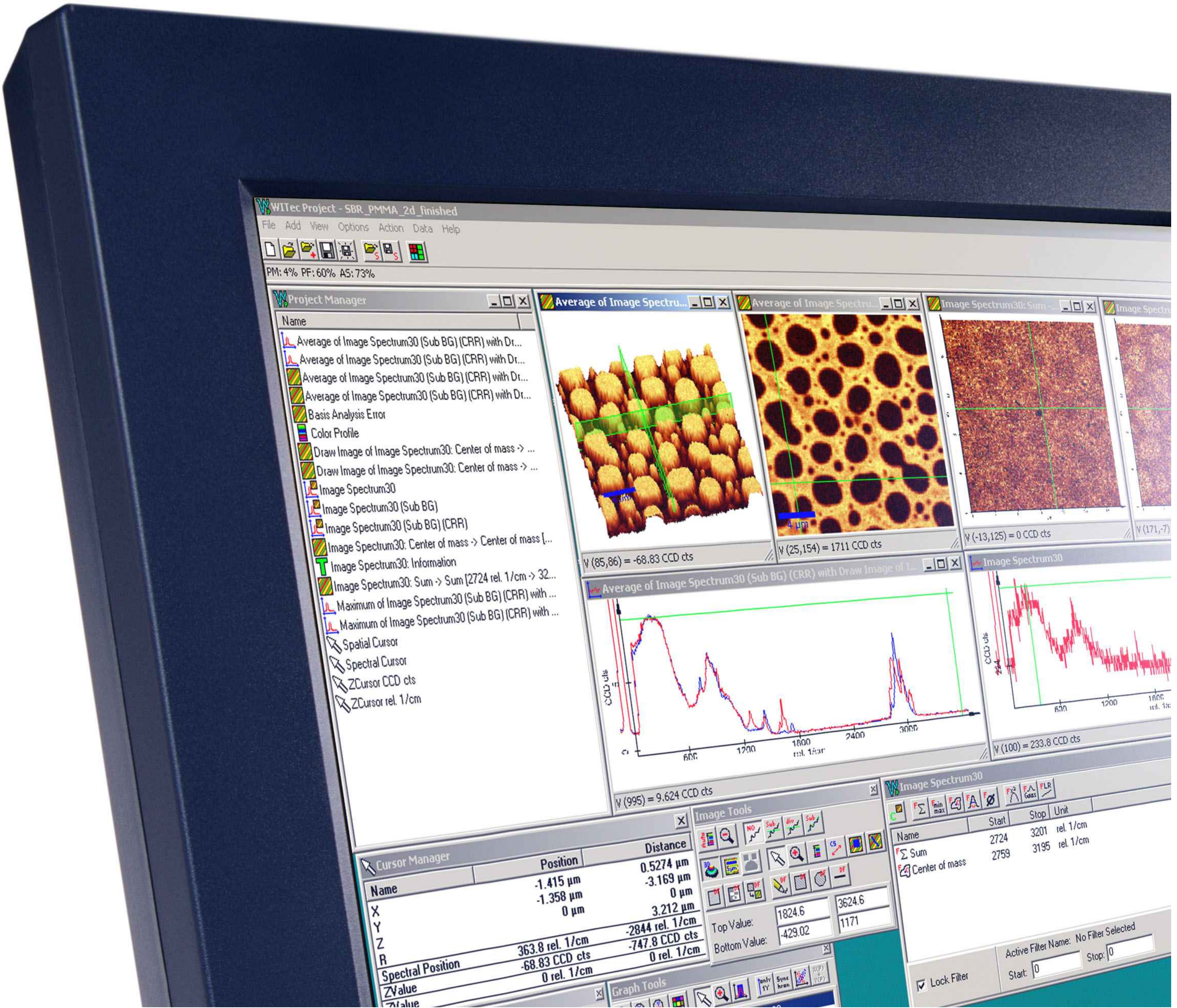
WITec Project

Data Evaluation Software

User Manual

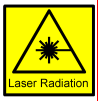
WITec
focus innovations



About this manual

This manual describes the WITec Project software. This software is designed for the analysis of scanning probe data sets (e.g. AFM, SNOM, and Raman data).

Warnings are marked with a red bar. Please read these warnings carefully to avoid problems that may otherwise occur.



If extra care should be taken by the operator due to the presence of intense laser radiation, this warning sign will be present.

HINT Throughout the manual, you will find text blocks with a blue **HINT** on the left–hand side of the text. These text blocks contain additional, useful information.

Text marked with a shaded rectangle such as Menu Item Name refer to a menu item in the software.

Text marked with a rectangle such as Button Name refer to a button or checkbox in the software.

Keyboard keys are highlighted as Key.

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Safety Information

Please read this manual carefully before using the software.

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Introduction

Chapter 2

Appearance

After opening the WITec Project software, the window in Fig. 2.1 will be displayed. It contains the window title, the main menu, and a status bar.

