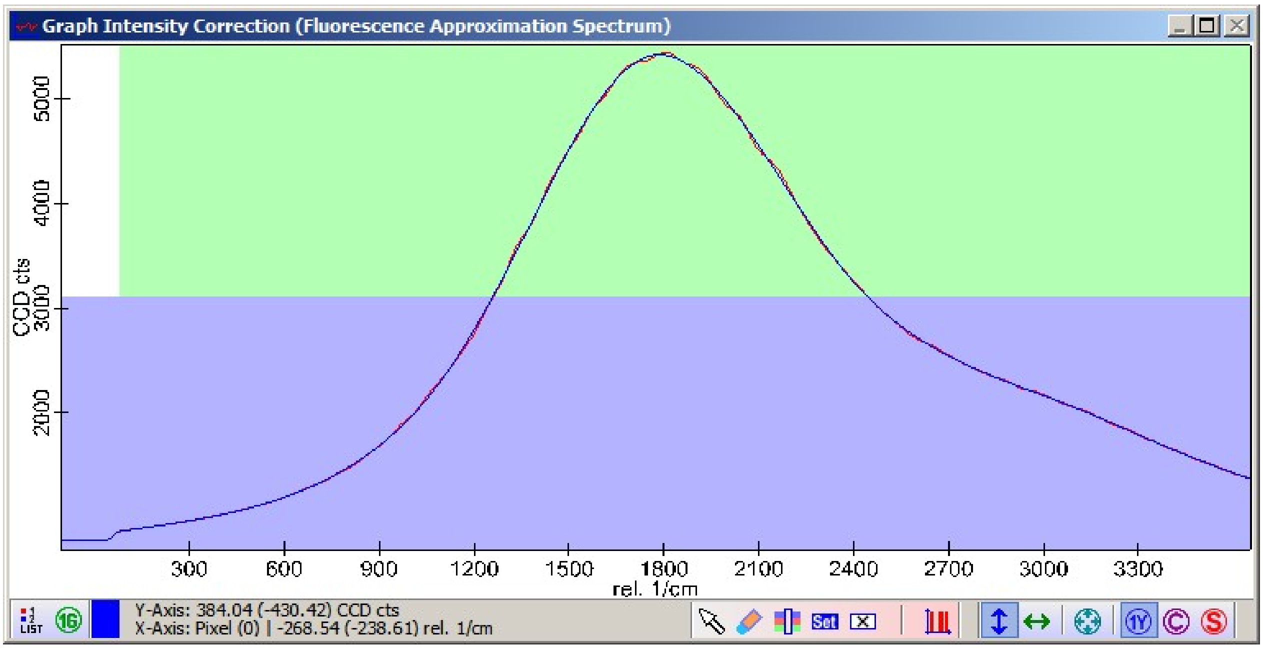
Extract (Button)

The corrected data will be exported to the project.
If more than one measurement have been acquired under same conditions, you can drop all measurements at once on this button.

Preview Windows



In the preview graph above the original and the corrected data is displayed. Normally you won't see any big difference for noisy spectra.



In this preview graph you can see the average fluorescence spectrum and the spline fit. The ratio of both is the correction used for the data.

The green mask defines the region that is used to calculate this ratio. If the green mask is not set, the correction factor will be 1. Note that the mask will be considered as one big region without gaps in between.

The blue mask can be used to define the offset of the fluorescence using the "Get Mask Average" button.

Image Background Subtraction Dialog

Description

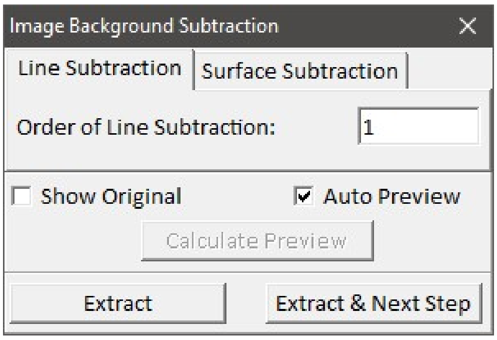
With the Image Background Subtraction Dialog you can subtract the background for each line (one dimensional) or for a whole surface (two dimensional) using polynomial functions with a adjustable order.

Input and Results

Input:
one image data object.

Results:
one background subtracted image data object.

User Interface



Line Subtraction Tab
If the line subtraction tab is selected, the image is being line subtracted (each single line is corrected using a one dimensional polynomial curve).

Surface Subtraction Tab
If the surface subtraction tab is selected, the image is being surface subtracted (a whole surface is subtracted using a two dimensional polynomial function).

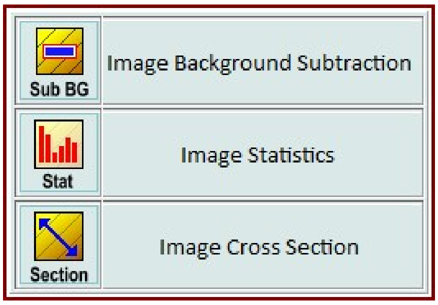
Order of Line / Surface Subtraction (Integer Edits):
sets the polynomial order for the line or surface subtraction.

Show Original (Check Box):
If checked, the preview image viewer shows the original image (for a fast comparison).
Don't forget to uncheck this check box afterwards to see the background subtracted image again.

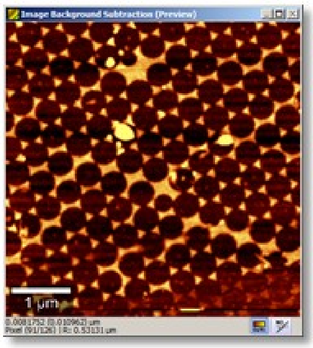
Calculate Preview (Button), Auto Preview (Check Box):
See Automatic Preview.

Extract (Button):
calculates and extracts the result to the current project.

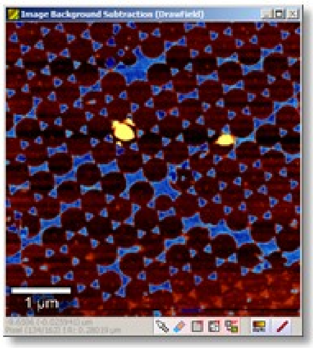
Extract & Next Step (Button):
Wizard feature: here you can choose to use the result image for another background subtraction, do some image statistics or an image cross section:



Preview Windows



The first preview window shows the background subtracted image.



The second preview window shows the original image and a draw mask.
Change the mask in order to define which pixels should be considered for calculating the the polynomial background fit function.

Image Statistics Dialog

Description

The Image Statistics Dialog can be used to analyze images by showing histograms and several statistic parameters.

Input and Results

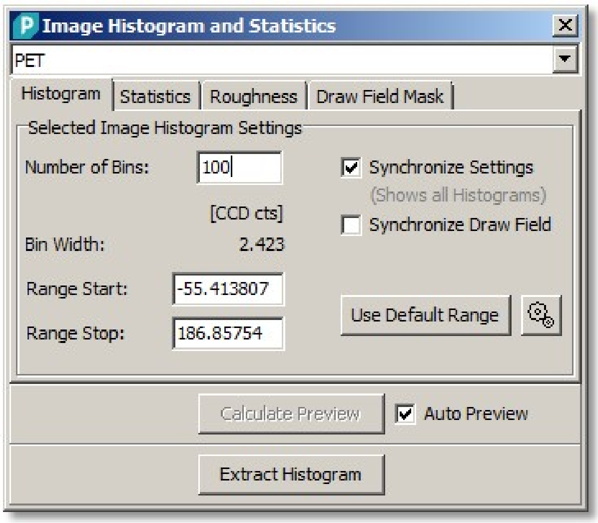
Input:
Any number of images.

Results:
Histograms or text objects containing statistic or roughness information.

User Interface

- Histogram Tab
- Statistics and Roughness Tab
- Draw Field Mask Tab
- Preview Windows

Histogram Tab



Number of Bins (Integer Edit):
Sets the number of bins or "vertical lines" for the histogram.

[CCD cts] (Label):
Shows the value unit of the currently selected image.

Bin Width (Label):
Shows the bin width of one histogram line.

Range Start/Stop (Float Edits):
Define the start and stop range of the histogram.
Both values are calculated automatically upon startup; each dropped image has its own range.

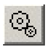
Synchronize Settings (Check Box):
Only enabled if all images share the same value unit kind.
If checked:

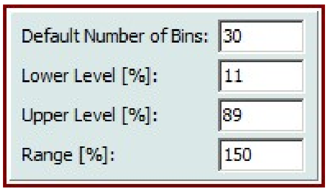
- all histograms of all dropped images are shown together in one graph preview
- all histograms share the same ranges and number of bins.

If not checked, each histogram has its own number of bins and range.

Synchronize Draw Field (Check Box):
Only enabled if all images share the same spatial transformation (same measurement).
If checked, the current draw field is used for all dropped images.
Otherwise each image has its own draw field that defines which pixels are used for the histogram and statistics calculation.

Use Default Range (Button):
resets the start and stop ranges of the current histogram using default settings for range determination (see below).

 **Default Range Settings (Tool Button)**



Default Number of Bins (Integer Edit):
This is the number of bins which is used when the dialog opens.

Lower Level (Float Edit):
The lower level of all sorted image values for default range value determination.

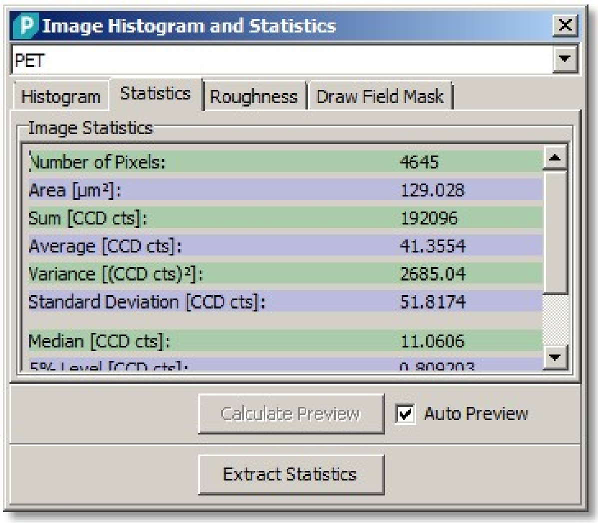
Upper Level (Float Edit):
The upper level of all sorted image values for default range value determination.

Range (Float Edit):
The range which is used to spread the range after using the lower and upper level.

Calculate Preview (Button), Auto Preview (Check Box):
See Automatic Preview.

Extract Histogram (Button):
calculates and extracts all histograms from all images.

Statistics and Roughness Tab



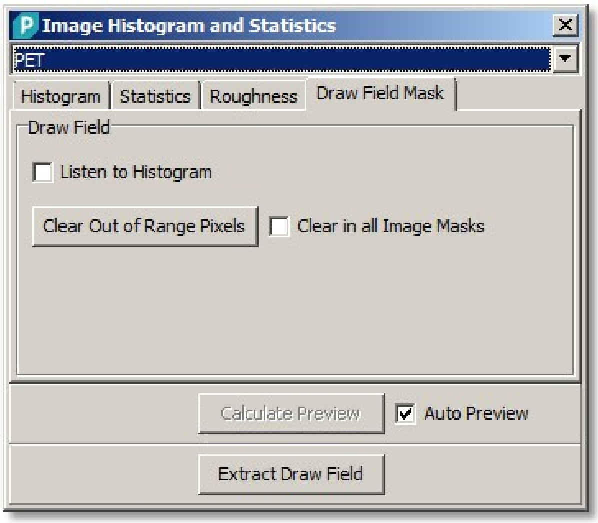
The **Statistics Tab** shows several image statistic values like the Average or Variance.
The values are calculated for all pixels that are set in the current image mask (see preview image viewer).

Extract Statistics (Button)
Creates a new text object containing all statistic parameters.

The **Roughness Tab** is very similar. Instead of standard statistical parameters it shows special roughness parameters (particularly used for topography images).

For a detailed description of the roughness parameters, see Image Statistics (Math).

Draw Field Mask Tab



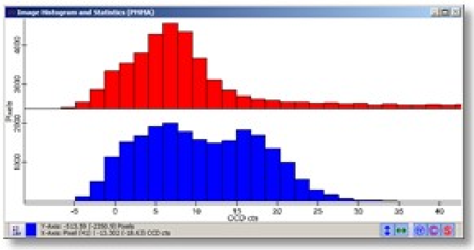
Listen to Histogram (Check Box):
If checked, you can set or clear (hold the shift key down) an area in the histogram in the preview graph viewer in order to set or clear the corresponding pixels from the image mask.

Clear Out of Range Pixels (Button)
This will clear all pixels from the image mask, that have values outside the current ranges of the histogram.

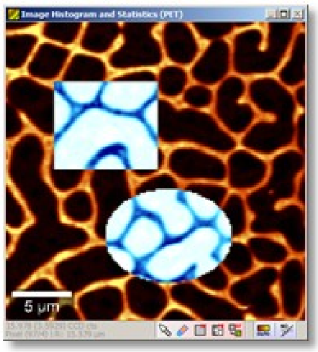
Clear in all Image Masks (Check Box)
If checked, the above button effects all image masks (if the mask is not synchronized anyway).

Extract Draw Field (Button)
Extracts all draw fields as a new boolean image data object to the current project.

Preview Windows



The graph preview window shows the histograms.
Hint: You can turn on or off the cascade mode in order to see the histogram lines side-by-side or cascaded.



The image preview window shows the currently selected image and the mask that defines which pixels are used for the histogram and statistics calculation.

Image Cross Section Dialog

Description

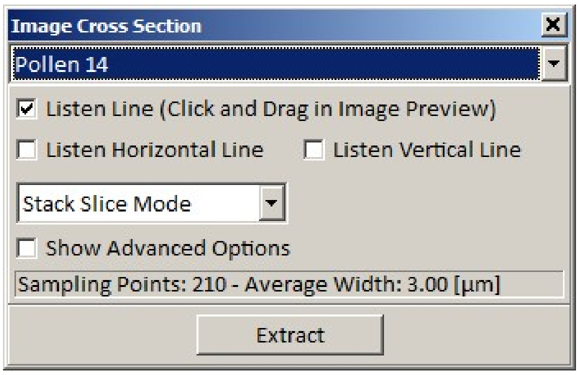
The Image Cross Section Dialog allows to display image intensities along a line as a graph object. This enables to analyze the structure of an image.
Additionally, a complete stack of images can be dropped in order to create a stack slice image.

Input and Results

Input:
Any number of image data objects.

Results:
One cross section graph object for each dropped image.

User Interface



"Pollen 14" (Combo Box):
selects the current preview image here (if you dropped more than one image).

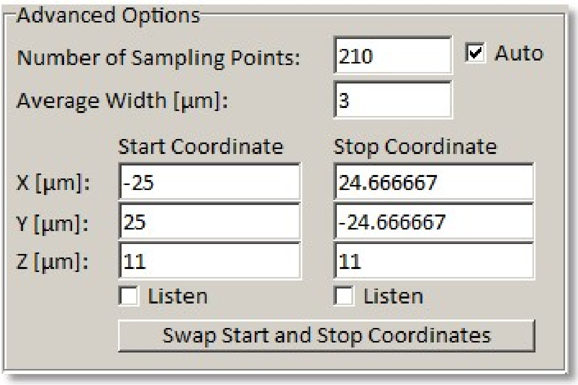
Listen Line (Check Box):
If checked, you just can draw a line in any image viewer in order to set a new cross section line position for this dialog.
This option is automatically checked upon starting the dialog, so you can directly draw your cross section line e.g. in the preview image viewer.

Listen Horizontal Line (Check Box):
If checked, you can click in a image viewer in order to use the clicked image line as a cross section. The dialog automatically sets the number of sampling points to the number of pixels in a line to use the exact supporting points of the image.

Listen Vertical Line (Check Box)
If checked, you can click in a image viewer in order to use the clicked image column as a cross section. The dialog automatically sets the number of sampling points to the number of pixels in a column to use the exact supporting points of the image.

Stack Slice Mode (Combo Box):
Only shown, if a image stack was dropped. Can be used to switch between stack slice mode and cross section mode.

Show Advanced Options (Check Box):
shows the advanced options:



Number of Sampling Points, Auto (Integer Edit, Check Box):
sets the number of pixels of the cross section graph object.
If the Auto Check Box is checked, this value is automatically determined (~3 times image pixel resolution).

Average Width (Float Edit):
If the average width is larger than zero, some pixels perpendicular to the cross section position with a distance of smaller or equal than <average width> are averaged and used for calculating one cross section value.

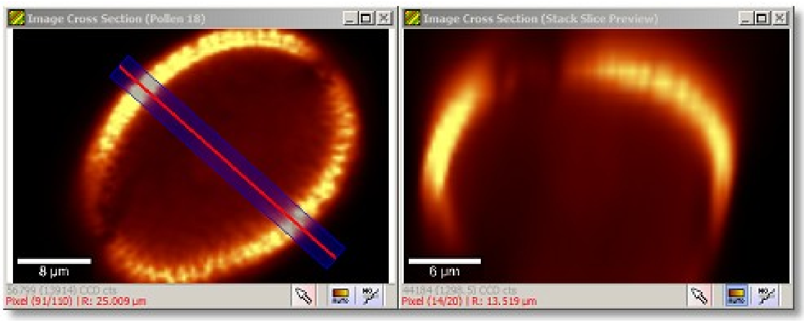
Start/Stop Coordinate (Float Edits):
Here you can exactly define an absolute spatial position for the start and stop coordinate of the cross section.

Listen Start/Stop Coordinate (Check Boxes):
If checked, you can click on an image in order to set the start or stop coordinate using the listen cursor mechanism.

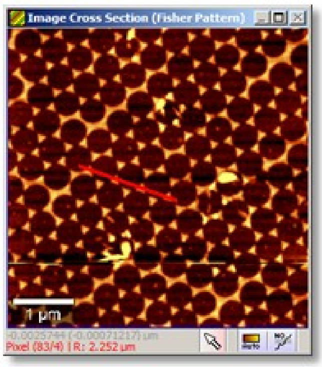
Swap Start and Stop Coordinates (Button):
simply swaps the start and stop coordinates in the result cross section.

Stack Slice Mode

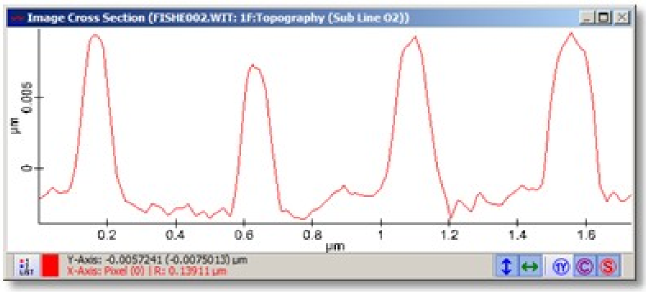
In the stack slice mode, a stack of images can be used to calculate a stack slice image (e.g. a depth image).
You can define a line in the cross section preview image window (lateral image) and see the stack slice preview in the second image window.
Click somewhere in the Stack Slice Preview Window in order to select the current stack image.



Preview Windows



The preview image viewer shows the selected input image and also the cross section line in red.
If the average width parameter is larger than zero, the image viewer shows a blue area which is used for averaging.



The preview graph viewer shows the cross section (or multiple cross sections if more than one image is dropped).

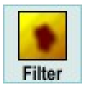


Image Filter Dialog

Description

The Image Filter Dialog offers several image smoothing and edge filters as well as a sharpen filter and a user definable custom filter.

Input and Results

Input:
Any number of image Data Objects.

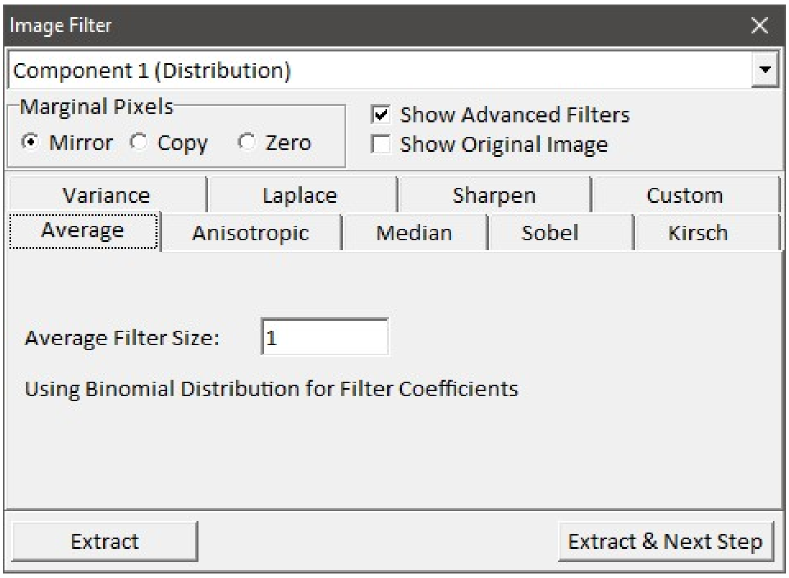
Results:
Smoothed images or edge filter images.

User Interface

- Average Tab and General UI
- Anisotropic Tab
- Median Tab
- Sobel Tab
- Kirsch Tab
- Variance Tab
- Laplace Tab
- Sharpen Tab
- Custom Tab
- Preview Windows

Average Tab and General UI

If the average tab is selected, the image is smoothed by a 2D averaging algorithm using binomial distribution for filter coefficients.



PET (Combo Box):
If multiple images are dropped, you can select the current preview image here.

Marginal Pixels (Radio Buttons):
Most filters use a certain window size using multiple pixels of the input image for calculating the result pixel. For marginal pixels / if the filter window is outside the image, you can select if

- the pixels are mirrored
- the border pixels are copied
- the pixels will be set to zero.

Show Advanced Filters (Check Box):
This will make all edge filters and the custom filter visible to the user.

Show Original Image (Check Box):
If checked, the preview image viewer shows the selected original image instead of the filter preview.
Don't forget to turn off this mode if you would like to see the filter preview again e.g. when changing some filter options.

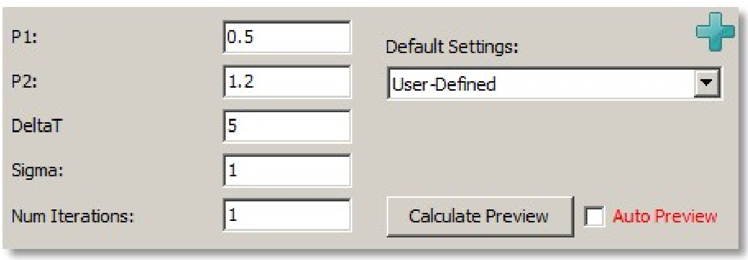
Average Filter Size:
sets the filter size for the average filter. The total average window size is (2 * <filter size> + 1)^2.

Extract (Button):
Calculates and extracts the result image(s) into the current project.

Extract & Next Step (Button)
Wizard Feature: you can use the result images of this dialog as an image combination:

Anisotropic Tab

If the anisotropic tab is selected, the image is smoothed using an anisotropic smoothing filter which also preserves the edges (see D. Tschumperle, Lecture Notes in Computer Science, 3952, 295 [2006]).
This is a WITec Project Plus feature.

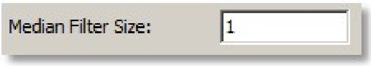


P1, P2, DeltaT, Sigma, Num Iterations (Edits):
Change the behavior of the anisotropic image filter.

Default Settings (Combo Box):
Chooses predefined settings for small and large structures.

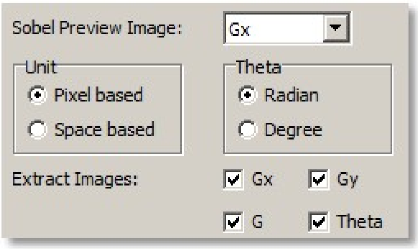
Calculate Preview (Button), Auto Preview (Check Box):
See Automatic Preview.
The automatic preview is disabled if the dialog opens.

Median Tab
If the median tab is selected, the image is smoothed by a 2D median algorithm.



Median Filter size (Integer Edit):
Sets the median filter size. The total median window size is (2*<filter size>+1)^2.

Sobel Tab
If the Sobel tab is selected, the edges in an image can be detected by searching in different directions using the Sobel operator. Additionally, the angle of maximum gradient can be shown.
This is a WITec Project Plus feature.



Sobel Preview Image (Combo Box):
You can select which Sobel result should be shown in the preview:
- Gx (Shows edges in x-direction)
- Gy (Shows edges in y-direction)
- G (Shows edges in x- and y-direction)
- Theta (Shows the edge angle as intensity)

Unit (Radio Buttons):
Changes the edge unit: pixel or space based (unit µm).

Theta (Radio Buttons)
Changes the angle unit: radians or degrees.

Extract Images (Check Boxes):
Select which of the Sobel results should be extracted when using the Extract Button.

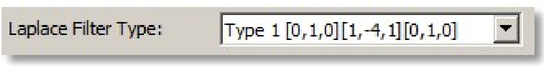
Kirsch Tab
If the Kirsch tab is selected, the edges of an image can be detected by searching in different directions using the Kirsch operator.
This is a WITec Project Plus feature.

Kirsch Filter Direction (Combo Box):
You can change the edge angle of the Kirsch filter (G1 - G8 and GMax which uses all directions).

Variance Tab
If the Variance tab is selected, the edges of an image can be detected by calculating the 2D variance.
This is a WITec Project Plus feature.

Variance Filter Size (Integer Edit):
You can change variance filter size. The total filter window size is (2*<filter size>+1)^2.

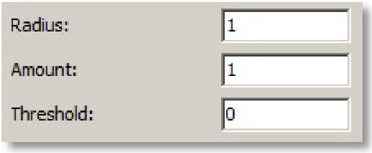
Laplace Tab
If the Laplace tab is selected, the edges of an image can detected using the Laplace operator.
This is a WITec Project Plus feature.



Laplace Filter Type (Combo Box):
Chooses between predefined Laplace filter coefficients.

Sharpen Tab

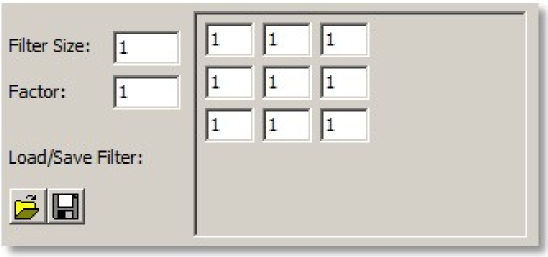
If the Sharpen tab is selected, the image is filtered using the Unsharp Masking technique.
This is a WITec Project Plus feature.



Radius, Amount, Threshold (Edits):
Changes the behavior of the sharpen image filter.

Custom Tab

If the Custom tab is selected, the image is filtered using user defined filter coefficients.
This is a WITec Project Plus feature.



Filter Size (Integer Edit)
Changes the filter size for the user defined filter. The total filter window size is (2*<filter size>+1)^2.

Factor (Float Edit):
A factor all filter coefficients are multiplied with.

Load/Save Filters (Tool Buttons):
You can save the current custom filter and reload it later on.

Filter Coefficients (Float Edit Matrix):
Enter your filter coefficients in the float edit matrix on the right side.

Preview Windows

The preview image viewer shows the preview of the smoothing/sharpen/edge algorithm.
You can toggle the "Show Original" checkbox in order to compare the result with the original image.

Image Repair Dialog

Description

The Image Repair Dialog can be used to replace unwanted pixels or areas in images using different replacement algorithms.

Input and Results

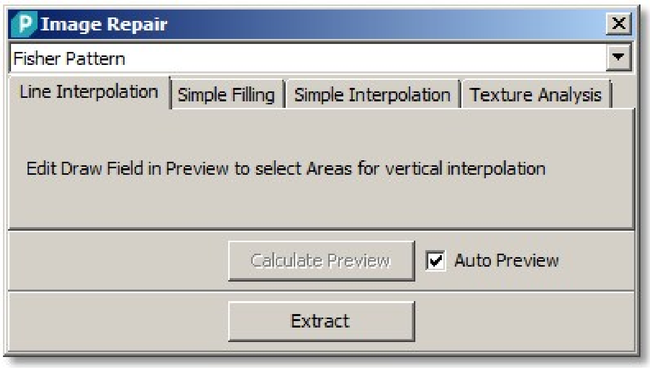
Input:
any number of image data objects.

Results:
repaired image data objects.

User Interface

Line Interpolation Tab and General UI

If the line interpolation tab is selected, the area which is set in the mask of the mask preview window will be interpolated using the lines above and below the masked area.



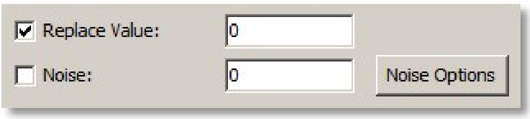
"Fisher Pattern" (Combo Box):
If multiple images are dropped, you can select the current preview with this combo box.

Calculate Preview (Button), Auto Preview (Check Box):
see Automatic Preview.

Extract (Button):
calculates and extracts the repaired image to the current project.

Simple Filling Tab

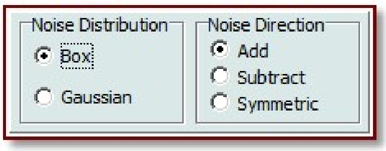
If the simple filling tab is selected, the area which is set in the mask of the mask preview window will be replaced using a given value which is optionally added with some random noise.



Replace Value (Check Box and Float Edit):
If checked, the masked areas are replaced using the replace value.

Noise (check Box and Float Edit):
If checked, the replaced values are furnished with noise of a given noise level/strength.

Noise Options (Button):
opens the noise options window:



Noise Distribution (Radio Buttons):
Here you can choose a noise distribution (Box or Gaussian noise).

Noise Direction (Radio Buttons):
Here you can chose a noise "direction", that means the noise is added or subtracted asymmetric or added symmetric.

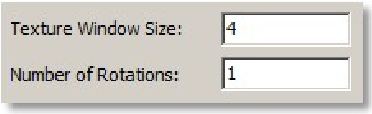
Simple Interpolation Tab

If the simple interpolation tab is selected, the area which is set in the mask of the mask preview window will be replaced using a simple interpolation algorithm that uses the borders of the mask areas for interpolation.

Number of Iterations (Integer Edit):
Sets the number of iterations for interpolation. The more iterations, the smoother the transition of image intensities.

Texture Analysis Tab

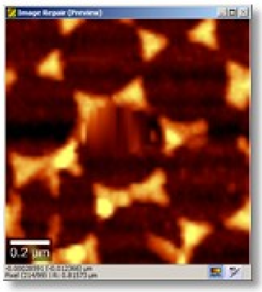
If the texture analysis tab is selected, the area which is set in the mask of the mask preview window will be replaced using a texture analysis algorithm that uses areas of the same image that fit best the areas to be replaced.



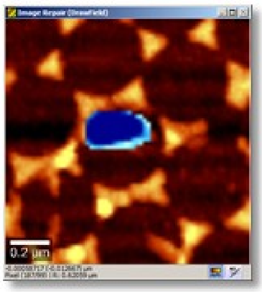
Texture Window Size (Integer Edit):
defines a texture window size which is used to search an appropriate replacement texture.

Number of Rotations (Integer Edit):
defines the number of rotations in order to find a better fitting replacement texture.
Both parameters have a strong influence on the calculation time.

Preview Windows



The first preview image viewer shows the repair preview.



The second preview image viewer shows the original image and the mask, that can be changed to define which pixels should be replaced or repaired.

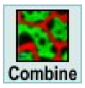


Image Combination Dialog

Description

The Image Combination Dialog can be used to combine multiple intensity images into a combined color bitmap using a different color table for each image.

Input and Results

Input:
Any number of image data objects.

Results:
One color combined bitmap object.

User Interface

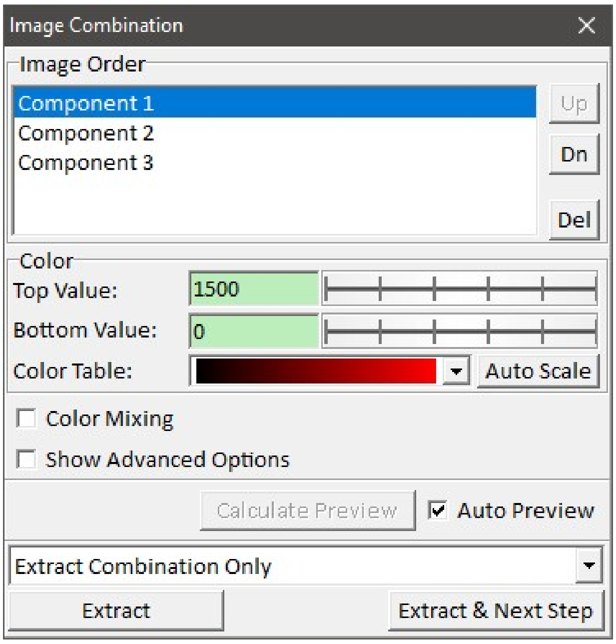


Image Order (List Box)
Shows the image list. You can select an image here in order to define its color scale, color table and - in advanced - mode the transparency thresholds.

Up/Dn (Buttons)
These buttons allow you to change the image order. This is only needed when using top or bottom transparency in the advanced mode.

Del (Button)
Removes the currently selected image (from the dialog only).

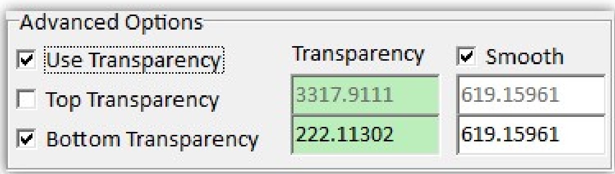
Top/Bottom Value (Edits and Sliders)
Changes the top and bottom color scale of the currently selected image.
In advanced mode, you can also use the preview image viewer ("Transp. Mask") color scale features to set the color scale of the current image.

Color Table (Combo Box)
Changes the color table for the currently selected image.

Auto Scale (Button)
This will do an automatic color scale for the currently selected image.

Color Mixing (Check Box)
If checked, the colors of all images are summed up / mixed for each image pixel.
If not checked, the dialog automatically decides which image will be shown at a certain pixel: the image with the brightest color will be displayed. This can be considered as an automatic mask algorithm.

Show Advanced Options (Check Box)
Shows the advanced options which are used to define a custom transparency:



Use Transparency (Check Box)
If checked, it's possible to use user defined transparency thresholds that define which parts of the images are transparent (letting images that "lay below" shine through the other image).

Use Top Transparency (Check Box)
If checked, all pixels with a higher value than the entered top transparency value are transparent.

Use Bottom Transparency (Check Box)
If checked, all pixels with a smaller value than the entered bottom transparency value are transparent.
Usually only this value has to be increased for each layer to create nice images.

Transparency (Edits)
The thresholds that define which pixels should be transparent.

Smooth (Check Box and Edits)
With these parameters the transparency transitions are drawn more smoothly.
A value of zero means that the border of transparency/no transparency is not smoothed.

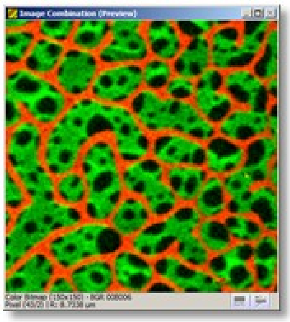
Calculate Preview (Button), Auto Preview (Check Box)
See Automatic Preview.

Extract Mode (Combo Box)

- Extract Combination Only: Extracts the combination bitmap only
- Extract All Images: Extracts the combination bitmap and every single image as a separate bitmap
- Extract All Images using Viewer Export Settings: Extracts the combination bitmap and every single image as a separate bitmap using the Image Viewer Export. This allows you to add a color scale bar next to each image and the "µm scalebar overlay" on the image. The current image graphic export options are used. You can also change those options using the image viewer export circle menu.
  Note that the result images will have no spatial transformation.

Extract (Button)
Calculates the result bitmap (if not already calculated) and adds it to your current project. Depending on the Extract Mode, also all bitmaps of all images are extracted as well.

Preview Windows



The first preview image viewer shows a preview of the combined color bitmap.

The second preview image viewer shows the selected image and its transparency mask.
This viewer is only visible in the advanced mode or if the extract mode "Extract All Images using Viewer Export Settings" is selected.
You can use the color scale features of this viewer in order to set the color scale of the currently selected image.

Image Fourier Filter Dialog

Description

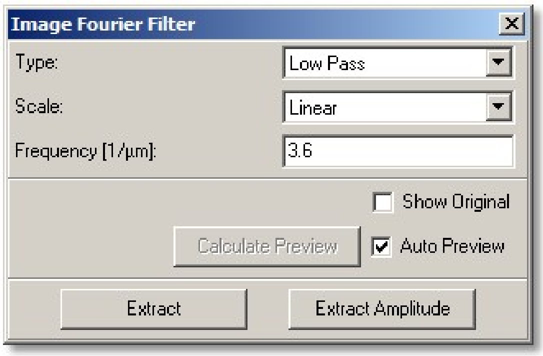
The Image Fourier Filter Dialog transforms an image into Fourier space (showing an amplitude image) and allows to change a mask in order to cut certain frequencies for a back-transformation.

Input and Results

Input:
one image data object.

Results:
the Fourier amplitude image or a back-transformed image.

User Interface



Type (Combo Box):
Depending on this option, you can change the mask in the amplitude image in order to cut frequencies in Fourier space for the back transformation:

- Free Hand: allows to change the mask directly in the image viewer using the draw tools.
- Low Pass: removes high frequencies using the frequency parameter.
- Low Pass Line: removes high frequencies line per line using the frequency parameter; only vertical mask.
- High Pass: removes low frequencies using the frequency parameter.
- High Pass Line: Removes low frequencies line by line using the frequency parameter; only vertical mask.
- Remove Harmonics: Removes harmonics for a given frequency.

Scale (Combo Box):
changes the scale of the amplitude image:

- Linear: linear scale
- Log: logarithmic scale
- Sqrt: square root scale.

Frequency (Float Edit):
defines the frequency for low pass (line), high pass (line) and remove harmonics mask creation.

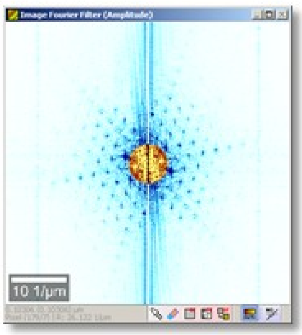
Show Original (Check Box):
if checked, the preview image viewer shows the original image instead of the back-transformed preview (for comparison).

Calculate Preview (Button), Auto Preview (Check Box):
see Automatic Preview.

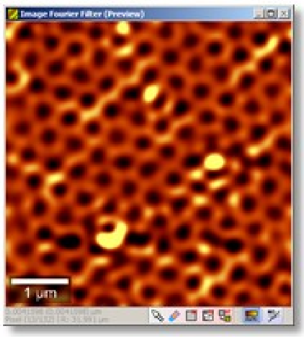
Extract (Button):
calculates and extracts the back-transformed image to the current project.

Extract Amplitude (Button)
extracts the amplitude image to the current project.

Preview Windows



The first preview image viewer shows the Fourier amplitude image. This viewer can be used to define a mask in order to cut frequencies for a back-transformation. Depending on the Type Parameter (Combo Box), this mask is automatically created.



The second preview image viewer shows the back-transformed image using the cut frequencies from the mask in the first preview image viewer.

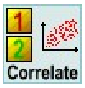


Image Correlation Dialog

Description

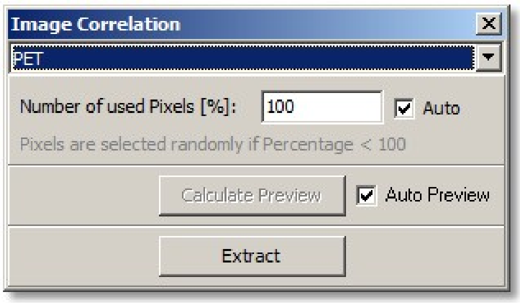
The Image Correlation Dialog creates graph objects containing information about the correlation of the intensity values of two different images.

Input and Results

Input:
at least two image data objects with the same spatial transformation.

Results:
one graph object for each dropped image object that can be shown as a correlation point cloud using the parametric display feature of the graph viewer.

User Interface



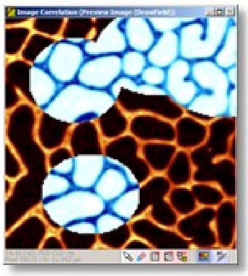
PET (Combo Box):
Selects the current image for the preview image viewer (e.g. as a helper for for mask manipulation).

Number of used Pixels (Float Edit), Auto (Check Box):
Sets the percentage of image pixels, that shall be used for the correlation plot / for the graph object.
If not all pixels are used (<100%), the pixels are selected randomly each time the mask changes or the dialog opens.
For very large images, it's not possible to use all pixels (overall limit is 100000 or ~300x300 pixels), therefore the upper limit could be smaller than 100%.

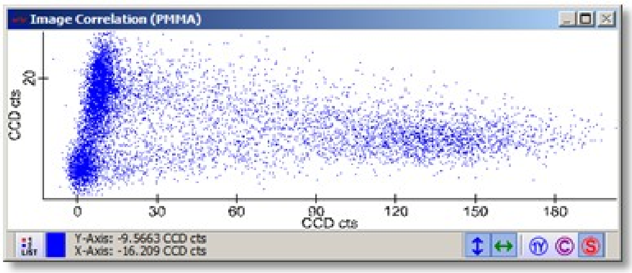
Calculate Preview (Button), Auto Preview (Check Box):
see Automatic Preview.

Extract (Button):
Extracts one graph object for each dropped image.
Open the graph objects in the same graph viewer window in order to show a correlation plot.

Preview Windows



The preview image viewer shows the current selected image and the mask, that can be changed in order to define which image pixels should be used for the correlation plot.



The preview graph viewer shows the preview correlation plot.
Hint: Turn off the automatic zoom features if you don't want the automatic zoom when changing the mask or pixel percentage (e.g. if you zoomed manually because of extreme valued points).

Image Auto/Extended Focus Dialog

Description

The Image Auto/Extended Focus Dialog can be used to combine multiple images from a whole image stack in order to have a nice sum image (Extended Focus) or a maximum image (Auto Focus).

Input and Results

Input:
Any number of images that belong to the same stacked measurement.

Results:
One extended or auto focus image and a position image (for auto focus).

User Interface

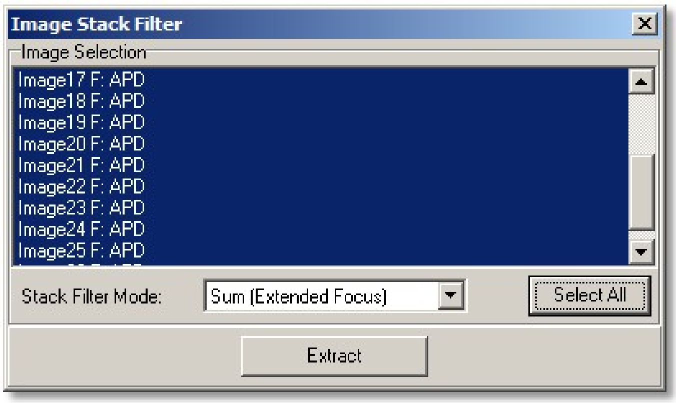


Image Selection (List Box):
You can select which images shall be used for the extended or auto focus operation. Use the shift or control keys to select more than one object.

Select All (Button):
Selects all images that were dropped.

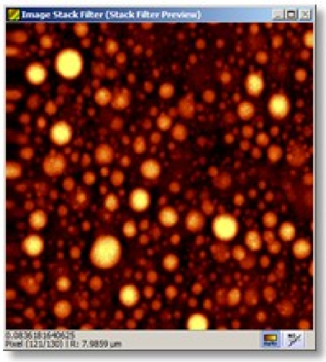
Stack Filter Mode (Combo Box):
Select a filter mode here:

- Sum: sums all selected images in order to provide an extended focus image

- Maximum: looks for the maximum intensity among all stacked images for each single xy-position; the found maxima are used in a so called "auto focus" image
- Position of Maximum: uses the spatial z-position of the image which has the maximum value of all images at each pixel

Extract (Button):
Calculates and extracts the results.

Preview Windows



The preview image viewer shows the sum or maximum or position of maximum image.

Image Stack Export Dialog

Description

The Image Stack Export allows to export multiple images as equally scaled bitmap files using a desired color profile and a fixed top/bottom for the color scale.
Stack layers get interpolated automatically in order to ensure cubic pixels - having a XYZ size ratio of 1.

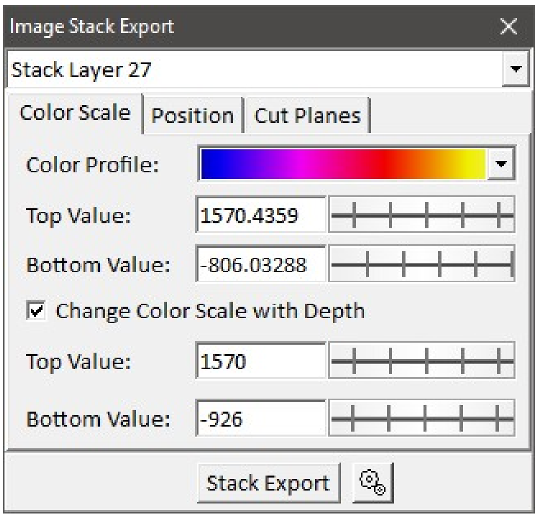
Input and Results

Input:
Any number of images that belong to the same stack measurement.

Results:
TIF image file containing all stack layers or multiple bitmap files on hard drive. Automatic transfer to external program available.

User Interface

Color Scale Tab



"Stack Layer 27" (Combo Box)
Here you can select which of the images should be shown in the XY preview window.

Color Profile (Color Combo Box)
Changes the color profile for all images.

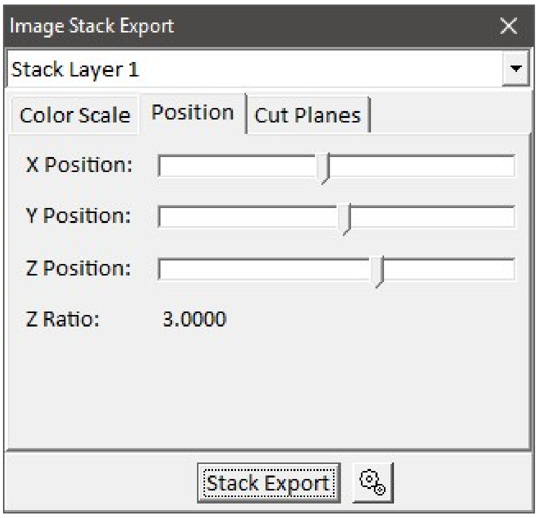
Top/Bottom Value (Edits and Sliders)
Changes the color scale for all images.

Change Color Scale with Depth (Check Box)
If checked, a second pair of Top/Bottom value edits appear and you have the chance to compensate changing intensities along the Z-Axis.
The upper Top/Bottom values define the color scale for the first layer of your stack, the lower Top/Bottom values for the last layer. Layers between will get interpolated color scales.

Export (Button)
Exports the stack according to the Image Stack Export Options.

Options (Button)
Opens the Image Stack Export Options.

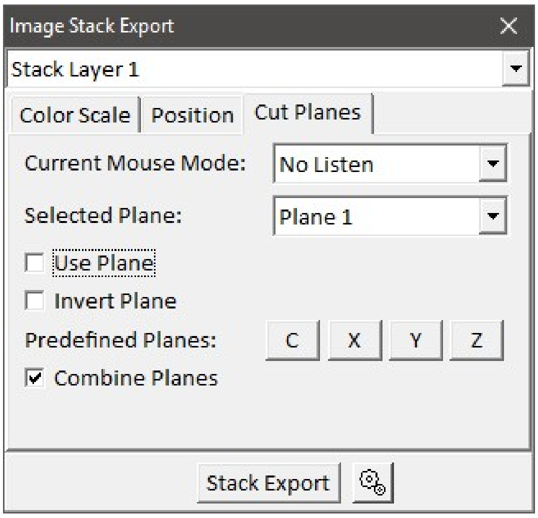
Position Tab



X/Y/Z Position (Slider)
Those sliders let you select the preview position in each direction.

Z Ratio (Label)
Shows the ratio between the xy pixel size and the z layer distance.

Cut Planes Tab



The cut planes tab allows you to "cut away" pixels from the stack (they will get black) in order to make them transparent in a volume or surface presentation.

Current Mouse Mode (Combo Box)
- No Listen: a mouse click into the preview images selects the preview position
- Listen Position: a mouse click into the preview images changes the position of the selected cut plane
- Listen Orientation: a mouse click into the preview images changes the orientation of the selected cut plane (angle)

Selected Plane (Combo Box)
Here you can select up to 3 different planes

Use Plane (Check Box)
If checked, the currently selected plane will be used for cutting away pixels.

Invert Plane (Check Box)
If checked, the currently selected plane will cut away pixels on the opposite side of the plane.

Predefined Planes ("C" Button)
Sets the plane position to the center of the image, keeping its orientation.

Predefined Planes ("X/Y/Z" Buttons)
Configures different default planes.

Combine Planes (Check Box)
If checked, multiple planes are combined which allows you to cut e.g. a "cube" out of your stack.

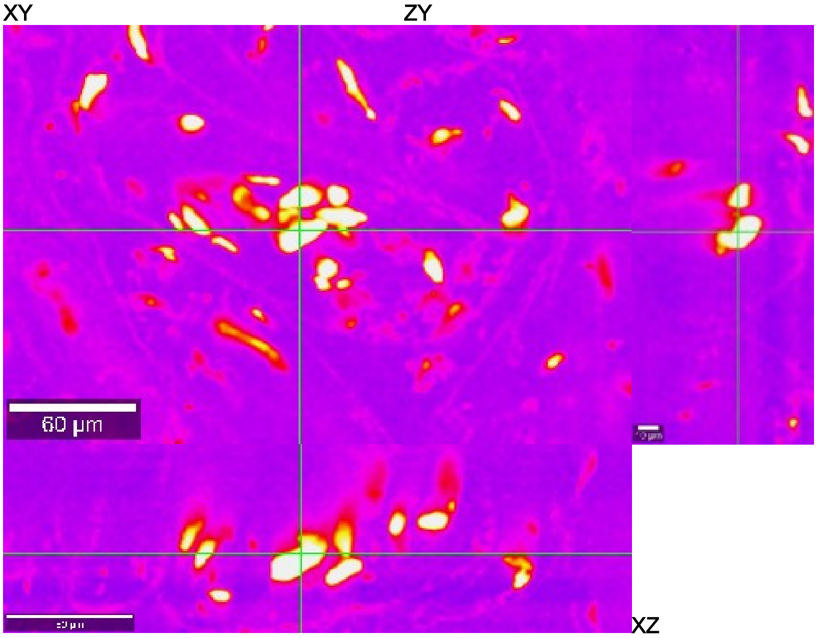
Preview Windows

Preview XY
Shows the XY Plane. If you click in this image, the XZ and ZY Images will change.

Preview ZY
Shows the ZY Plane. If you click in this image, the XY and XZ Images will change.

Preview XZ
Shows the XZ Plane. If you click in this image, the XY and ZY Images will change.

XY ZY



XZ

Inverse Basis Analysis Dialog

Description

This dialog uses intensity distribution images together with an image spectrum measurement to calculate demixed basis spectra and an offset spectrum.

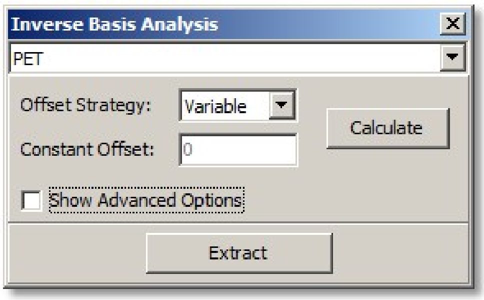
Input and Results

Input:
- One image spectrum data object
- <n> image data objects that belong the the image spectrum.

Note that the images must be background subtracted and demixed (demixed means that the images must show high/bright values only for 1 component)

Results:
- One basis spectrum for each dropped image and the offset spectrum.
- Optionally, an error image can be extracted.

User Interface



PET (Combo Box):
Here you can select one of the input images. It will be shown in the preview image viewer in order to being able to define an image mask.

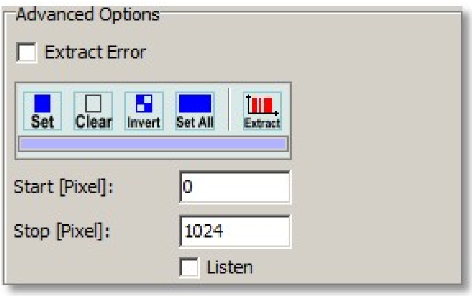
Offset Strategy (Combo Box):
Here you can select one of the offset strategies (chose the strategy depending on the offset of your spectra):
- Variable
- Constant

Constant Offset (Float Edit):
Enter a constant offset value, if your spectra have a constant offset.
Offset Strategy must be "Constant".

Calculate (Button)
This will start the inverse basis analysis and show the result in the preview windows.
Before you can calculate the inverse basis analysis, you have to chose which spectra should take part in the algorithm by drawing a mask in the image preview window.

Extract (Button):
Extract the current results.

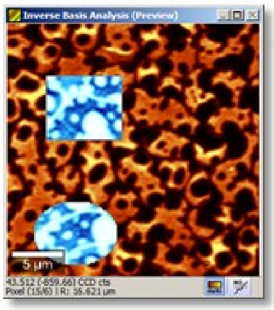
Show Advanced Options (Check Box):
Shows some advanced Options:



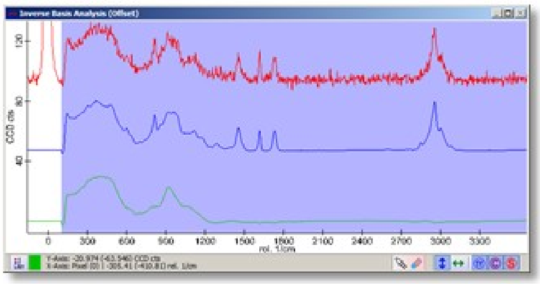
Extract Error (Check Box):
If checked, an additional error image is created when pressing the "Extract" Button.

Mask Controls (Tool Buttons and Edits):
You have to change the mask to define which spectral pixels should be used for the inverse basis analysis.
These edits are optional, you can change the masks directly in the preview graph viewer.

Preview Windows

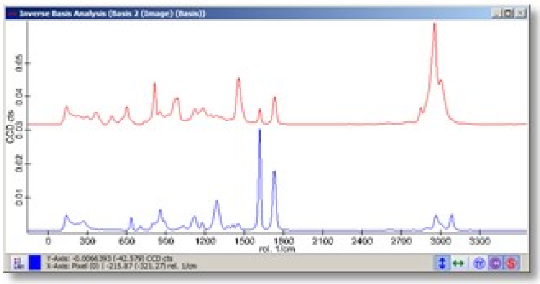


The preview image form shows the currently selected input image. You have to draw a mask here in order to define which image pixels should be used for the inverse basis analysis.



The first graph preview window shows:

- Original spectrum as a red graph
- The fit preview as a blue graph
- The offset preview as a green graph



The second graph preview window shows the preview basis graphs, one for each dropped image.

Image Transform and Overlay Dialog

Description

The Image Transform and Overlay Dialog has the following abilities:

- To create an overlay of two images/bitmaps (e.g. show the chemical Raman image on a video image)
- To change a spatial transformation data object for correcting displacements (Position, Scale, Rotation) or just to change it in the preview for bitmap creation
- Advanced Transformations for bitmap creation: Affine mapping, Bilinear mapping, Multiple-Affine mapping via triangle mesh

Input and Results

Input:

- Background Image (Image or Bitmap Data Object)
- Overlay Image (Image or Bitmap Data Object)

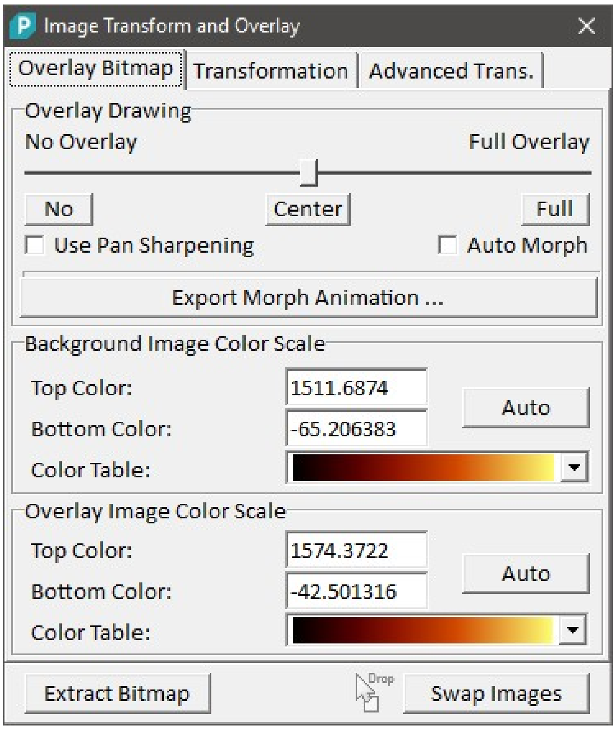
Results:

- Overlay Bitmap
- Changed Space Transformation of an existing data object

User Interface

- Overlay Bitmap tab
- Transformation tab
- Advanced Transformation tab
- Preview windows

Overlay Bitmap Tab



Overlay Drawing (Slider):
With this slider you can change the opacity of the overlay image.

Use Pan Sharpening (Check Box):
If checked, the background image defines the brightness (therefore only black and white) and the overlay image defines the color:

- an overlay slider position from "No Overlay" to "Center" defines the opacity of the overlay color.
- an overlay slider position from "Center" to "Full Overlay" defines the opacity of the overlay intensity.

If not checked, the background image keeps its colors and the overlay image is just overlayed.

Auto Morph (Check Box):
If checked, the overlay image opacity is automatically changed smoothly (this can be helpful e.g. for adjusting the transformation while comparing features in the overlay image with features of the background image).

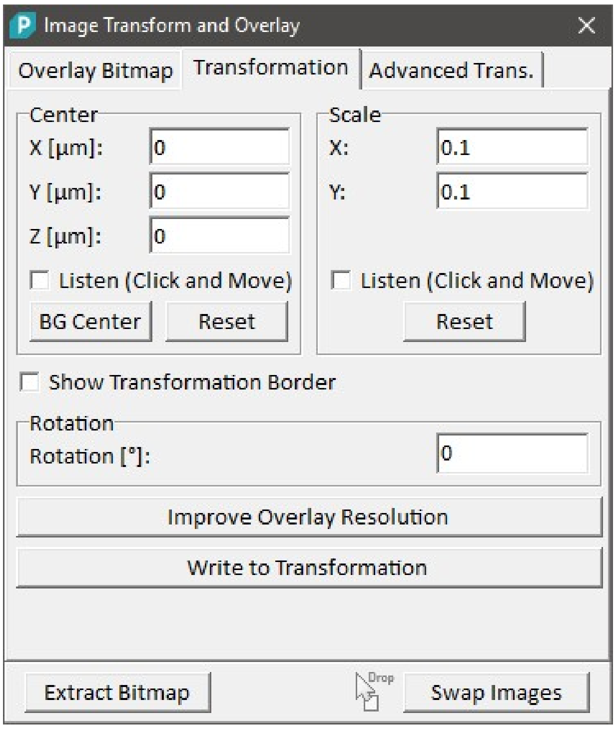
Export Morph Animation (Button):
Opens the Animation Editor for exporting an animation. Uses only the Overlay Parameter for the animation.

Background/Overlay Image Color Scale (group boxes):
The contrast/brightness of a color bitmap or the color scale of an floating point image can be changed - depending on what kind of data objects are used for this dialog.

Swap Images (Button, Drop Zone):
Pressing this button causes the dialog to re-initialize using the current overlay image as the background image and vice versa. This is also a drop zone. You can drop another overlay image onto this button in order to preserve all settings and transformations. This only works if the dropped image uses the an equal spatial transformation.

Extract Bitmap (Button):
Pressing this button extracts the current preview as a new color bitmap data object and adds it to the current project.

Transformation Tab



Center (Group Box):
With the X/Y/Z edits the current absolute position of the overlay image can be seen and changed.
Note: A much better way to change the position is the following described Listen mechanism.

Listen (Check Boxes):
If checked, the overlay image in the preview image viewer can be clicked and moved in order to change the absolute position or the scale of the overlay image.

BG Center (Button):
Sets the center position of the overlay image to the center of the background image (makes sense if the transformation of the overlay image is completely different, e.g. when importing an image).

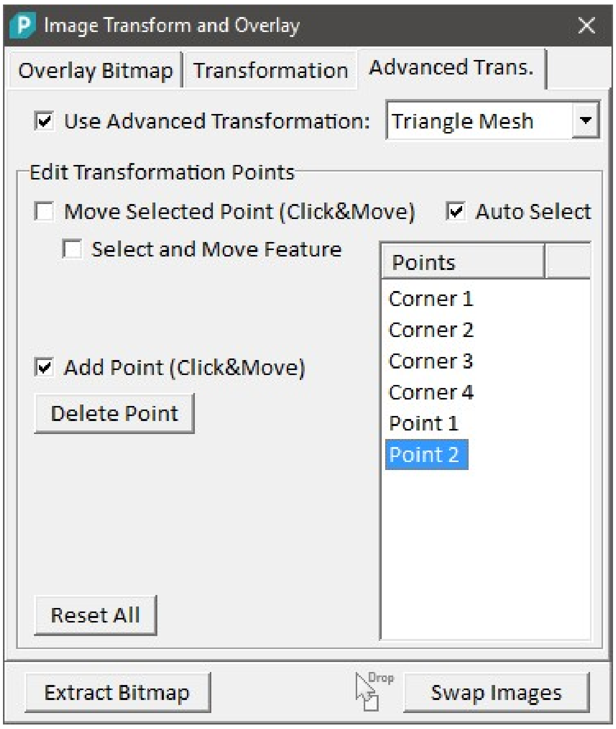
Reset (Button):
Resets the center or scale position of the overlay image using the original transformation.

Rotation (Float Edit):
Changes the rotation of the overlay image (this parameter will only rotate the image on the axis perpendicular to the image plane).

Improve Overlay Resolution (Button):
Creates a new background image or bitmap by increasing its resolution.
This is useful if the overlay image has a higher resolution than the background image (on the overlay region).
After the improvement, the background image has enough pixels such that the overlayed image can be displayed in its full resolution. Note that you will only see a difference in the overlay region.

Write to Transformation (Button):
This will overwrite the spatial transformation data of the overlay image (not only the preview transformation!).
This may affect other data objects that use the same spatial transformation (images and image graph objects). In general this means objects created by the same measurement or were results of an analysis of the same measurement. You'll get a list of all affected data objects before you can confirm or cancel the permanent transformation change.

Advanced Transformation Tab



Use Advanced Transformation (Check Box):
Turns on or off the advanced transformation.

Advanced Transformation Selector (Combo Box):
One can chose between the following advanced transformations:

- Affine (Affine mapping of 3 points, see Affine Transformation Math)
- Bilinear (Bilinear mapping of 4 points, see Bilinear Transformation Math)
- Triangle Mesh (Any number of points that create a triangle mesh; using affine mapping for each triangle, see Triangulation Math)

Move Selected Point (Check Box):
Turns on the listen mechanism to change the position of a single point. If the **Auto Select Check Box** is checked, the point next to the mouse cursor will listen to the cursor position; otherwise, the currently selected point in the Point List will listen.

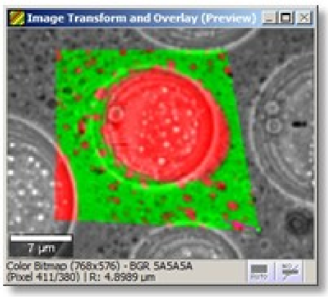
Select and Move Feature (Check Box):
If checked, the mouse cursor position at the moment of pressing the mouse button down will be used as the source position for distortion. Use this feature if you would like to click on a feature in the overlay image and want to "move" it onto the corresponding feature on the background image.

Add Point (Check Box):
Adds a new point in the Triangle Mesh mode. When pressing the mouse down the point is added using the source position of the clicked position. If you move the mouse afterwards the target of the point is changed.

Delete Point (Button):
Deletes the currently selected point in the point list. Corner points can't be deleted.
Be careful: if the Auto Select Check Box is checked, you might accidentally select another point before deleting.

Reset All (Button):
Deletes all custom points and resets the corner positions tho the original image corner positions.

Preview Windows



The preview image form shows the background and overlay image.
In Advanced Transformation Mode, it also shows the currently selected point which makes it easy to use customized distortion effects.

Automatic Preview

All data analysis dialogs (drop action dialogs) have preview windows showing a preview of the result(s).
Some of the dialogs need some calculation time if very large data objects are used.
They show the following options:

Auto Preview (Check Box):
With this check box you can turn off the auto preview in order to change settings or masks without being disturbed by a longer running automatic calculation.
This option is automatically turned off if the dialog opens with a very large objects (e.g. images with > 700 x 700 Pixels).

Calculate Preview (Button):
If the auto preview mode is turned off, you can manually do the preview calculation once by pushing that button.

Listen Cursor Mechanism

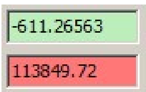
Some parts of the software can listen to a cursor position that was sent from another window, e.g. from the Graph- or Image-Viewer.

There are implicit and explicit listening modes:

Implicit listening happens automatically, e.g. if you click into an image viewer, a graph viewer listens to the spatial position and shows the corresponding spectrum of a image graph data object.

Explicit listening is activated by a dialog or and edit automatically or has to be activated by the user. There are the following possibilities for this explicit listening:

Edits with Listen Capability



All edit controls in the software that have a green background color are "listenable".
That means their value can be changed by sending a cursor position from other windows.
You can **turn on or off the listening mode by double-clicking** into the edit control.
Edit controls that are currently listening have a red background color.

It depends on the value kind to which unit or cursor the edit control will listen.

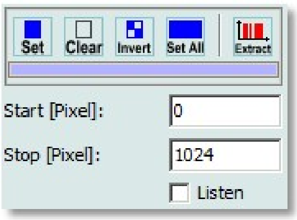
Manipulating Masks via Listen Cursor Mechanism

See Mask Manipulation Tools.

Mask Manipulation Tools

Although masks can be manipulated very fast directly in the Graph Viewer (see Graph Viewer Mask Manipulation), it is possible to set or clear a pixel range exactly defined by the user.

All data analysis dialogs that support mask manipulation offer a belonging mask user control:



Set (Tool Button)
sets a mask at the range given by the Start/Stop Pixel Edits aside.

Clear (Tool Button):
clears the mask at the range given by the Start/Stop Pixel Edits aside.

Invert (Tool Button):
inverts the complete mask.

Set All (Tool Button):
sets all pixels in the mask.

Extract (Most Right Tool Button):
extracts the mask as a single graph object to the project.
You can drag and drop such a mask graph object onto the mask in the graph viewer (see Graph Viewer Drag and Drop) or onto one of the mask tool buttons to reuse it.

Color Bar:
The Color Bar below the tool buttons shows the color in the preview graph window of the mask that is being changed by the buttons above.
If multiple masks are changed, no color bar is visible.

Start [Pixel] (Integer Edit);
the beginning of the range that will be cleared or set in the mask using the Set or Clear Tool Buttons.

Stop [Pixel] (Integer Edit):
the end of the range that will be cleared or set in the mask using the Set or Clear Tool Buttons.

Listen (Check Box):
If the Listen Check Box is checked, the start and stop pixel edits will listen to a spectral range sent by any Graph Viewer window using the Mouse Marker.

See also Listen Cursor Mechanism

Image (Def)

The following symbols are used for 2-dimensional image data:

$$
\begin{array}{ll}
I_{i,j} & : Image\ value \\
i,j & : Pixel\ position \\
x_{i,j} & : X - Coordinate \\
y_{i,j} & : Y - Coordinate \\
z_{i,j} & : Z - Coordinate \\
N & : Pixels\ per\ row\ i = 0..N-1 \\
M & : Pixels\ per\ column\ j = 0..M-1
\end{array}
$$

Average Spectrum (Math)

The following formulas are used to calculate an average spectrum from a set of spectra with given weighting factors:

$$
\vec{S}_{Ave} = \frac{1}{W}\sum_{i=0}^{N-1} w_i \vec{S}_i \qquad W = \sum_{i=0}^{N-1} w_i
$$

$$
\begin{array}{ll}
N & : Number\ of\ spectra \\
\vec{S}_i & : i - th\ spectrum \\
w_i & : i - th\ weighting\ factor \\
\vec{S}_{Ave} & : Average\ spectrum \\
W & : Sum\ of\ weighting\ factors
\end{array}
$$

See also

- Spectrum (Def)

Remarks

No Weighting

The weighting factors equal 1 if no weighting is used. In this case the sum of weighting equals the number of spectra.

Boolean Weighting

In most cases the weighting factors are given by a mask that was set by the user or by some algorithm. In this case the weighting factor equals one if the mask is set, and equals zero if the mask is not set. The sum of the weighting factors equals the number of spectra selected by the mask.

Filter Viewer (Math)

This section describes the math behind the Filter Viewer. This includes the background subtraction which is done before the Filter is calculated.

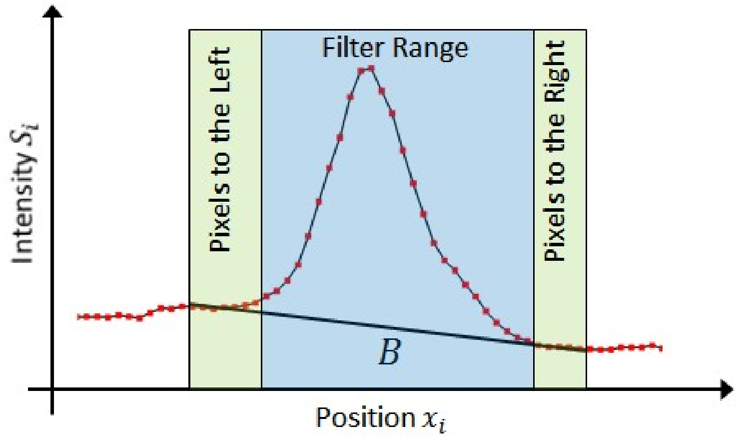
Background Estimation

$$S_i = \tilde{S}_i - B(x_i)$$

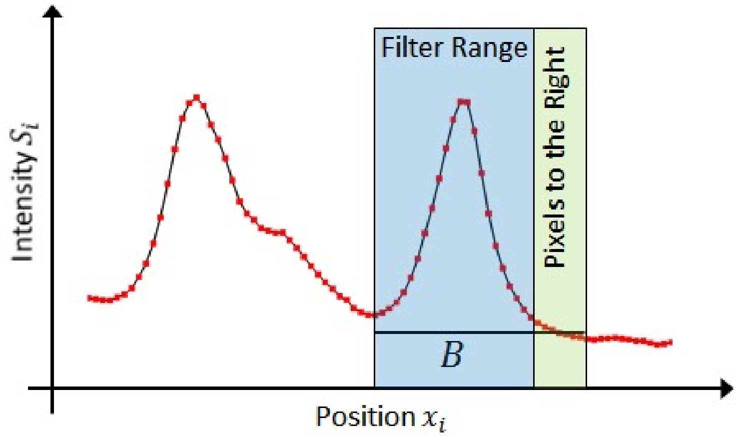
$$\begin{array}{ll} \tilde{S}_i & : Spectrum\ with\ background \\ S_i & : Spectrum\ without\ background \\ B(x_i) & : Background\ estimation\ at\ position\ x_i \\ x_i & : Spectral\ position\ at\ pixel\ i \end{array}$$

The background B is calculated using the neighbor pixels of the filter range. The number of pixels to the right and to the left can be defined in the Filter Viewer.

If the number of pixels to both sides is larger than 0 a slope is calculated. The average intensity and the average positions on both sides define the coordinate for the slope calculation.



If the number of pixels is zero on one side a horizontal line is used as background estimation. It is calculated by the intensity average of the other side.



If both number of pixels are 0, no background subtraction is performed.

Filter Calculation

The following notation is used for the filter calculations.

$$\begin{array}{ll} n_l & : leftmost\ pixel\ inside\ the\ filter\ range \\ n_r & : rightmost\ pixel\ inside\ the\ filter\ range \end{array}$$

Sum Filter

$$F_{sum} = \sum_{i=n_l}^{n_r} S_i$$

Average Filter

$$F_{ave} = \frac{1}{n_r - n_l + 1} \sum_{i=n_l}^{n_r} S_i$$

Average minus Minimum Filter

$$F_{ave-min} = F_{ave} - F_{min}$$

Standard Deviation Filter

$$F_\sigma = \sqrt{\frac{1}{n_r - n_l + 1}\sum_{i=n_l}^{n_r}(S_i - F_{ave})^2}$$

Center of Mass Filter

$$F_{CoM} = \frac{1}{F_{sum}}\sum_{i=n_l}^{n_r} x_i S_i$$

Peak Width Filter (FWHM)

Starting from the F(pos of max) the algorithm searches to the right and the left direction at which the signal falls below 0.5*F(max). The neighbor pixels of these two positions are used in a linear model to calculate the FWHM.

Minimum Filter

$$F_{min} = min\{S_i : n_l \le i \le n_r\}$$

Maximum Filter

$$F_{max} = max\{S_i : n_l \le i \le n_r\}$$

Position of Minimum Filter

$$F_{pos\,of\,min} = first\{x_i : S_i = F_{min}, n_l \le i \le n_r\}$$

Position of Maximum Filter

$$F_{pos\,of\,max} = First\{x_i : S_i = F_{max}, n_l \le i \le n_r\}$$

Line Correction (Math)

Each line of an image is subtracted by a k-order polynomial. The coefficients of the polynomial are calculated by fitting the polynomial to the line data.

$$I_i^{sub} = I_i - P_k(\vec{a}|i)$$

$$P_k(\vec{a}|i) = \sum_{m=0}^{k} a_m (i)^m$$

$$\sum_{i=0}^{N-1} w_i (I_i - P_k(\vec{a}|i))^2 = Minimum$$

I_i : *Image value*

I_i^{sub} : *New image value*

$P_k(\vec{a}|i)$: *Polynomial of order k*

$\vec{a}$: *Fit parameter*

i : *Pixel position*

w_i : *Weighting factor*

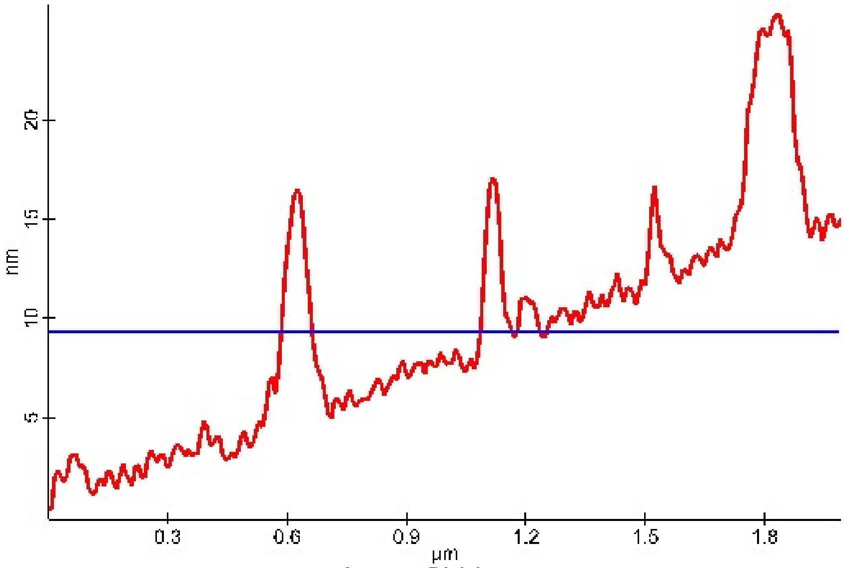
See also

- Image (Def)
- Surface Correction (Math)

Remarks

Average Subtraction

Average subtraction is a special case of the above formula. Here the polynomial is of the order zero. The polynomial is a constant and is equal to the average of the image values.



Average Division

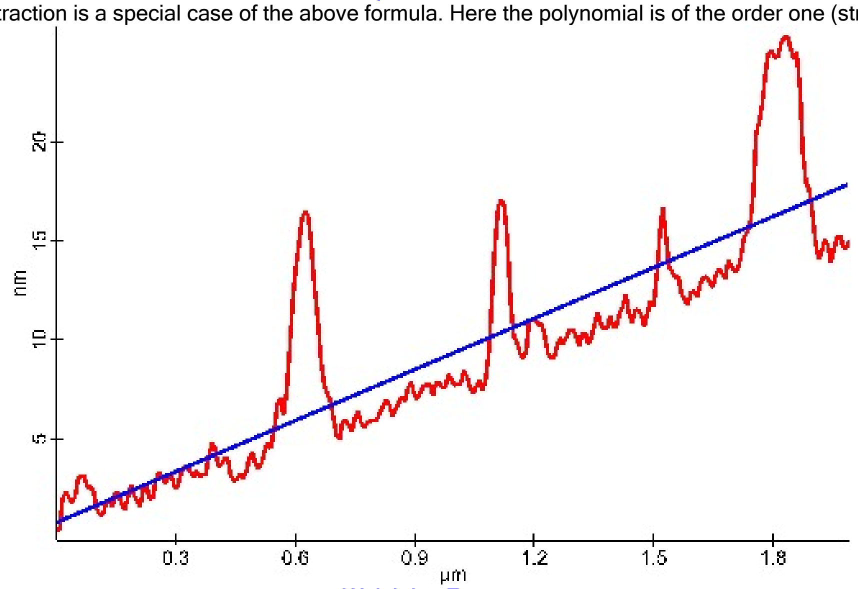
Instead of subtracting the average from the line data, the line data is divided by the average.

$$I_i^{div} = \frac{I_i}{\langle I \rangle}$$

$$\langle I \rangle = \frac{1}{N} \sum_{i=0}^{N-1} I_i$$

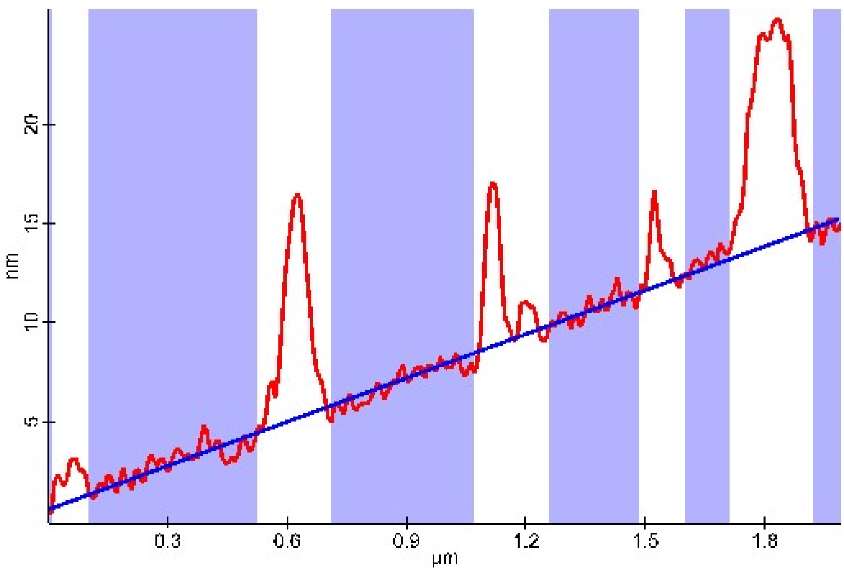
Slope Subtraction

Slope subtraction is a special case of the above formula. Here the polynomial is of the order one (straight line).



Weighting Factors

Using weighting factors ensures that the calculated slope is parallel to some flat surface. Usually the weighting factors are a boolean mask set by the user.



Surface Correction (Math)

To correct the slope of an complete image a 2-dimensional polynomial of k-order can be subtracted.

$$I_{i,j}^{sub} = I_{i,j} - P_k^{2D}(\vec{a}|i,j)$$

$$P_k^{2D}(\vec{a}|i,j) = \sum_{m=0}^{k}\sum_{n=0}^{m} a_{m,n}(i)^n(j)^{m-n}$$

$$\sum_{j=0}^{M-1}\sum_{i=0}^{N-1} w_{i,j}\left(I_{i,j} - P_k^{2D}(\vec{a}|i,j)\right)^2 = Minimum$$

$I_{i,j}$: Image value
$I_{i,j}^{sub}$: New image value
$P_k^{2D}(\vec{a}|i,j)$: 2D − Polynomial of order k
$\vec{a}$: Fit parameter
i,j : Pixel position
$w_{i,j}$: Weighting factor

See also
- Image (Def)
- Line Correction (Math)

Spatial Transformation (Math)

This transformation converts the pixel coordinates into real world space coordinates and vice versa.

$$\vec{x} = \hat{R}\hat{S}(\vec{b} - \vec{b}_0) + \vec{x}_o$$

$\vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$: Spatial position
$\vec{x}_o$: Spatial offset
$\vec{b} = \begin{pmatrix} i \\ j \\ k \end{pmatrix}$: Pixel position
$\vec{b}_0$: Pixel offset
$\hat{R}$: Rotation matrix
$\hat{S}$: Scale matrix

Remarks

Scaling Matrix

$$\hat{S} = \begin{pmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & s_z \end{pmatrix}$$

$$s_x, s_y, s_z \quad : Pixel\ size\ (e.g.\ \mu m/pixel)$$

Rotation Matrix

$$\hat{R} = \hat{R}_\alpha \hat{R}_\beta \hat{R}_\gamma$$

$$\hat{R}_\alpha = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}$$

$$\hat{R}_\beta = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix}$$

$$\hat{R}_\gamma = \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\hat{R} = \begin{pmatrix} \cos\beta\cos\gamma & -\cos\beta\sin\gamma & \sin\beta \\ \sin\alpha\sin\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\sin\beta\sin\gamma + \cos\alpha\cos\gamma & -\sin\alpha\cos\beta \\ -\cos\alpha\sin\beta\cos\gamma + \sin\alpha\sin\gamma & \cos\alpha\sin\beta\sin\gamma + \sin\alpha\cos\gamma & \cos\alpha\cos\beta \end{pmatrix}$$

$$\alpha \quad : Rotation\ angle\ of\ x-axis$$
$$\beta \quad : Rotation\ angle\ of\ y-axis$$
$$\gamma \quad : Rotation\ angle\ of\ z-axis$$

Redundancy and Limitations

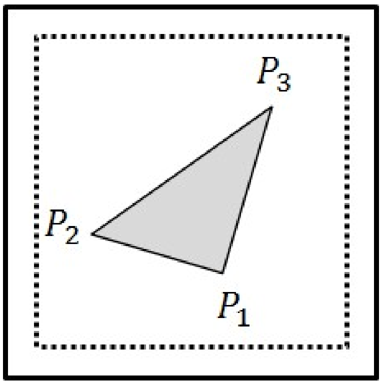
This form of a 3D linear transformation has some redundant parameters, but it is more convenient. The pixel position offset belongs directly to the spatial position. Also the separation of scaling and rotation makes it easier to analyse the transformation. A shearing matrix is not implemented in order to keep the main spatial directions perpendicular to each other.

Affine Transformation (Math)

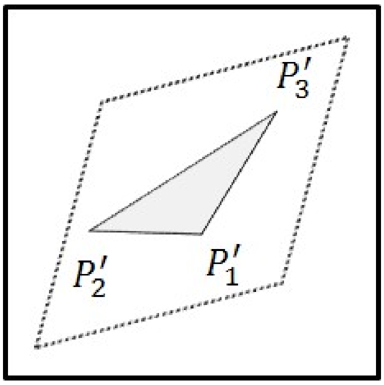
The coordinates of 3 points are transformed into coordinates of 3 new points. The transformation is a linear transformation which includes
translation, scaling, shearing and rotation. The affine transformation transforms a line into a line, a triangle into a triangle and a square into parallelogram.

$$\vec{x}' = \hat{M}\vec{x} + \vec{x}_0$$

$$\vec{x}' \quad : New\ point$$
$$\vec{x} \quad : Old\ point$$
$$\hat{M} \quad : Matrix\ for\ scaling, shearing\ and\ rotation$$
$$\vec{x}_0 \quad : Translation$$



Original Image



Transformed Image

See also

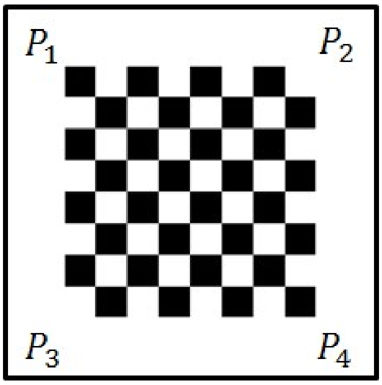
- Bilinear Transformation (Math)
- Spatial Transformation (Math)

- Delaunay-Triangulation (Math)

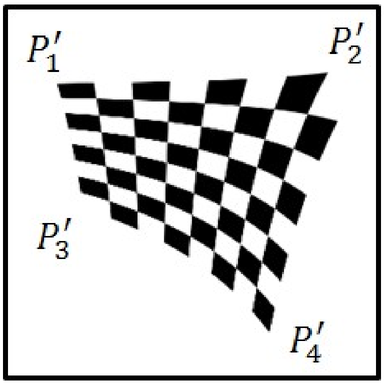
Bilinear Transformation (Math)

The coordinates of 4 points are transformed into coordinates of 4 new points.

$$x' = a_1 x + a_2 y + a_3 xy + a_4$$
$$y' = b_1 x + b_2 y + b_3 xy + b_4$$
$$\vec{x}' \quad : New\ point$$
$$\vec{x} \quad : Old\ point$$
$$\vec{a}, \vec{b} \quad : Fit\ parameter$$



Original Image

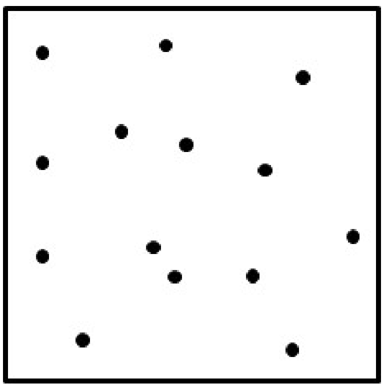


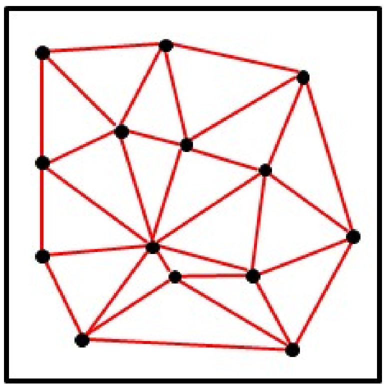
Transformed Image

See also
- Affine Transformation (Math)
- Spatial Transformation (Math)
- Delaunay-Triangulation (Math)

Delaunay-Triangulation (Math)

Beginning from a set of points in 2D-space, the Delaunay-Triangulation creates a triangle mesh. This mesh is always a convex area of all points. At each point a additional information is stored. This information together with the coordinates of the points allows to interpolate into the free space between the points.


Set of Points


Delaunay-Triangulation

Remarks
Local Affine Transformations
Together with the Affine Transformation a mesh which describes local deformation can been defined. The old point coordinates are used for triangulation, the new point coordinates as additional information. This allows to calculate the deformation inside a triangle.

Superposition of Spectra (Geometric View)

Many mathematical descriptions are made easier to understand by using a geometric model of a hyperspectral dataset. This geometric model works for data that follows the superposition principle, particularly Raman spectra which contain a mixture of components.

A complete hyperspectral dataset of two components can be described by three spectra: a constant background spectrum and two component spectra with their corresponding mixing values:

$$\vec{S}_i = h_i^{B_0}\vec{S}_{B_0} + h_i^{B_1}\vec{S}_{B_1} + \vec{S}_{BG}$$

$\vec{S}_{BG}$: *Constant background spectrum*

$\vec{S}_{B_0}, \vec{S}_{B_1}$: *Component Spectra*

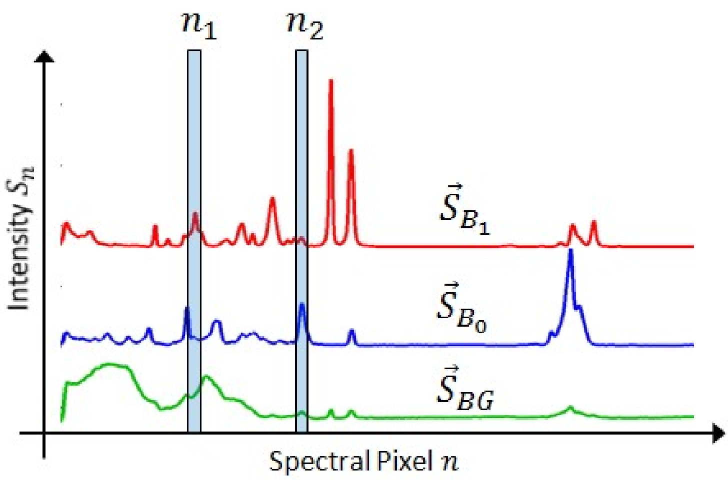
S_{n_1}, S_{n_2} : *Intensity at spectral pixel* n_1, n_2

$\vec{S}_i$: *Spectrum i from the hyper spectral dataset*

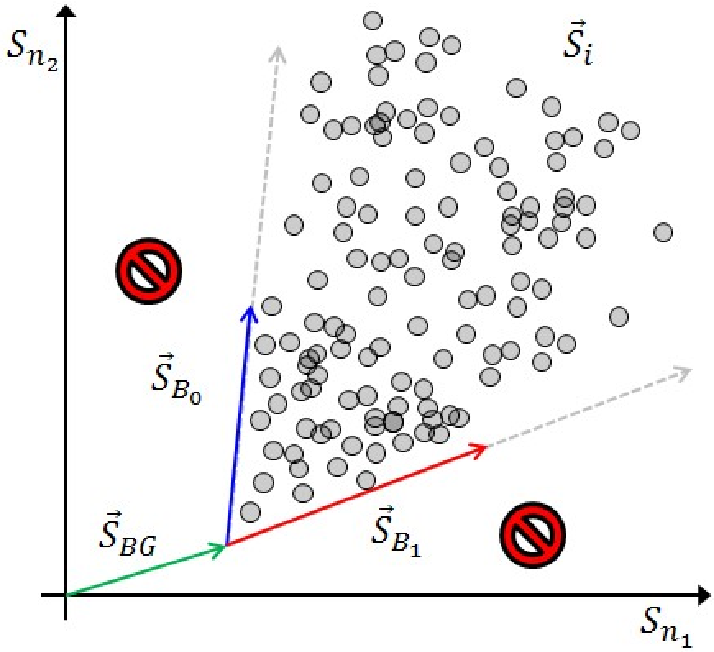
$h_i^{B_0}, h_i^{B_1}$: *Mixing values for spectrum i*

Usually, the component spectra are normalized to one (area normalization). In this case, the mixing values are exactly the amount of signal that belongs to the corresponding component.

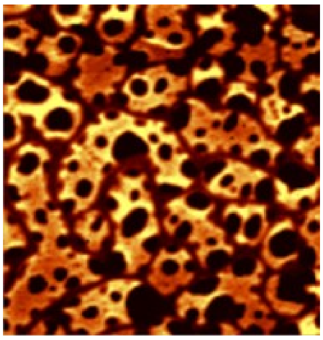
In order to plot the high dimensional vector equation above, a reduction of the dimensions i.e. projection into 2D space is necessary. Two intensity values at spectral pixels n1 and n2 are used as coordinates for the 2-dimensional projection plane:



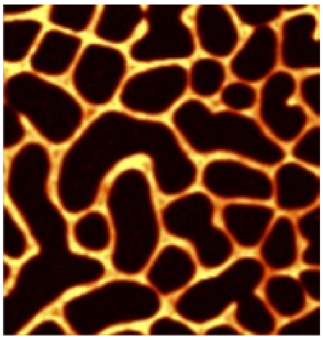
Using these two coordinates, each grey dot in the image below represents a spectrum of the hyperspectral dataset:



If the hyperspectral data is extracted from an image scan, the mixing values can be displayed as images:



$h_i^{B_0}$



$h_i^{B_1}$

Remarks

Limitations

The vector equation is **not** adequate for Raman spectra with Peak-shift, PFM-curves or CARS spectra.

Constant Background Spectrum

The origin of the background spectrum is unimportant as long as it is constant. Examples of constant background spectra are:

- Offset from CCD Camera
- Thermal generated electrons
- Signal from substrate if it is constant (planar scan).

Superposition of Spectra (Math)

One of the models that describe a hyper spectral dataset is based on the principle of superposition. Usually the spectra from the hyper spectral dataset are mixed spectra from different components. Each component points in a different direction of the high dimensional vector space. These spectra or a linear combination of them form a basis which describes only a sub-space of the complete vector space. With this basis all measured spectra can be described as linear combinations.
In addition a constant spectrum, which is equal for all spectra of the dataset, is introduced. Noise from data acquisition and signal which can not be described will be added to the error. Please read Superposition of Spectra (Geometric View) for a further understanding.

$$\hat{S} = \hat{B}\hat{H} + \vec{S}_C\vec{1}^T + \hat{E}$$

$\hat{S}$: Hyper spectral dataset matrix
$\hat{B}$: Matrix of Basis spectra
$\hat{H}$: Mixing values as matrix
$\vec{S}_C$: Constant spectrum
$\vec{1}^T$: Vector filled with 1
$\hat{E}$: Error matrix

Matrix Representation of Hyper Spectral Dataset

$$\hat{S} = (\vec{S}_0 \quad \cdots \quad \vec{S}_m \quad \cdots \quad \vec{S}_{M-1})$$

$\vec{S}_m$: Spectrum m from the hyper spectral dataset
M : Number of spectra in dataset

See also: Spectrum (Def)

Matrix Representation of Component Spectra (Basis)

$$\hat{B} = (\vec{S}_{B_0} \quad \cdots \quad \vec{S}_{B_n} \quad \cdots \quad \vec{S}_{B_{N-1}})$$

$\vec{S}_{B_n}$: Basis spectrum n
N : Number of basis spectra

Matrix Representation of Mixing Values

$$\hat{H} = \begin{pmatrix} h_0^{B_0} & \cdots & h_m^{B_0} & \cdots & h_{M-1}^{B_0} \\ \vdots & \ddots & \vdots & & \vdots \\ h_0^{B_n} & & h_m^{B_n} & & h_{M-1}^{B_n} \\ \vdots & & \vdots & \ddots & \vdots \\ h_0^{B_{N-1}} & \cdots & h_m^{B_{N-1}} & \cdots & h_{M-1}^{B_{N-1}} \end{pmatrix}$$

$h_m^{B_n}$: *Mixing value for basis spectrum n and spectrum m*
M : *Number of spectra in dataset*
N : *Number of basis spectra*

Basis Analysis (Math)

The idea of the basis analysis is to describe a measured spectrum or a complete hyper spectral dataset by a linear combination of spectra, which are already known. The mixing values, which are used for the linear combination, is the result of this analysis. In addition to the basis spectra the constant background spectrum must also be known in advance. Usually the latter one is subtracted before using the basis analysis algorithm. This algorithm is based on the basic equation, which is explained in the article Superposition of Spectra (Math):

$$\hat{S} = \hat{B}\hat{H} + \vec{S}_C\vec{1}^T + \hat{E}$$

For basis analysis the equation can be reduced to:

$$\vec{S}_i = \hat{B}\vec{H}_i + \vec{E}_i$$

$\vec{S}_i$: *Spectrum i from the hyper spectral dataset*
$\vec{H}_i$: *Mixing values spectrum i*
$\vec{E}_i$: *Error spectrum*
$\hat{B}$: *Matrix of Basis spectra*

The mixing values are fitted by the method of least squares minimizing the following expression:

$$(\vec{S}_i - \hat{B}\vec{H}_i)^2 = Minimum$$

See also

- Inverse Basis Analysis (Math)
- Non-Negative Matrix Factorization (Math)

Remarks

Choosing the Correct Basis

In order to analyse Raman spectra it is important first to use a basis matrix including all present components and second that the basis spectra are pure spectra. This assures that the result makes physical sense. If the basis spectra are taken from an average process of a hyperspectral dataset, a decomposing process might be necessary (see Decomposing of Basis Spectra (Math)) before using the basis analysis.

In most cases the best way to get the basis spectra is to use the same hyperspectral dataset instead taking the spectra from a database or an old measurement. This guarantees that the basis spectra are recorded using the same experimental conditions and the fit does not include any systematic error (same spectrograph, grating, spectral center position, calibration, objective, laser excitation, fiber, etc...).

Constrained Minimization (Fitting)

When using the basis analysis often only positive mixing values are reasonable: In the case of Raman analysis, negative values belong to negative matter, which physically makes no sense. Therefore it is possible to fit the above equation constrained by allowing only positive mixing values:

$$h_m^{B_n} \geq 0$$

Constrained fitting can be used to find out whether the basis components are mixed.

Inverse Basis Analysis (Math)

The idea behind inverse basis analysis is to calculate the basis spectra and a constant spectra from a hyper spectral dataset if only images (distribution maps) from the belonging components are known.
Inverse basis analysis is base on the basic equation, which is explained in the article Superposition of Spectra (Math).

$$\hat{S} = \hat{B}\hat{H} + \vec{S}_C\vec{1}^T + \hat{E}$$

The following equation has to be solved separately for each spectral position.

$$\sum_{j=0}^{N-1} \left| S_i^j - \left(\sum_{k=0}^{M-1} B_i^k H_k^j + S_i^C \right) \right|^2 = Minimum$$

i : $i-th\ spectral\ position$
N : $Number\ of\ spectra\ in\ hyper\ spectral\ dataset$
M : $Number\ of\ basis\ spectra$
S_i^j : $j-th\ spectrum\ in\ hyper\ spectral\ dataset$
B_i^k : $k-th\ basis\ spectrum$
H_k^j : $k-th\ mixing\ value$
S_i^C : $Constant\ spectrum\ at\ i-th\ spectral\ position$

See also

- Basis Analysis (Math)
- Non Negative Matrix Factorization (Math)

Remarks

Choosing the right Images

Similar to the basis analysis a complete set of images is necessary which describe all components inside the hyper spectral dataset. In addition each image must contain the background free signal from only one component in order to get physical meaningful spectra.

Constant Spectrum

If the constant background spectrum is flat and there is no need for fitting, the user can set its offset value.

Basis Spectra Reconstruction

In some cases it is possible to get nice images only from a very small part of the spectra. Especially when using non negative matrix factorization. In this case inverse basis analysis can be used to reconstruct the basis spectra over the whole spectral range.

Non-Negative Matrix Factorization (Math)

Non-Negative Matrix Factorization (NMF) is a method used to evaluate distribution maps, demixed basis spectra and constant background spectra from a hyperspectral dataset. This multivariate analysis requires the constraint of only positive values inside the distribution maps, the basis spectra and the constant background spectrum. It is based on the basic equation explained in the article Superposition of Spectra (Math):

$$\hat{S} = \hat{B}\hat{H} + \vec{S}_C \vec{1}^T + \hat{E}$$

Constraints:

$$B_i^k > 0$$
$$H_k^j > 0$$
$$S_i^C > 0$$

i : $i-th\ spectral\ position$
k : $k-th\ basis\ spectrum$
j : $j-th\ spectrum\ of\ hyper\ spectral\ dataset$

The NMF algorithm is iterative and converges to a solution with minimal error by:

1. Initializing basis spectra, distribution maps and the constant background spectrum.
2. Optimizing the basis spectra
3. Normalizing the basis spectra
4. Optimizing the distribution maps
5. Optimizing the constant spectrum
6. If it is not the final iteration:

To pull the constant spectrum and basis spectrum into the data of the hyperspectral dataset

7. Repeat steps 2 to 6 until the error is small enough or final iteration is reached

See also

- Basis Analysis (Math)
- Inverse Basis Analysis (Math)

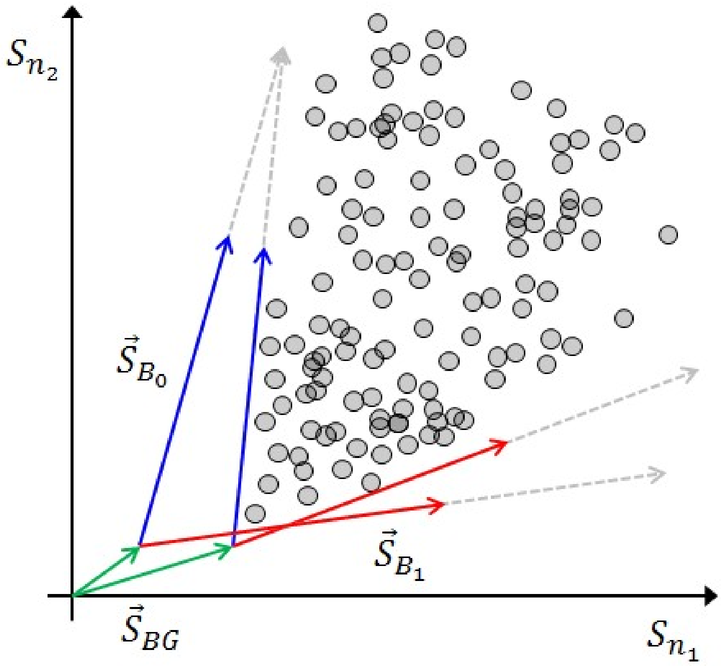
Remarks

Constant Spectrum

If the constant spectrum is flat, a spectral independent offset can be optimized in step 5.

Uniqueness of solution

In general there is no unique solution because an infinite number of solutions exist fulfilling the constraints above.



By pulling the constant spectrum and basis spectra into the cloud of the hyperspectral dataset, a unique solution which is close to pure spectra can be determined. In addition this guarantees that the solution describes the hyperspectral dataset symmetrically to the noise (e.g. readout noise).
The strength of the pulling must be adjusted by the user.

Spectrum Normalization (Math)

It is sometimes necessary to normalize a spectrum. If a spectrum is interpreted as a vector there are usually many ways this can be done. For spectral analysis the so-called L1-Norm and L2-Norm are often used, the more general form is the Lp-Norm.

$$\|\vec{S}\|_p = \sqrt[p]{\sum_{i=0}^{N-1} |S_i|^p}$$

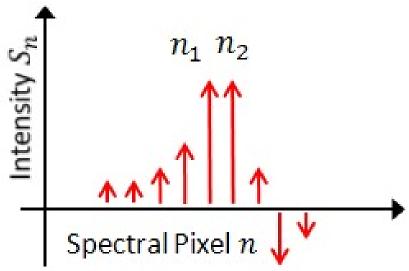
$$\vec{S}_{Norm} = \frac{1}{\|\vec{S}\|_p}\vec{S}$$

$\|\vec{S}\|_p$: $L^p - Norm$
$\vec{S}_{Norm}$: $Normalized\ spectrum$
$\vec{S}$: $Spectrum$
p : $Normalization\ parameter$

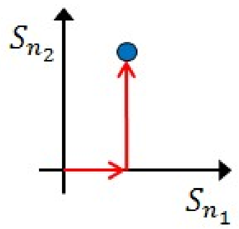
See also: Spectrum (Def)
Remarks

Manhattan Norm

For p equals 1, the norm is sometimes called the Manhattan norm. In this case it is equal to the area below the spectrum and therefore proportional to the signal. This type of normalization should be used if proportionality to the signal is important.



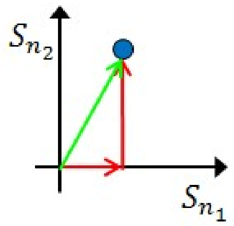
Spectrum



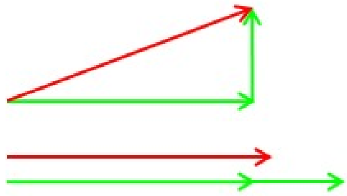
Projection of spectrum into 2D space showing the Manhattan norm

Euclidean Norm

If p equals 2 the norm is called the Euclidean norm. In this case it is equal to the length of the vector, i.e. the influence of a small value inside a vector is smaller compared to a large value. This type of Normalization is appropriate if the influence of small values should be suppressed.



Projection of spectrum into 2D space showing the Euclidean norm



Comparison between Manhattan and Euclidean norm

Decomposing of Basis Spectra (Math)

If the basis spectra are not pure component spectra, a demixing process might be necessary before using them for algorithms, database searching or publication. It does not matter why the spectra are mixed unless the basis is complete and acquired under the same experimental conditions. In this case a decomposition is possible through the following equations:

$$\hat{B}_1 = (\hat{B}_0 - \vec{1}\vec{C}_O^T)\hat{D}_0$$

$$\hat{B}_k = \hat{B}_{k-1}\hat{D}_{k-1} = (\hat{B}_0 - \vec{1}\vec{C}_O^T)\hat{D}_0\hat{D}_1 \dots \hat{D}_{k-1}$$

$$\hat{D}_k = \begin{pmatrix} 1 & \cdots & d_{n,0}^k & \cdots & d_{N-1,0}^k \\ \vdots & \ddots & \vdots & & \vdots \\ d_{0,m}^k & & 1 & & d_{N-1,m}^k \\ \vdots & & \vdots & \ddots & \vdots \\ d_{0,N-1}^k & \cdots & d_{n,N-1}^k & \cdots & 1 \end{pmatrix}$$

$$\hat{B}_k = \left(\vec{S}_{B_k^0} \quad \cdots \quad \vec{S}_{B_k^n} \quad \cdots \quad \vec{S}_{B_k^{N-1}}\right)$$

$\hat{B}_0$: *Initial set of spectra*
$\hat{B}_k$: *Final set of spectra after k − th iteration*
$\vec{S}_{B_k^n}$: *n − th basis spectrum of k − th iteration*
$\vec{C}_O^T$: *Constant Offset*
$\vec{1}$: *Spectrum filled with 1*
$\hat{D}_k$: *Decomposition matrix*
$d_{n,m}^k$: *Elements of decomposition matrix*
N : *Number of basis spectra*

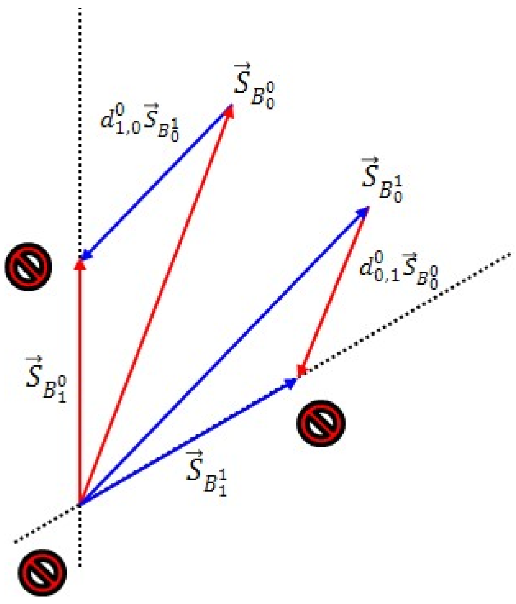
See also: Basis Analysis (Math)

Remarks

Justification

The initial set of basis spectra is only a sub-space of the completely possible vector space. By subtracting or adding the spectra it is not possible to exit this sub-space, i.e. this procedure can not create new components.

The following plot shows how this works for a set of two basis spectra. It is not possible to leave the plane defined by the initial set of basis spectra.



Principal Component Analysis (Math)

Principal component analysis (PCA) is a multivariate analysis. This analysis calculates a new orthogonal basis and transforms the original data into this basis. Similar to other technics the basis equation Superposition of Spectra (Math) can be used as a starting point.

$$\hat{S} = \hat{B}\hat{H} + \vec{S}_c\vec{1}^T + \hat{E}$$

The only difference is that the symbol of right side have a different meaning. The constant spectrum is calculated by the average of the hyper spectral dataset (see Average Spectrum (Math)). The matrix of basis spectra is filled by the eigenvectors with the highest eigenvalues of the covariance matrix. The mixing values are just calculated by the new coordinate transformation.

The eigenvectors and eigenvalues are calculated by the following equation.

$$\hat{C} = \begin{pmatrix} cov(S_0,S_0) & \cdots & cov(S_0,S_m) & \cdots & cov(S_0,S_{M-1}) \\ \vdots & \ddots & \vdots & & \vdots \\ cov(S_n,S_0) & & cov(S_n,S_m) & & cov(S_n,S_{M-1}) \\ \vdots & & \vdots & \ddots & \vdots \\ cov(S_{M-1},S_0) & \cdots & cov(S_{M-1},S_m) & \cdots & cov(S_{M-1},S_{M-1}) \end{pmatrix}$$

$$cov(S_n,S_m) = cov(S_m,S_n) = \frac{1}{N-1}\sum_{k=0}^{N-1}(S_n^k - S_n^{Ave})(S_m^k - S_m^{Ave})$$

$$\hat{C}\vec{X}_k = \lambda_k\vec{X}_k$$

$$\hat{B} = (\vec{X}_0 \quad \cdots \quad \vec{X}_m \quad \cdots \quad \vec{X}_{M-1})$$

$\hat{S}$: Hyper spectral dataset matrix
$\hat{C}$: Covarianz matrix
$\vec{X}_k$: Eigenvector of $\hat{C}$
λ_k : Eigenvalues of $\vec{X}_k$ and $\hat{C}$ ($\lambda_k > \lambda_{k+1}$)
$\hat{B}$: Complete matrix of eigenvectors
N : Number of spectra in hyper spectral dataset
M : Dimension of spectra
$\vec{S}^{Ave}$: Average spectrum of hyper spectral dataset

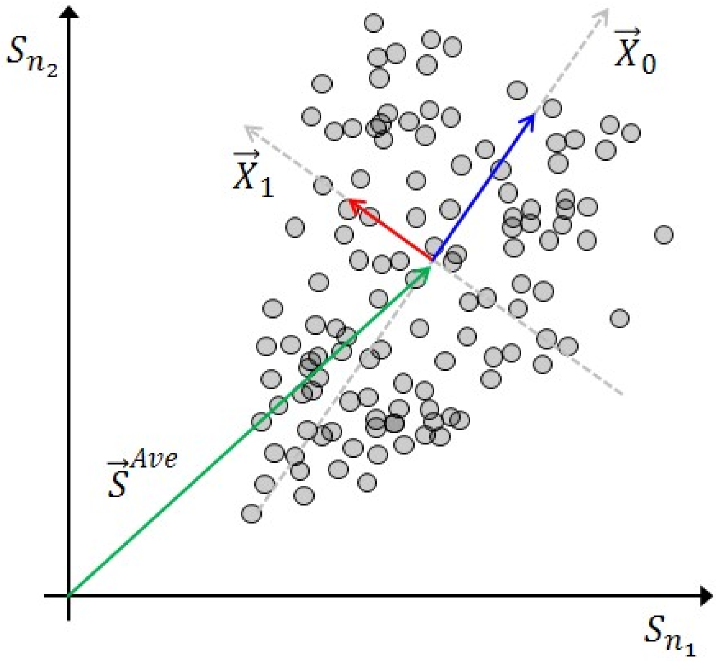
See also

- Non Negative Matrix Factorization (Math)

Remarks

Basis of Eigenvectors

Due to the properties of the covariance matrix the eigenvectors are orthogonal to each other. PCA can be seen as a shift and rotation of the old coordinate system.



If all eigenvector are taking as a new basis, there is no loss of information. In general only the eigenvector with the highest eigenvalues are chosen. In this case not the complete information is preserve. The goal is to chose as many eigenvectors necessary to preserve the measured signal, but take as less to remove the noise.

Principle component Analysis can be used to reduce dimensionality for further analysis or just as a noise filter.

Eigenvalues and Eigenvectors

The eigenvalue can be seen as the variance of the data into the direction of the eigenvector. In this context the meaning of variance is not error but content information.

Uniqueness

For a given hyper spectral dataset a principal component analysis will always give the same result, but a similar dataset with a different e.g. concentration distribution will lead to a different basis. There is no intrinsic physical meaning of the eigenvectors. In addition the elements of the eigenvectors and the mixing values can have negative values.

Cluster Analysis K-Means (Math)

The k-means cluster algorithm splits a hyper spectral dataset into a user defined number of sets (cluster). The sets are chosen by minimizing the following equation.

$$\sum_{k=1}^{N} \sum_{\vec{S}_i \in \Gamma_k} \left| \vec{S}_i - \vec{S}_{Ave}^{k} \right|^2 = Minimum$$

N : Number of clusters

$\vec{S}_i$: Spectrum i from the hyper spectral dataset

Γ_k : Set of all spectra inside cluster k

$\vec{S}_{Ave}^{k}$: Average spectrum of cluster k (cluster center)

For a large number of spectra it is not possible to solve the above equation in a reasonable amount of time. Therefore a iterative algorithm is used to find the minimum. This minimum is not necessarily equal with global minimum. The algorithm performs the following steps.

1. Initialize all cluster center.
2. Compare each spectrum of the complete hyper spectral dataset with all cluster centers. Put the spectrum into the most similar set.
3. Calculate new cluster center.
4. Repeat step 2-3 until the sets keep unchanged.

See also

- Average Spectrum (Math)
- Cluster Analysis K-Means (Geometric View)

Remarks

Similarity of two Spectra

In order to calculate the similarity of two spectra the length of the difference spectrum can be used. the inverse of the length is a measure for the similarity. Usually the Euclidean norm is used for k-means clustering, but sometimes the Manhattan norm gives better results (see Spectrum Normalization (Math)).

Pre-Transformations

Instead of using the original spectra for clustering a applied pre-transformation to all spectra inside the hyper spectral dataset can make sense.

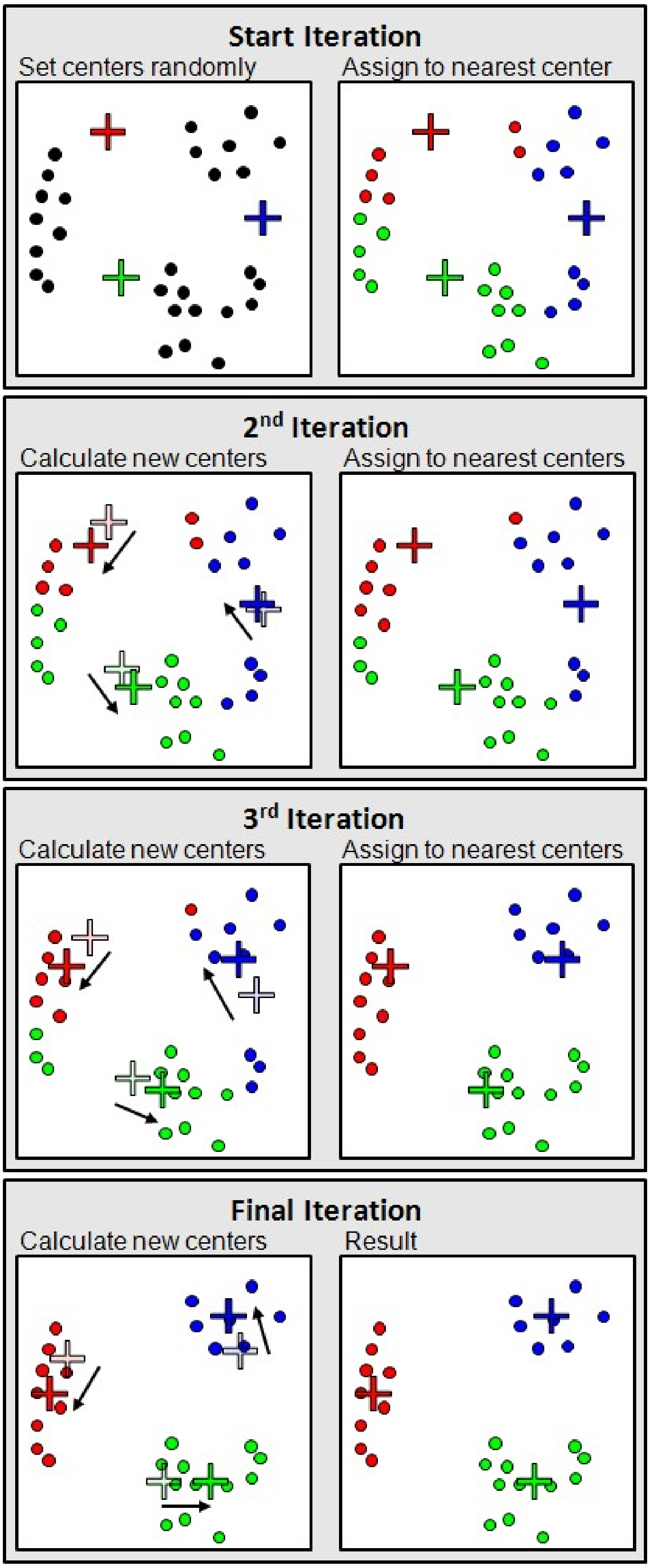
- Data Reduction (speed up and more distinct clusters because of less noise)
- Normalization (only sensitive to spectra shape, insensitive to intensity, integration time and material density)

- Derivative (only sensitive to sharp Raman Lines, insensitive to fluorescence)

These pre-transformed spectra are only used for the clustering process. In order to get a nice averaged spectrum from the original spectra the set information (mask) can be used.

Cluster Analysis K-Means (Geometric View)

In order to solve the k-means clustering condition (see Cluster Analysis K-Means (Math)) a iterative algorithm is used. Below a visualization of the algorithm is shown for three clusters. The crosses show the cluster centers. Each dot is a individual spectrum of the hyper spectral dataset. Please read Superposition of Spectra (Geometric View) for further understanding.



Spectrum (Def)

Many mathematical algorithms for spectral analysis can be described with vector and matrix algebra. The N pixels of a spectrum determine the coordinates of the N-dimensional vector:

$$\vec{S} = \begin{pmatrix} S_0 \\ \vdots \\ S_{N-1} \end{pmatrix}$$

$$N \quad : Number\ of\ spectral\ pixels$$
$$S_i \quad : Intensity\ of\ i-th\ pixel$$
$$\vec{S} \quad : Spectrum$$

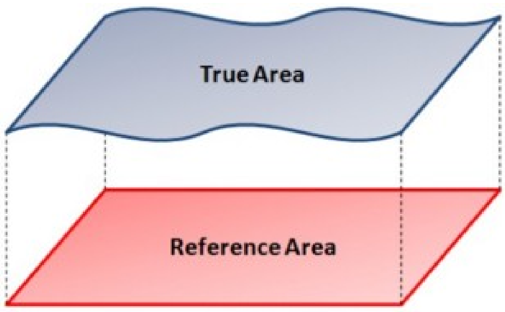
Image Statistics (Math)

Histogram | Statistics | Roughness | Draw Field Mask

Image Roughness Parameters

Number of Pixels:	262144
True Area [µm²]:	3125.68
Reference Area [µm²]:	2490.24
SDR [%]:	27.5646
SDQ [µm]:	1.24282
SSC [1/µm]:	0.693558
Average [µm]:	1.26278
SA [µm]:	1.02088
SQ [µm]:	1.17234
SSK:	0.0125672
SKU:	1.85145
Peak-Peak [µm]:	7.3184
# Local Maxima:	1583

True Area / Reference Area:



The roughness average, SA, is defined as:

$$\text{SA} = \frac{1}{<MN>} \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} |z(x_i, y_j) - \bar{z}|$$

with $\bar{z}$ representing the mean hight.

$$\bar{z} = \frac{1}{<MN>} \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} z(x_i, y_j)$$

The root mean square SQ is defined as:

$$\text{SQ} = \sqrt{\frac{1}{<MN>} \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} [z(x_i, y_j) - \bar{z}]^2}$$

The surface skewness SKK, describes the asymmetry of the height distribution histogram and is defined as:

$$\text{SSK} = \frac{1}{<MN> \text{SQ}^3} \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} [z(x_i, y_j) - \bar{z}]^3$$

If $\text{SSK} = 0$, a symmetric height distribution is indicated, e.g. Gaussian.

If $\text{SSK} < 0$, it can be a bearing surface with holes and if $\text{SSK} > 0$, it can be a flat surface with peaks. Values of SSK numerically greater than 1.0 may indicate extreme holes or peaks on the surface.

The surface kurtosis SKU, describes the peaked-ness on the surface topography and is defined as:

$$\text{SKU} = \frac{1}{<MN> \text{SQ}^4} \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} [z(x_i, y_j) - \bar{z}]^4$$

For Gaussian height distributions SKU approaches 3.0 when increasing the number of pixels. Smaller values indicate broader height distributions.

The extreme values are defined by:

$$\text{Max} = \max\{z(x_i, y_j) : 1 \leq i \leq M, 1 \leq j \leq N, \epsilon_{i,j} = 1\}$$
$$\text{Min} = \min\{z(x_i, y_j) : 1 \leq i \leq M, 1 \leq j \leq N, \epsilon_{i,j} = 1\}$$

The peak-peak parameter is defined as:

$$\text{Peak-Peak} = |\text{Max} - \text{Min}|$$

Pearson Correlation Coefficient

The following formula is used to calculate the Pearson Correlation Coefficient:

$$r = \frac{\sum_{i=0}^{N-1} (S_i - \bar{S})(S_i^{Ref} - \bar{S}^{Ref})}{\sqrt{\sum_{i=0}^{N-1} (S_i - \bar{S})^2} \sqrt{\sum_{i=0}^{N-1} (S_i^{Ref} - \bar{S}^{Ref})^2}}$$

$$\bar{S} = \frac{1}{N} \sum_{i=0}^{N-1} S_i \qquad \bar{S}^{Ref} = \frac{1}{N} \sum_{i=0}^{N-1} S_i^{Ref}$$

$\vec{S}^{Ref}$: *Reference Spectrum*
$\vec{S}$: *Spectrum*

Creating Raman Overlay

Raman Overlay on Video Image

1. Open your video image in an image viewer.
2. Drag and drop your Raman image on the image viewer and select "Use as Overlay".
3. Adjust the overlay in the Image Transform and Overlay Dialog. Press "Extract Bitmap".

Video Image on Topography

1. Open your topography image in an image viewer.
2. Drag and drop your video image on the topography and select "Use as Overlay".
3. Adjust to full overlay in the Image Transform and Overlay Dialog. Press "Extract Bitmap".
4. Drag and drop the new bitmap on the image viewer showing the topography and select "Use as Color Image".

Using Graph Intensity Correction

To execute a proper intensity correction, the following steps have to be done.

Note: For all measurements you have to use the same laser, the same spectral position and the same CCD camera settings !

Preparation

- Measure a series of fluorescence spectra (≈ 500 to 2000, time series)
  There must be no Raman signal on the fluorescence!

- The correction only works if the background can be subtracted from the fluorescence.
  If the background can't be determined using the fluorescence spectrum itself (from an area without any signal, e.g. near Rayleigh) or if the background has a strong variation coming from the CCD, you have to measure a series of dark spectra (≈ 500 to 2000, time series). The average of those dark spectra can be used to subtract the background.

Measurement and Correction

1. Execute your Raman measurement under the same conditions as the fluorescence spectra.

2. If necessary, remove cosmic rays from your Raman measurement.
   Don't do any background subtraction. Only use 0-order polynomial / horizontal line subtraction in case you see that the offset had drifted during the measurement.

3. Drop your Raman measurement on the Graph Intensity Correction Dialog Drop Action

4. Drop your fluorescence series on the "Drop Fluorescence" Button

5. Subtract the background from the fluorescence:
   - Set the blue mask in the Fluorescence preview graph viewer to an area without any signal and press "Get Mask Average" in the Fluorescence Offset Group Box.
     or
   - Drop the dark spectra series on the "Drop Spectrum" button in the Fluorescence Offset Group Box.

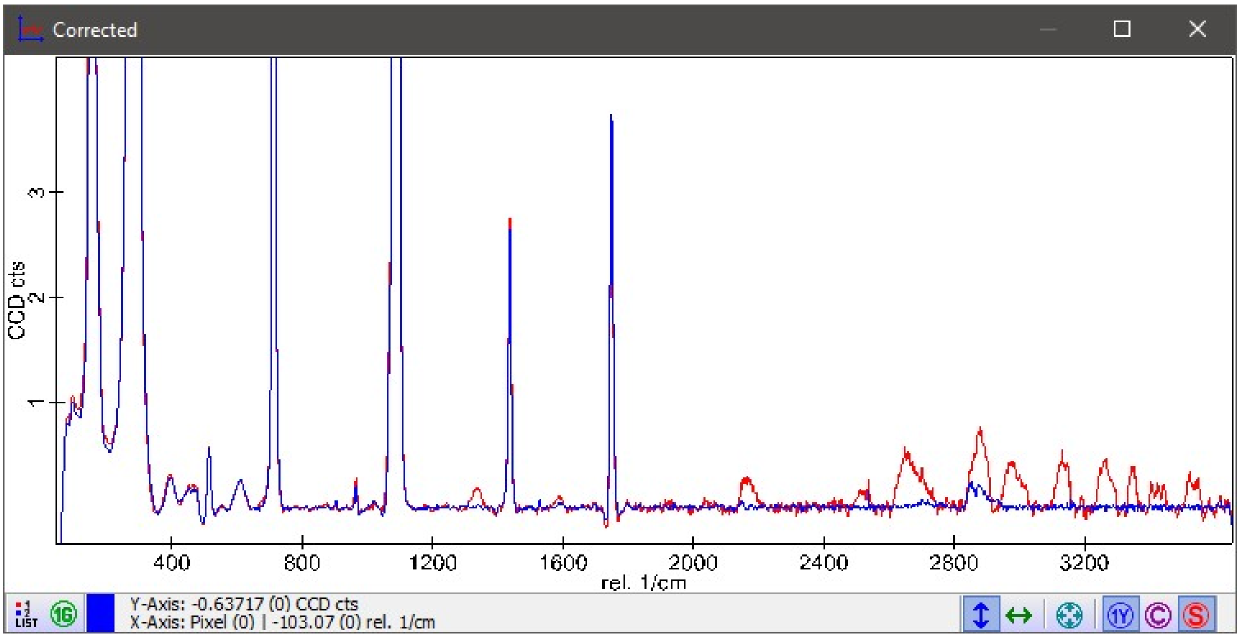
6. Subtract the background from your Raman measurement:
   - Set the blue mask in the result preview graph viewer to an area without any signal and press "Get Mask Average" in the Measurement Offset Group Box.
     or
   - Drop the dark spectra series on the "Drop Spectrum" button in the Measurement Offset Group Box.

7. If your fluorescence spectrum has a region without any signal, remove it from the green mask

8. Press Extract.

How does the result look like?

In the graph viewer below you can see the result of an intensity correction.
You won't see the difference in a single noisy spectrum, but in a spectrum with high intensity or in averaged spectra.
Both spectra show an average Raman spectrum having a fluorescence offset which is subtracted using the shape background subtraction.
The red one shows the result without the intensity correction, the blue one with the correction:



Creating Image Masks - Overview

Image Masks are needed to select which pixel (or spectra of a hyper-spectral data) set should be considered for a calculation, e.g. for Averaging Spectra, Cluster Analysis, Image Statistics and so on.

You can create Image masks using several software features:

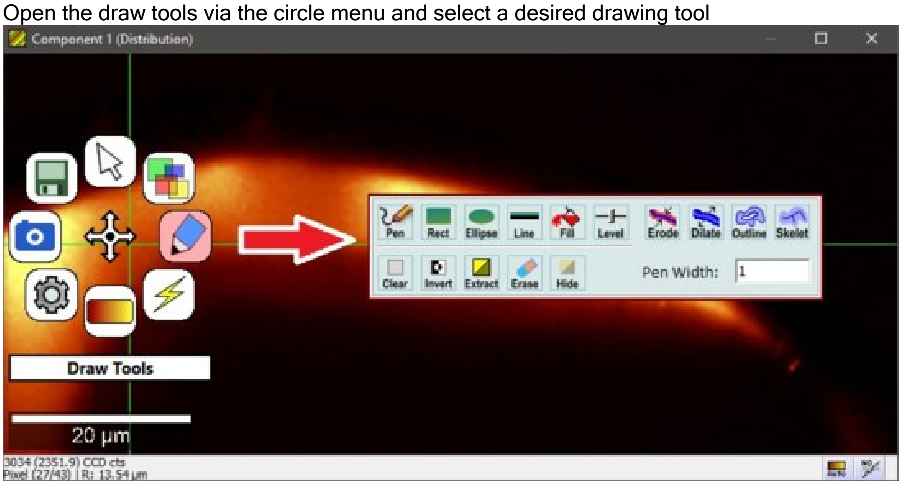
Features	Examples
Image Viewer Draw Tools (manual + thresholding)	Creating Image Masks using the Draw Tools
Calculator Dialog (boolean formulas)	Creating Image Masks using the Calculator
Advanced Graph Average Dialog (advanced thresholding)	

Creating Image Masks using the Draw Tools

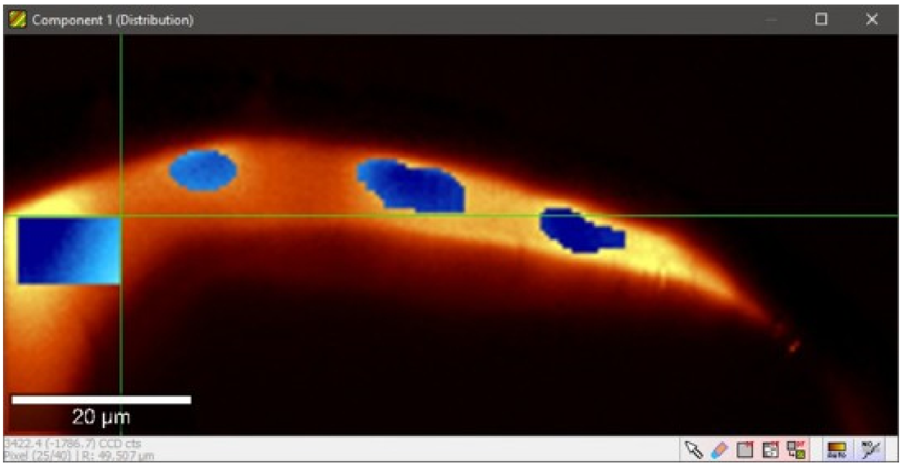
You can create Masks using the Draw Tools in any Image Viewer.

Steps

1. Open a new Image Viewer or select an existing Image Viewer
2. Open the draw tools via the circle menu and select a desired drawing tool



3. Draw on the image using the left mouse button or select a threashold in the threshold tool



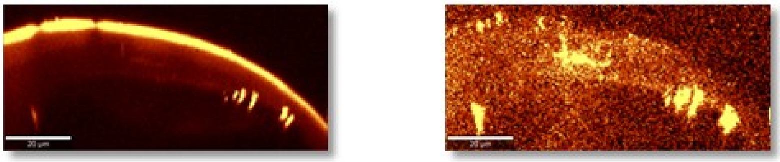
Hint: If the mask is used for averaging multiple spectra, make sure you only mask pixels that contain only one component.

4. Extract the mask using the tool button in the Image Viewer status bar or via the draw tools circle menu > Extract button
5. Switch back to the Mouse Move mode by pressing the tool button with the mouse icon or by using Circle Menu Up.

Creating Image Masks using the Calculator

You can create masks using a boolean formula in the Calculator Dialog.
The formula gives you the chance to combine any kind of logic in order to create a mask from different images also.

For example we could have a sum image showing a Raman component with flluorescence and a sum image showing fluorescence only:

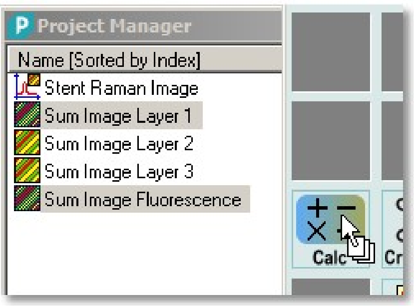


Sum Image Layer 1 Sum Image Fluorescence

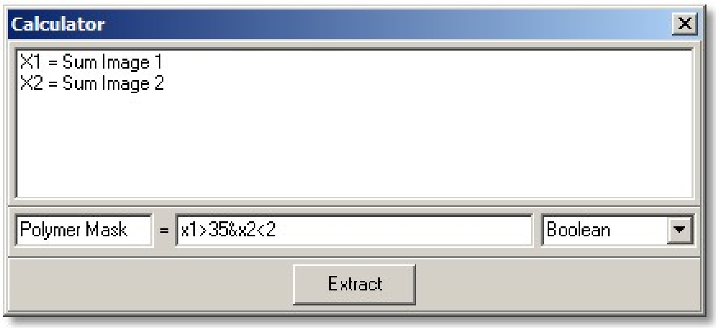
The calculator could be used to create a mask where only the Raman component of the first image is masked.

Steps

1. Drag and drop both images on the Calculator Drop Action.



2. Now you can type a boolean formula (leading to a mask result with values of 0 and 1). This can be achieved by using the larger (>) and smaller (<) operator as well as the logical "and" (&) and "or" (|) operators:

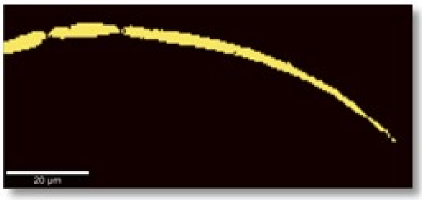


3. Use the formula "x1 > 150":
   This will set all pixels that have a value larger than 150 in the Sum Image Layer 1 (Polymer), thus selecting only bright pixels.
   The threshold (in this case 150) depends on the sum image. Move the mouse cursor over the original sum image to get an idea which value could be a good threshold for thresholding bright pixels and change the value to see what happens.
4. Use the formula "x2 < 30":
   This will clear all pixels that are larger or equal than 30 in the Sum Image Fluorescence, thus removing fluorescent pixels.
5. Use the "logical and" operator (&) to combine the two masks (both conditions have to be true to set the mask pixel), thus removing the fluorescent pixel from the Polymer mask.
6. Optional: Use the unit "Boolean" and rename the image to recognize the mask later on
7. You can calculate the masks also for the Polymer Layer 2 (Threshold 120) and Polymer Layer 3 (Threshold 350).
8. Compare your results with the predefined mask data objects Mask Layer 1/2/3.

Results

Calculator Result with Formula "x1 > 150"

Calculator Result with Formula "x2 < 30"

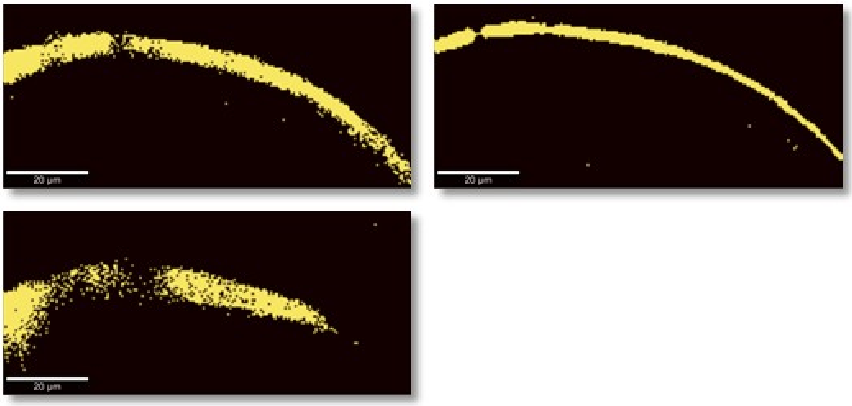


Calculator Result with Formula "x1 > 150 & x2 < 30"

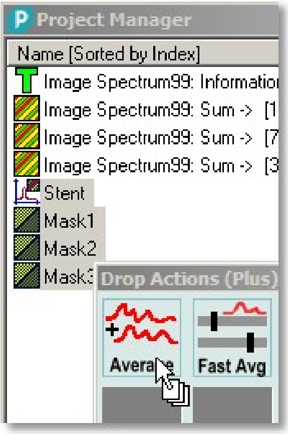
Creating Average Spectra using Masks

If you would like to create a nice, noise-free spectrum for each component, averaging multiple spectra from the same component is a suitable way.
To achieve that, you have to do the following steps:

1. Create Image Masks for each component.

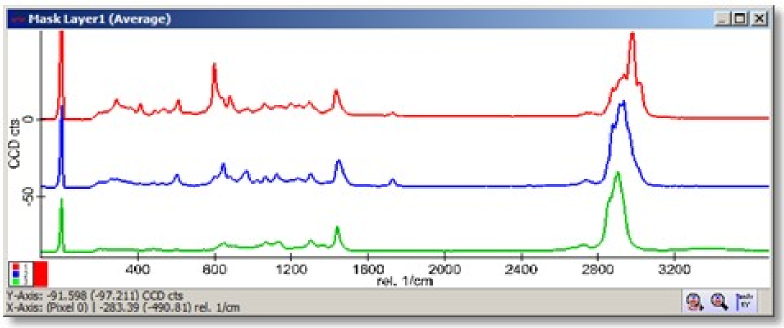


2. Having those masks, you can select the masks together with the spectral Raman image data set and drag and drop it onto the Average Spectrum Drop Action:



Result

The result is one nice average spectrum for each dropped mask:



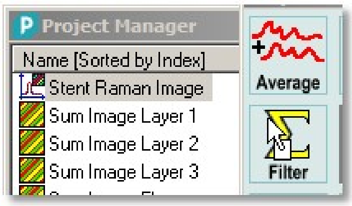
Creating Images using the Filter Viewer

During or after a Raman Image Scan measurement, you can create images with the Filter Viewer.
Hint: In WITec Control, a Filter Viewer might be automatically created upon starting an Image Scan or Large Area Scan.

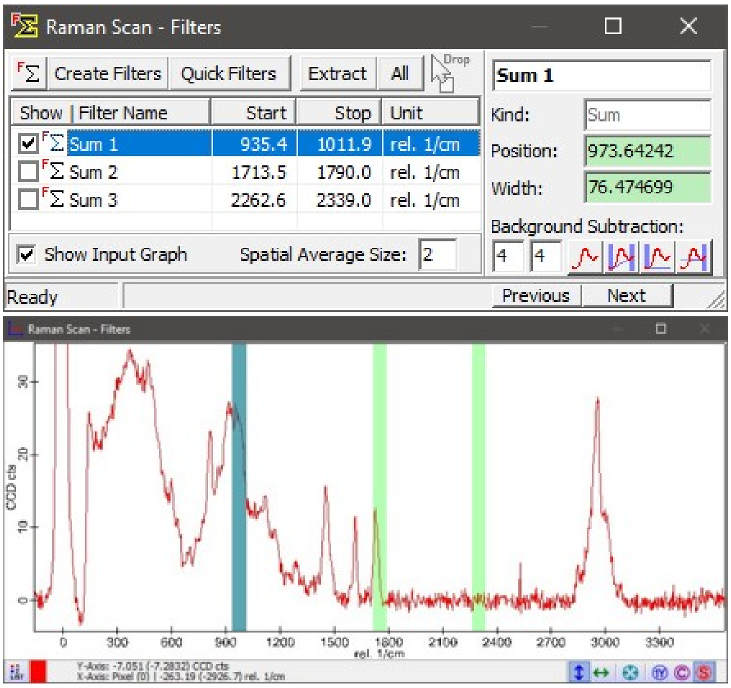
The Filter Viewer helps you finding the interesting Raman bands and creates images which show structures of your components.

Steps

1. Drag and drop the Raman Image Data Object onto the Filter Viewer Drop Action



2. Add new sum filters
3. Select a sum filter to change the filter parameters (position, width, background subtraction, ...)



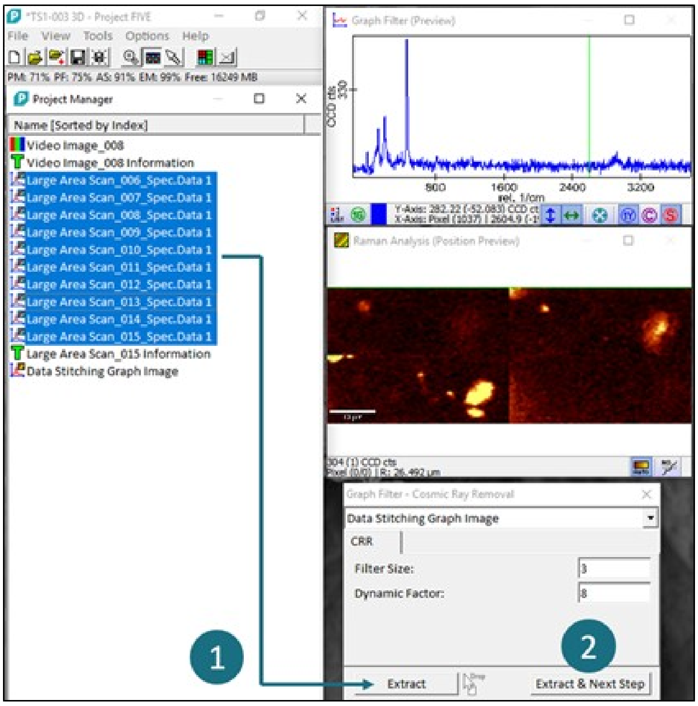
4. You can extract the currently selected filter image or all filters using the buttons "Extract" and "All".

3D Data Analysis

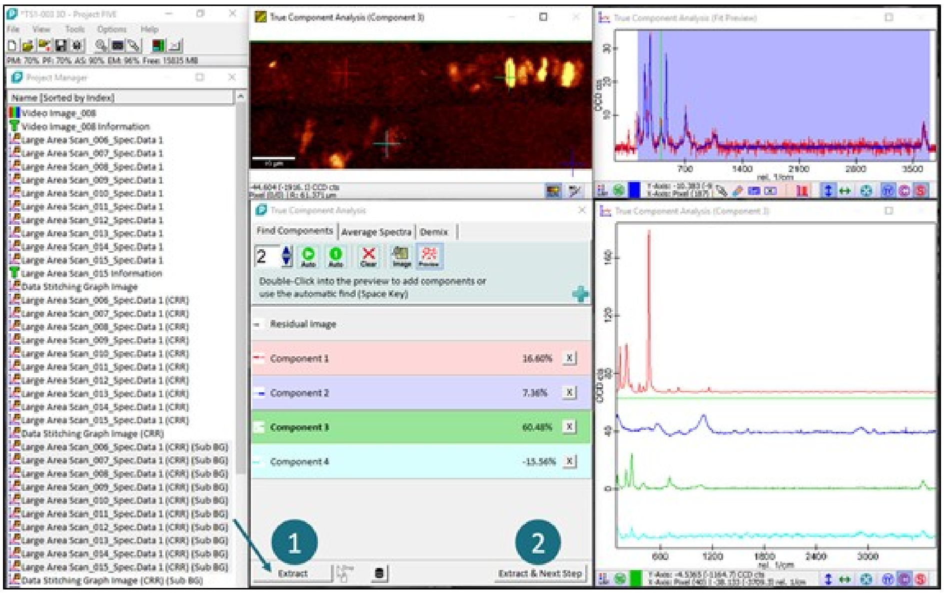
This article describes how to prepare 3D stack data in WITec Project for the export. An example of the data analysis procedure is given in the following. The best way to analyze a set of data will depend on the specific data and your requirements, so the following procedure might need to be modified and adjusted.
Our goal is to apply the same analysis steps like background subtraction and True Component Analysis (TCA) to all layers with the same parameters. However, TCA or other analysis tools need the whole dataset in order to find all components. The solution is to stitch the layers together in one image, and set the analysis parameters with this single stitched object. Then, we apply the analysis to all individual layers by drag and drop them to the Extract button.
If the number of stack layers is very high, it is better to choose only few representative layers (e.g. 2 or 4) for stitching, this makes the analysis much faster.
The procedure suggested here uses the TrueComponent analysis; however, other tools like the fitting tool can also be used.
The data in the figures show some inclusions (green, yellow) in a garnet sample (red) mounted on a glass slide (blue).

Data analysis

- Stitch the images to one object using the Stitching tool from the Drop Action Menu. In the example here, I choose two layers.
- Drag and drop the stitched image to the Raman Wizard, it will open a preview image showing your representative layers.
- The first step is cosmic ray removal (CRR). Set the values as usual.
- Important: Drag and drop all individual layers (not the stitched image) of your stack on the Extract (1) button before pushing the Extract & Next Step (2) button! (See figure below)



- Do the same for baseline correction: Choose the settings with the help of the preview image, then drag and drop all (CRR) corrected layers on the Extract button and finally push the Extract & Next Step button.
- Continue your data evaluation of the stitched data object with the TCA (as in our example):
- Drag and drop all single layers to the Extract button. This will create a (long) list of objects, namely one image for each component in each layer.



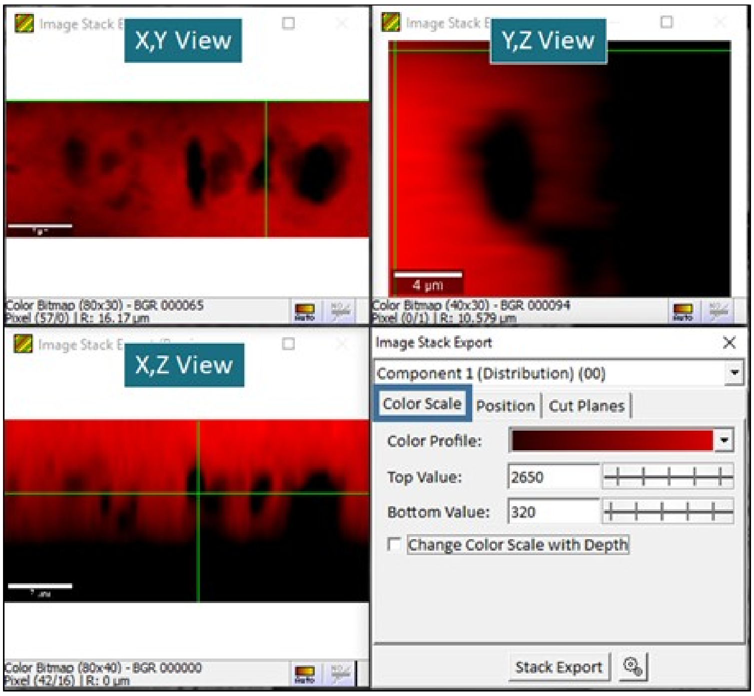
- Optional: Consider image smoothing at this point.

Data Export

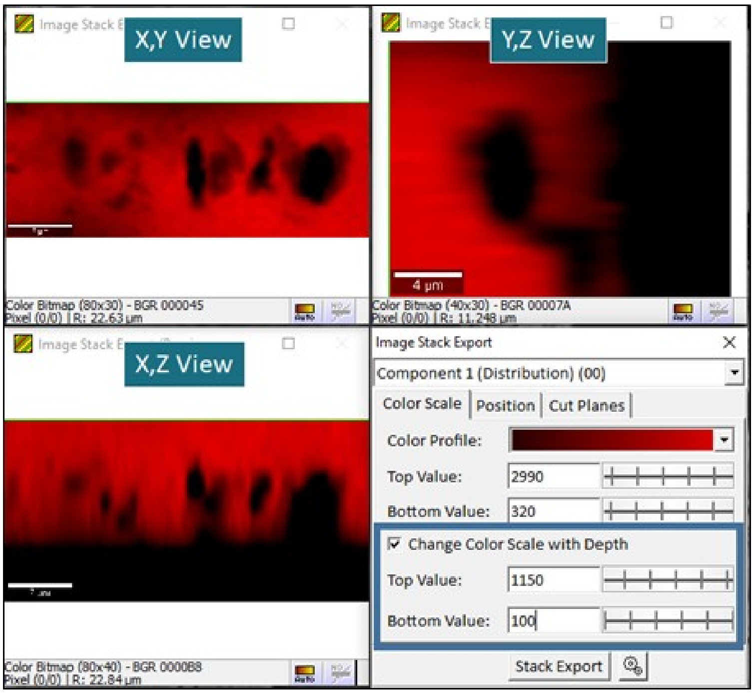
- Extract the images of each component by using the Image Stack Export button in the drop actions menu.

Sort the objects in the project manager by name first.

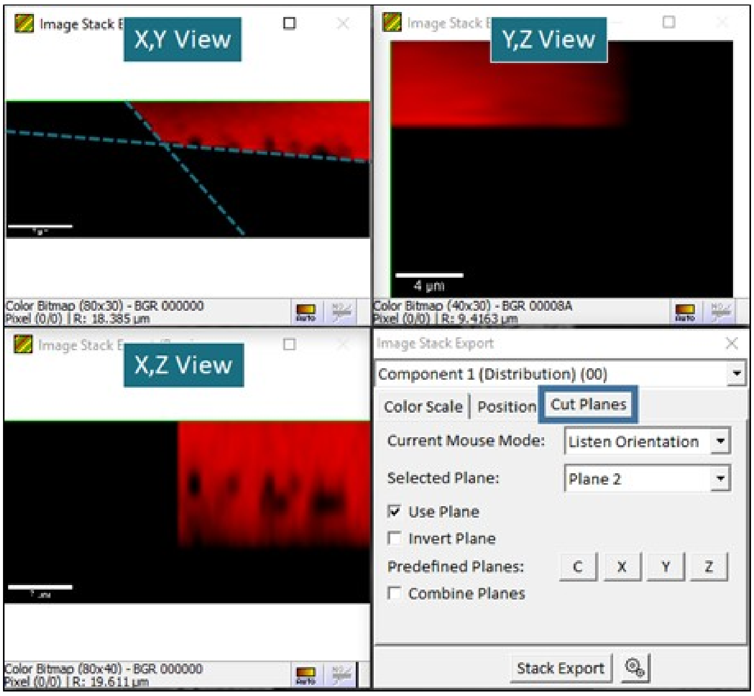
- The Image Stack Export tool provides x,y x,z and y,z views. The color and color scale can be adjusted



- To compensate for the typical intensity decrease when focusing deeper inside a sample, activate “Change Color Scale with Depth”.

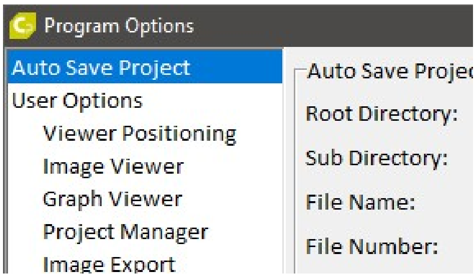


- Use “Cut Planes” to remove parts of single components, e.g. if you want to show only a part of a matrix with inclusions:



- Greyscale is fine - if you choose the color of each component later i.e. in the ImageJ 3D Viewer. (Note: if you choose another 3D Plugin, definition of the color scale might be necessary here.)
- Export as single tif file
- The data can be visualized in any 3D image software i.e. ImageJ

Program Options Window



You can open the Program Options window via the main menu **Options > Program Options**.

Notes:

- Options are not saved to the hard drive until the application is closed.
- Some options take effect immediately, some require a program restart.

There are several places in which options will be saved, depending on the option:

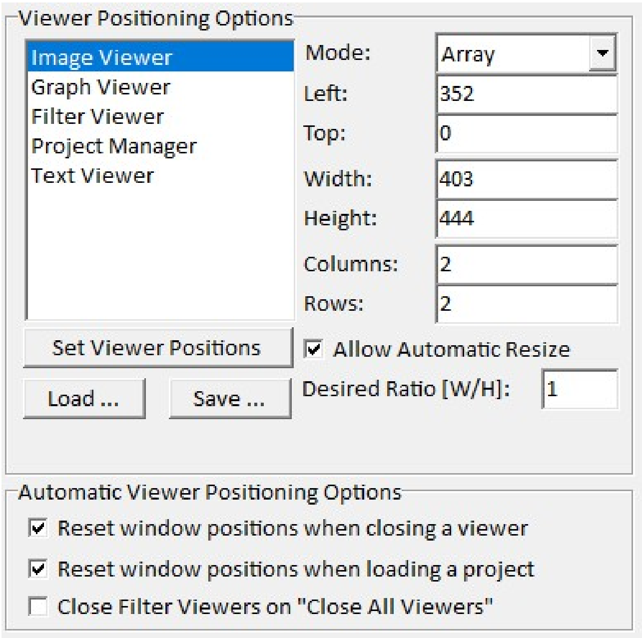
- Most options are saved for the current user only.
- Some options are saved for all users of the current application version.
- Some options are saved system-wide for all WITec applications and users.

The following options are available:

- Viewer Positioning Options
- Image Viewer Options
- Graph Viewer Options
- Project Manager Options
- Image Export Options
- User Interface Options
- OpenGL Options
- Graph ASCII to External Program Options
- Memory Options
- Auto Save Project Options

Viewer Positioning Options

You can change the way of automatic viewer positioning for each viewer category in the **Program Options > Viewer Positioning**.
To change the viewer positioning, first select a viewer category in the list box. Second, change the values in the edits on the right to adjust the positioning.



Viewer Positioning Options

Mode (Combo Box):

- None: No automatic positioning, use operating system default position (cascade).
- Array: Tile the windows side by side with a given number of columns and rows.
- Cascade: Cascade the windows with a given X and Y step size.
- Single Position: Use one static position and size for each viewer.

Left/Top (Integer Edits):
The most left and top position of the first viewer.

Width/Height (Integer Edits):
The width and height of each viewer;
in Array Mode, the maximum area for the viewers is <Width * Columns> x <Height * Rows>.

Columns/Rows (Integer Edits):
number of rows and columns for Array Mode.

Allow Automatic Resize (Check Box):
In Array Mode, window sizes are automatically scaled down if too many windows are open and no more tile is left, this is the case if Number of Viewers > Columns * Rows.

Desired Ratio (Float Edit):
If "Allow Automatic Resize" is turned on, the automatic resize algorithm tries to get a good number of rows and columns that fit best the desired ratio.

Set Viewer Positions
Resets all the viewer positions if one or more viewers were moved by the user.

Load/Save
Here you can save or load your current viewer positioning options.
The file name is important: the software automatically chooses the filename for the current screen/monitor resolution.
If you press "Save", the file name is automatically set to the file name that will be searched for for the current resolution.

Automatic Viewer Positioning Options

Reset window positions for a viewer kind when closing a viewer (Check Box):
If checked, the window positions for a viewer kind are automatically reset if a viewer of this kind is closed.

Reset window positions when loading/appending a project (Check Box):
If checked, the positions of all loaded viewers are reset after loading the project.

Close Filter Viewers when using "Close All Viewers" Button (Check Box):

If checked, all Filter Viewers will be closed when using the "Close All Viewers" feature in the main window.

Image Viewer Options

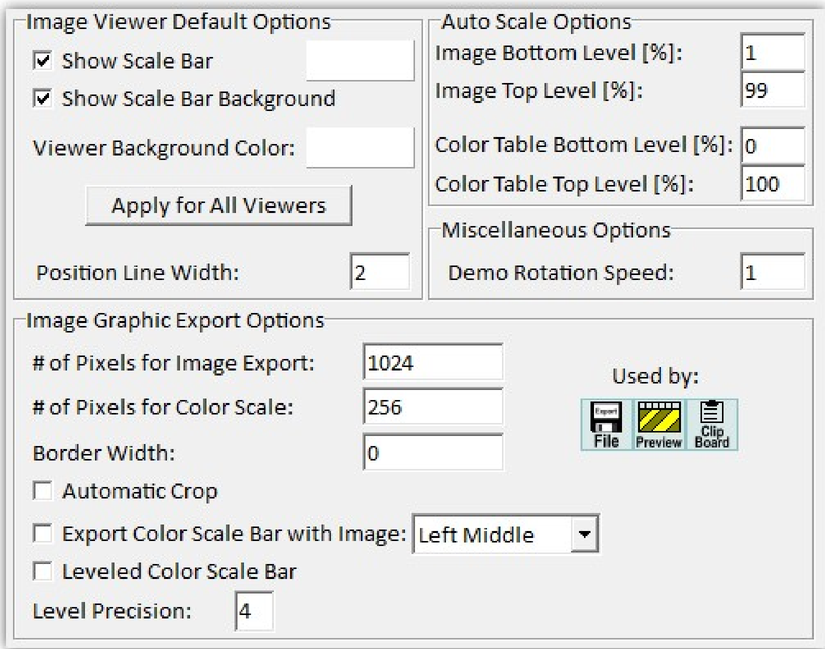


Image Viewer Default Options

Those options are used each time a new image viewer is opened.

Show Scale Bar (Check Box):
Changes the default visibility of the scale bar.

Default Scale Bar Color (Color Panel):
Click on the colored area to change the default scale bar color.

Show Scale Bar with Background (Check Box):
Changes the default visibility of the semi-transparent background of the scale bar (and other labels).

Viewer Background Color (Color Panel):
Changes the default background color for Image Viewers.

Apply for All Viewers (Button)
Applies the current default settings to all currently opened image viewers

Position Line Width (Integer Edit):
Sets the line width of transformation drawings (if you drop another measurement object onto an image viewer to see the measurement position).

Auto Scale Options

Image Bottom/Top Level (Float Edits):
set the bottom and top level for automatic color scale calculation. All values smaller than the bottom level or higher than the top level are ignored.

Color Table Bottom/Top Level (Float Edits):
set the bottom and top color table level for automatic color scale calculation. All values smaller than the bottom level or higher than the top level are ignored.

Miscellaneous Options

Demo Rotation Speed:
Changes the animation speed of the demonstration rotation function.

Image Graphic Export Options

of Pixels for Image Export (Integer Edit):
Defines the width in pixels of an exported bitmap. The height in pixels is automatically adjusted using the current viewer size ratio.

# of Pixels for Color Scale (Integer Edit)
Defines the width in pixels of an exported color scale bitmap.

Border Width (Integer Edit)
Defines the width in pixels for an additional border around the exported image.

Automatic Crop (Check Box):
If checked, the white border is removed automatically before exporting.

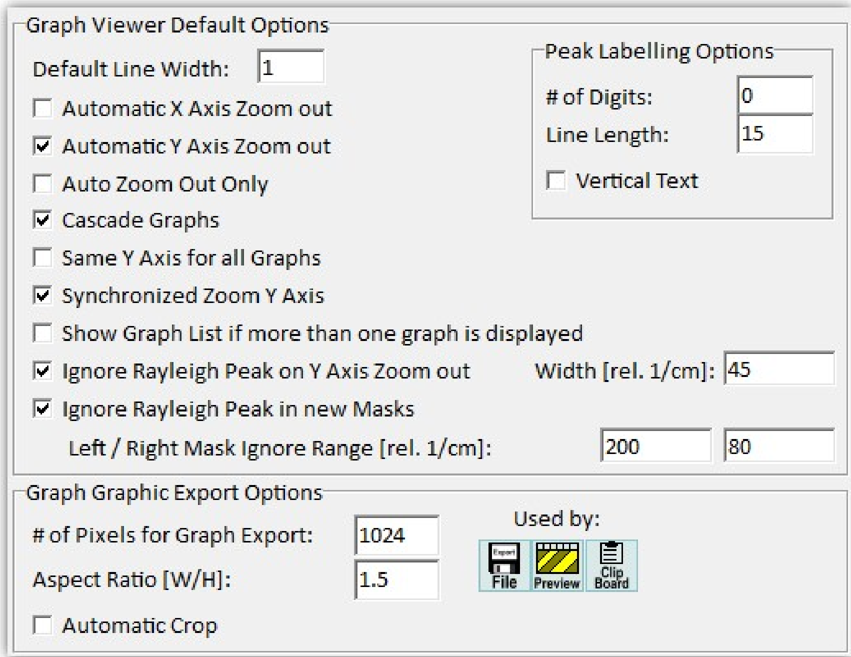
Export Color Scale Bar with Image (Check Box):
If checked, the color scale bar is automatically exported next to the image when exporting an image.

Color Scale Bar Position (Combo Box):
Defines the position of the exported color scale bar, if "**Export Color Scale Bar with Image**" is checked.

Leveled Color Scale bar (Check Box):
If checked, the values of the labels of the exported color scale bar are leveled to an absolute color scale value range (from 0 to <range>).

Level Precision (Float Edit):
Sets the precision of the numbers shown at the level bar.

Graph Viewer Options



Graph Viewer Default Options
These options are used each time a new Graph Viewer is created.

Default Line Width (Integer Edit):
Sets the default line with for drawing graph objects.

Automatic X Axis Zoom out (Check Box):
if checked, the X Axis is automatically zoomed when the displayed graph is changing.

Automatic Y Axis Zoom out (Check Box):
if checked, the Y Axis is automatically zoomed when the displayed graph is changing.

Cascade Graphs (Check Box):
if checked, the Y Axis is cascaded when showing multiple Graph Objects.

Same Y Axis for all Graphs (Check Box):
if checked, all Graph Objects in the same viewer share the same Y Axis scale.

Synchronized Zoom Y Axis (Check Box):
if checked, all Graph Objects are zoomed synchronously when using the mouse wheel for zooming.

Show Graph List if more than one graph is displayed (Check Box):
if checked, a list of displayed Graph Objects will be shown automatically if more than one graph is displayed.

Ignore Rayleigh Peak on Zoom out Y (Check Box and Float Edit):
if checked, the Y Axis zoom on spectral data automatically ignores the Rayleigh Peak.
In the float edit you can define the spectral range that should be ignored (in relative wavenumbers).

Ignore Rayleigh Peak in new Masks (Check Box and Float Edits):
if checked, the Rayleigh peak is automatically removed from masks in analysis dialogs. You can define the range that should be removed by setting the left and right distance from the excitation wavelength.

Peak Labelling Options

# of Digits (Integer Edit):
Sets the default number of digits for peak labels.

Line Length (Integer Edit):
Sets the default line length for peak labels.

Vertical Text (Check Box):
If checked, the peak label text is drawn vertically.

Graph Graphic Export Options

# of Pixels for Graph Export (Integer Edit):
defines the width of an exported bitmap in pixels.

Aspect Ratio (Float Edit):
defines the width/height ratio of an exported bitmap.

Automatic Crop (Check Box):
if checked, the white border is removed automatically before exporting.

Image Export Options

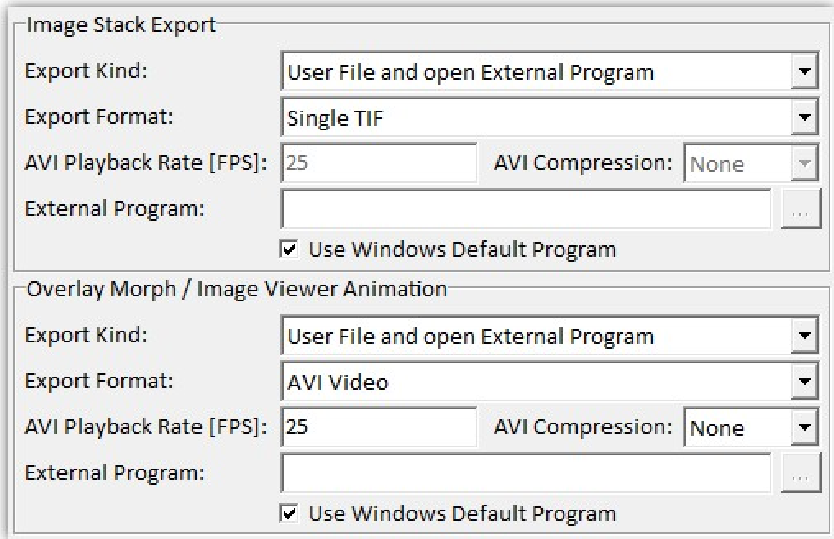


Image Stack Export

Used for the Image Stack Export Dialog.

Export Kind:
Here you can choose the following options:
- User File: just saves the file(s) to a user defined location
- User File and open External Program: saves the file(s) to a user defined location and opens the file using the program defined in "External Program"
- Temporary File and open External Program: saves the file(s) to a temporary folder and opens the file using the program defined in "External Program"

Export Format:
Defines the file format for the image export:
- Single TIF: Stores all images into a multi-frame TIF file
- Multiple Bitmaps: Stores all images into separate bitmap files, a number is automatically added to the file names (0001, 0002, ...)
- AVI Video: Stores all images to an AVI video file.

AVI Playback Rate:
Default playback rate for AVI videos.

AVI Compression:
Defines the compression for AVI videos:

- None: no compression
- MSVC: Simple Microsoft Video Compression - might not work with several video players.

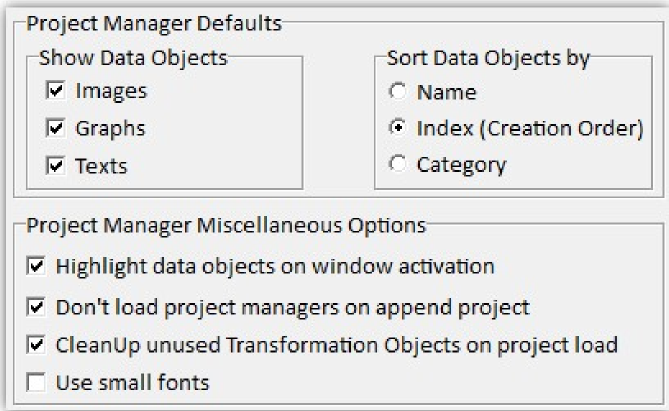
External Program:
Here you can define an external program file name that will be used for opening the stored image file.

Use Windows Default Program:
If checked, the windows default program is used instead of a user defined external program.

Overlay Morph / Image Viewer Animation

Parameters see above.
Used for the Image Viewer Animation Export and the Overlay Morph in Image Transform and Overlay Dialog.

Project Manager Options



Project Manager Defaults
Those options are used each time a new project manager is created.

Show Data Objects

Images:
If checked, Image Data Objects are shown

Graphs:
If checked, Graph Data Objects are shown.

Texts:
If checked, Text Data Objects are shown.

Sort Data Objects by

Caption:
If checked, Data Objects are sorted by their name / caption.

ID (Creation Order / Index):
If checked, Data Objects are sorted by their creation order. The newest object is at the end of the list.

Category:
If checked, Data Objects are sorted by their category.

Project Manager Miscellaneous Options

Highlight Data Objects in project managers on window activation.
If checked, each Project Manager will highlight data objects that are used by another software part upon clicking on a viewer or a data analysis dialog.

Don't load project managers when appending a project:
If checked, Project Manager windows of an appended project are not loaded.

CleanUp unused Transformation Objects on project load:
If checked, transformation objects (that are hidden by default) are deleted if not used by any image or graph object.
Can be turned off e.g. for special import actions.

Use small fonts:
If checked, Project Manager uses the old smaller font style. Create a new Project Manager to see the effect.

Image Export Options

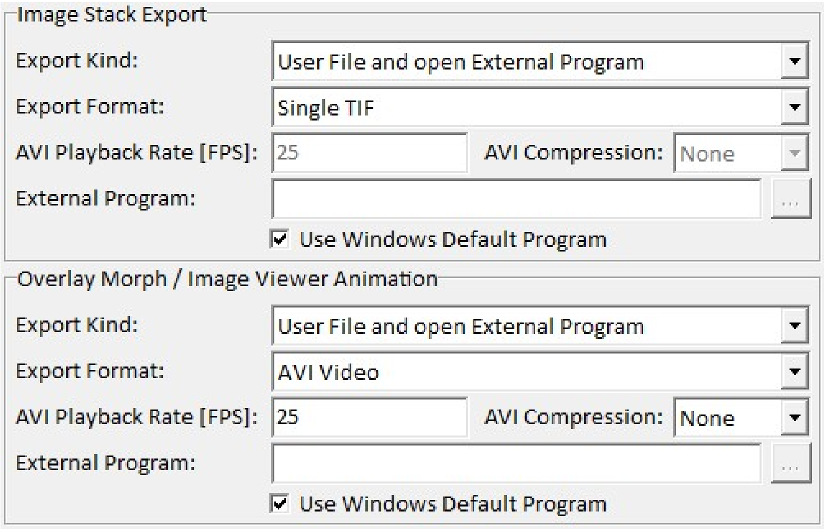


Image Stack Export
These settings are used for the Image Stack Export Drop Action.

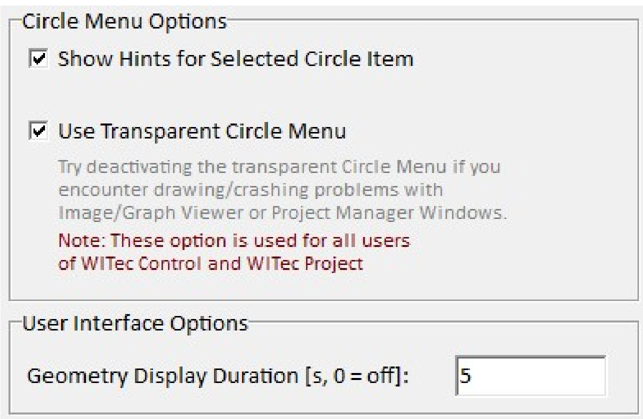
Overlay Morph / Image Viewer Animation
These settings are used for
- The Image Transform and Overlay Drop Action (Export Overlay Morph)
- The Image Viewer Animation Editor

Export Kind
User File: Just saves a file using a save file dialog.
User File and open External Program: Saves the file using a save file dialog, then opens the configured external program.
Temporary File and open External Program: Saves the file in the Temp-Directory, then opens the configured external program.

Export Format
Single TIF: Saves one or multiple images into a single (multi-frame-)TIF image file.
Multiple Bitmaps: Saves one or multiple images as one or multiple bitmap files.
AVI Video: Creates an AVI Video File for movie playback, using the AVI Playback Rate and AVI Compression options.

External Program:
Enter the full path of an external executable, e.g. ImageJ or another program of your choice.
Will be automatically opened depending on the Export Kind.

User Interface Options

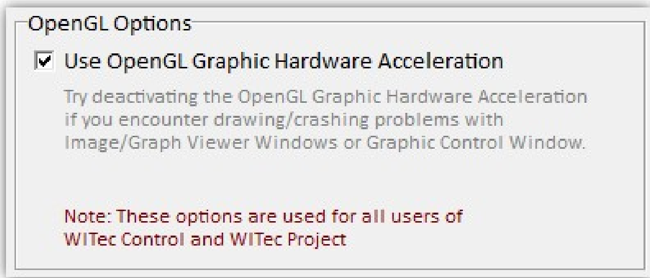


Show Hints for Selected Circle Item
If checked, the Circle Menu shows a text when moving over an option.

Use Transparent Circle Menu
Can be turned off if there are problems displaying the circle menu (e.g. remote sessions).

Geometry Display Duration
In image and graph viewers, you can press the "G" Button to send the current position to all other windows. This will define how long the position is shown in the other windows.

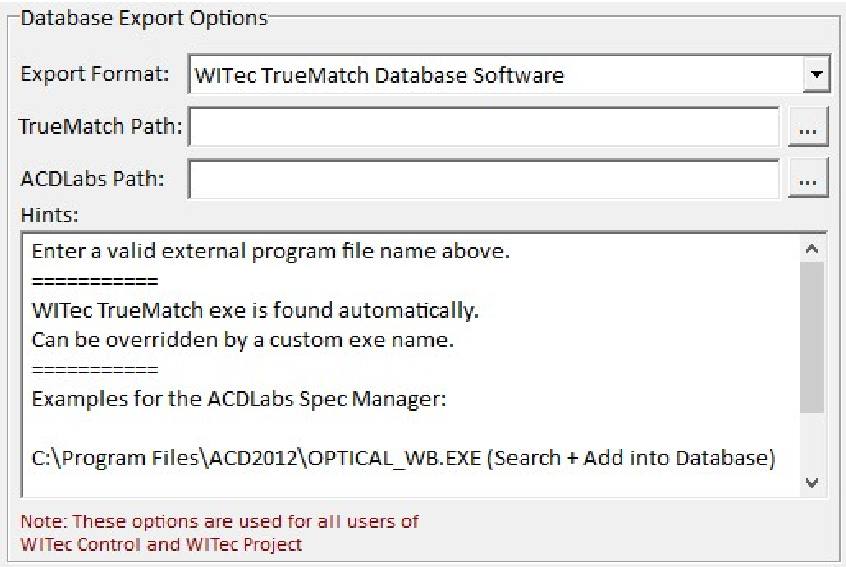
OpenGL Options



Use OpenGL Graphic Hardware Acceleration:
If checked, the software will use the graphic hardware acceleration to improve graphic performance (especially for large 3D presentations in Image Viewers).
This setting is used for **all users** and for both WITec Project and WITec Control from the same Suite Version.

Database Export Options

In the Database Export Options you can define which database software should used.
These options are shared for **all users** of the compter in WITec Control and WITec Project.
See Database Search in WITec Project.



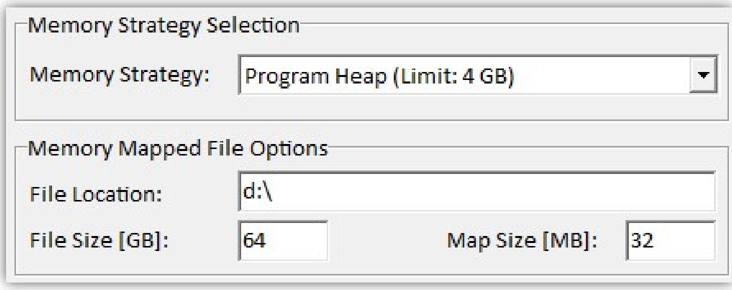
Export Format
Here you can choose between the WITec TrueMatch Database Software and ACDLabs.

TrueMatch Path
Should be empty. The TrueMatch executable will be found automatically for the WITec TrueMatch Database Software.

ACDLabs Path
Enter the path / executable file name for the ACDLabs Database Software.

The file name should be something like
C:\Program Files\ACD2012\OPTICAL_WB.EXE (Search + Add into Database)
C:\Program Files\ACD2012\SPECPROC.EXE (Search in Database Only)
C:\Program Files\ACD12\UVIRMAN.EXE (Search + Add into Database)

Memory Options



Memory Strategy

The Memory Strategy affects the way Data Objects are held in memory while the software is running and working with the data.
The main difference between the strategies is the amount of data that can be handled by the software as well as the performance while loading/saving/calculating.

Please take a look at the Data Object Memory Consumption article to get a feeling about the size of your measurement data.

These options are shared for **all users** of the computer.

Memory Strategy "Program Heap"

This is the standard "Memory Strategy"; if there are no memory problems this strategy should be used.
The software uses up to 4 GB of fast physical memory for data objects (the real maximum is < 4 GB).

Use this Memory Strategy if:

- you are working with small graph Data Objects (< 500 MB)
- you don't have a fast Solid State Disk (SSD) Hard Drive
- you have a 32-bit Operating System

Memory Strategy "Memory Mapped File"

This strategy enables the software to work with project data larger than 4 GB.
For this purpose the software uses a big file on a fast hard drive for Data Objects. This file is cached automatically by the operating system using the fast physical memory.

Use this Memory Strategy if:

- You have a 64-bit operating system
- The amount of installed physical memory is larger than your project size (e.g. > 8 GB)

Before using this Memory Strategy pay attention to the following notes:

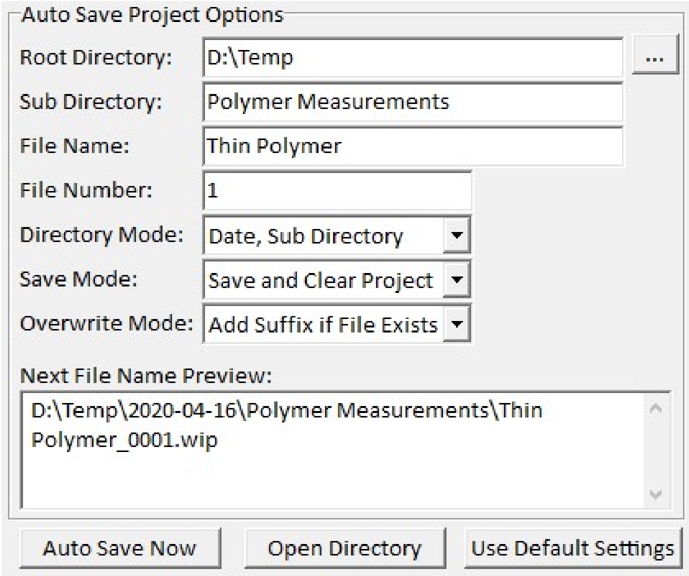
- For performance reasons, the "File Location" should be on a fast Solid State Disk (SSD) Hard Drive.
- The file size should be adjusted to the SSD size and to your project size needs.
- Each software instance will create a memory mapped file with the given size!

File Location:
The location of the memory mapped file; should be on a fast Solid State Disk (e.g. "E:\" if the drive letter of the SSD is E.)

File Size:
The size of the memory mapped file, i.e. the amount of space each instance of WITec Project/Control will need on the SSD.

Map Size:
The amount of physical memory used to map data between the memory mapped file and the application.
We recommend a value of 32 MB.

Auto Save Project Options



These options are used if you press the Auto Save Project Button:

Every time you perform the "Auto Save Project" action, the file number will be increased and a new file name will be generated.

Licensing Overview

The WITec Control as well as the WITec Project software components need valid license keys before they can be started.

WITec Project

WITec Project is the basic post-processing software for analyzing WITec microscope data. The WITec Project (basic version) License Key is delivered with a microscope system and can be used by the whole user group of this microscope. This Key is not bound to a computer and can be installed on a certain number of computers according to the license product. To install an existing license key onto a new computer, use the License Manager.

WITec Project Plus

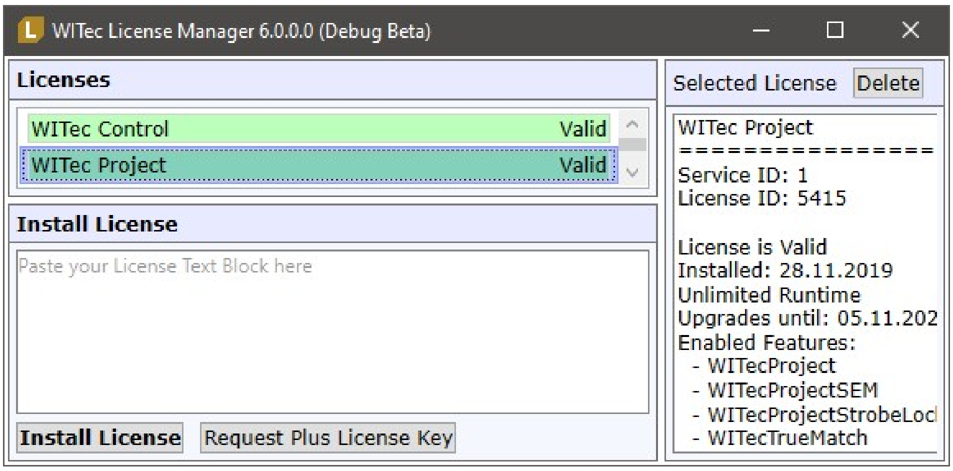
WITec Project Plus is an add-on to the basic WITec Project software containing sophisticated data evaluation algorithms (see WITec Project Plus Features). All Plus features are available with limitations (demonstration mode) if you don't have a license. To use the plus features without limitations, you have to buy a computer-bound license, see WITec Project Plus Activation. This Key is bound to exactly one computer and cannot be installed on a different one.

WITec Control

WITec Control is only installed on the microscope system computer that comes from WITec and should already have a valid license installed. In case of (remote) software upgrades the WITec support team will install this license.

License Manager

The License Manager shows the currently installed licenses and allows you to install or remove licenses:



License List
Click on a License to see the License details.

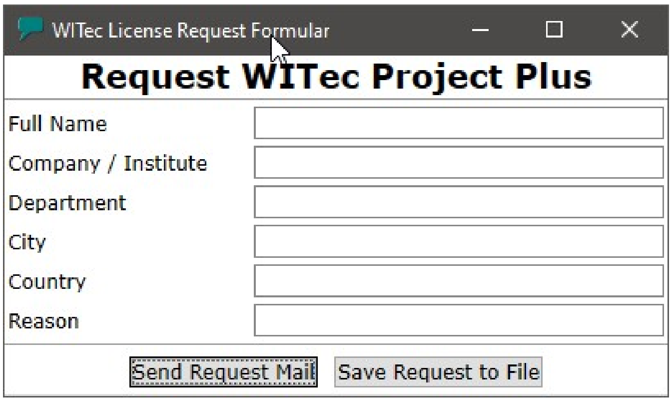
Delete
Removes the currently selected License.
Please only delete a license if it is no longer valid or you really know what you are doing!

Install License
Copy your license text from the windows clipboard into the white area beside the black key symbol (using the Ctrl-V shortcut or via right-click Context Menu -> Paste). Then press the "Install License" Button.

Request WITec Project or Plus License Key:
This will open a request window which allows you to send a request to WITec.

Before sending a WITec Project Key request, check whether your company/department already has a License Key. In general, a WITec Project license is shipped with the WITec System.

Before sending a WITec Project Plus Key request, make sure WITec already received a license order. The Request is needed to create a computer-bound license key for WITec Project Plus.



Please at least enter your full name and your company/university, wherever applicable also the other fields.

Send Request eMail:
If you have an eMail client installed and configured properly, you can press this button in order to automatically create a new eMail containing the request text.
If you don't have an eMail client on the certain computer, save the request to a file and take this file to a computer with an eMail client in order to send its contents to key@witec.de

Save Request To File:
Saves the request eMail Text to a file on hard drive.

WITec Project Plus Activation

Request Price Quotation

If you are interested in our Advanced Data Evaluation Software **WITec Project Plus**, feel free to ask for a price quotation: info@WITec.de.

Activation Process

Before you can use your WITec Project Plus License, you have to activate the license:

Send Request:

- Start the WITec Software on the computer on which the plus license should be activated.
- Open the License Manager via "Main Menu > Help > License Manager".
- Press the "Request WITec Project Plus Key" Button.
- Enter your contact information.
- If you bought multiple licenses to activate the software on more than one computer, enter the computer name in the reason field to be able to distinguish the keys later on.
- Press the "Send Request eMail" Button to send the Request to WITec if you have an eMail Client installed on the same computer; otherwise:
- Press the "Save Request To File" Button to store the request in a Text File and copy it to a computer with an eMail Client, then copy the content of the Text File into a new eMail addressed to key@witec.de.

Receive and Install License:

- WITec will send you a License Key via eMail (the Key is sent as an encrypted text block).
- Open the License Manager of WITec Project (or WITec Control) on the computer where the request was created.
- Copy the encrypted text block into the white empty field next to the key symbol and press "Install New License".
- Restart WITec Project. The splash screen should now display that WITec Project Plus is active ("Plus Version"). You can

check whether the Plus Version is active at any time by opening the About and Support Panel in the Help Menu of WITec Project.

Note that the WITec Project PLUS license only works on the computer from which you created the license request.

If you have problems activating your WITec Project Plus Software, please contact key@witec.de.

WITec Project Plus Features

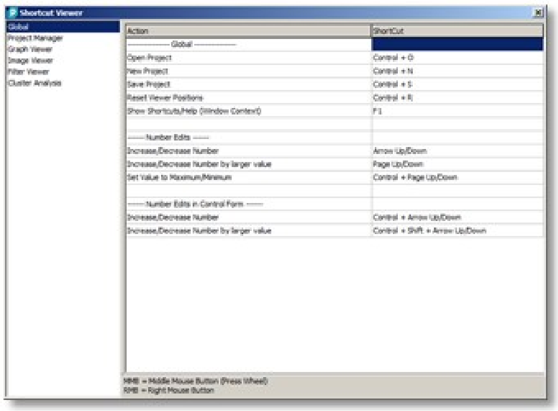
List of all WITec Project Plus Features

The following Drop Actions are features of the WITec Project Plus Software.
Some standard Drop Actions contain parts that only work with the Plus license.

Fast Avg	Advanced Graph Average fast threshold mask creation from images and "real-time" average spectra
Sub BG	Graph Background Subtraction (only parts) shape subtraction, automatic mask in polynomial subtraction, weighted constant spectrum subtraction
Analyze	True Component Analysis find components, demix spectra, create intensity images
Inv Basis	Inverse Basis Analysis create component spectra using intensity images and the original image spectra
Fitting	Advanced Fitting Tool (only parts) fit all spectra in a multi spectral data object in one step
Cluster	Cluster Analysis automatically find similar spectra in a multi spectral data object
NMF	Non-Negative Matrix Factorization automatic creation of component spectra and distribution images
PCA	Principal Component Analysis PCA Transformation of spectral image data objects
Repair	Graph Repair replace spectral pixels by a simple interpolation
Crop	Data Cropping and Reduction change the size of images, bitmaps, spectral data objects
Stitching	Graph and Image Stitching stitch multiple images or image spectral objects side by side into one larger image or spectral object
Overlay Transform	Image Transform and Overlay overlay 2 images, adjust Image position and scale including advanced transformations
Correlate	Image Correlation calculate correlation graphs to plot a correlation point cloud of two or more images
Filter	Image Filter (only parts) Anisotropic, Sobel, Kirsch, Variance, Laplace, Sharpen and Custom Image Filters
Fourier	Image Fourier Filter create Fourier Amplitude Images or remove noise frequencies in fourier space with back transform
Repair	Image Repair replace bad image pixels using user values with noise, interpolation or texture analysis algorithms

Shortcuts

There are a lot of shortcuts in WITec Project.
An overview is available in the Shortcut Viewer: **Main Menu > Help > Show Shortcuts.**



Here you can find:

- Global shortcuts
- Project Manager shortcuts
- Graph Viewer shortcuts
- Image Viewer shortcuts
- Text Viewer shortcuts
- Filter Viewer shortcuts
- Cluster Analysis shortcuts.

Some shortcuts are also shown in the hint of an UI element if the mouse is just moved over the element.