This chapter describes the functions and capabilities of these software elements.

HINT All other windows in this program are top-level windows and can be moved over the entire desktop. Therefore, minimizing all other running programs is advised.

2.1 Window Title

The window title contains useful information such as the logo and name of the software, followed by the name of the opened file. On the right side, the standard Windows® buttons are available: minimize, maximize, and the software exit button.

2.2 Main Menu

The main menu provides access to all of WITec Project's functions and menus. All functions can be accessed using either a mouse or via the hot keys using the Alt - key on the keyboard in combination with the appropriate letter of the desired menu.

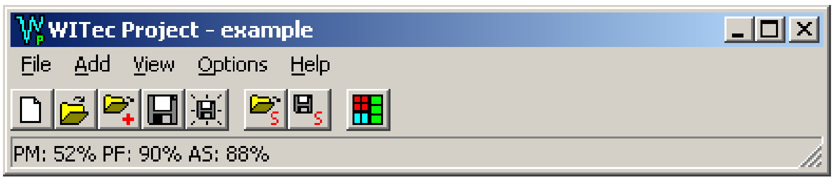


Fig. 2.1: Appearance of the WITec Project software.

2.2.1 File

The file menu contains all functions concerning file management.

Open Project

This function starts the Windows® standard open-dialog for WITec Project files (*.wip). Using this dialog, a saved data project can be opened. The data will be displayed on the screen as it was saved. Previously opened projects will be closed.

Save Project

This menu function allows a project to be saved. The filename will be the actual name displayed in the window title line.

Save Project As

This function is similar to the save project function, while offering the possibility to change the filename. The Windows® standard save-dialog for WITec Project files is activated.

Append Project

Using this function, an additional project can be appended to the opened file. This procedure is also available via the Windows® standard open-dialog.

Append Data

Using this function, a WITec data file (*.wid) can be appended to the opened file. This procedure is also available via the Windows® standard open-dialog.

Open Recent WIP Files

This sub menu shows a list of recently used WITec project files (*.wip). Clicking on a filename will open this project file. Previously opened projects will be closed.

Import

Allows the user to import data acquired with ScanCtrl, WinSpec, and the DPFM software. This data can be imported either to an already opened project to become part of the project, or as independent files to be evaluated with the WITec Project software. The modified (evaluated) data can be saved as WITec Project files (Section 6).

New Project

Opens a new ”untitled” project. Already opened projects will be closed.

Exit

Closes the program.

2.2.2 Add

The Add menu allows the user to add additional viewers, managers, and data objects to the project screen.

Project Manager

The project manager displays a user-defined selection of data objects stored in the current project. It allows the sorting of data objects based on several properties. The project manager is the starting point for all drag and drop operations. For a more detailed description of the project manager, see Section 4.2.

Filter Manager

The filter manager organizes a collection of filter data objects. These filters can be applied to a spectrum in order to create images, graphs, and single point information. For a more detailed description of the filter manager, see Section 4.8

Color Profile

The color profile, represented by the button , is added to the project. It allows the user to change the color of individual images. For a more detailed description, see Section 3.9.

Text

The text menu item adds an empty text data object to the current project (Section 3.8), in which the user can add text information. Simultaneously, the appendant text viewer is opened, see Section 4.6.

Spatial Cursor

The spatial cursor menu item adds a spatial cursor data object to the current project (Section 3.2.1).

2.2.3 View

The view menu provides access to image and graph processing functions.

Tool Windows

The following tool windows are available:

- **Image**
  Image tools are required to change the display parameters of images in the image viewer. The image tools window provides quick access to the image viewer functions. A detailed description of the available functions can be found in Section 4.3.4

- **Graph**
  Graph tools are required to change the scaling and display parameters of graphs in the graph viewer. The graph tools window provides quick access to the graph viewer functions. A detailed description of the available functions can be found in Section 4.5.4

- **Drop Action**
  The drop action enables the user to modify images and graphs, perform operations with graphs and images, and much more. A detailed description of all functions is given in Section 7.1.

Graphic Export 

Shows or hides the graphic export window. This window is used for all bitmap export functions in the software (see Section 5.1).

Reset Viewers 

Sets all viewers to user-defined positions.

2.2.4 Options

The options menu allows the user to change, load, and save all project settings. These can be parameters concerning appearance, data processing, and export functions. The parameters are categorized based on their functionality. In this section, a description of each function is provided.

Viewer Positions

This function opens a dialog box in which the settings for the viewer positions on the screen can be defined. With Reset Viewers, these rules are applied to all viewers.

Filter

The filter function shows the actual settings of the filters.

- **Graph**
  The graph function opens a dialog box displaying the filter parameter settings for the Savitzky-Golay filter (see also Section 7.1.2), the matrix filter used by the median graph filter (Section 7.1.3), and the average graph filter (Section 7.1.4)

▶ **Image**
The image function opens a dialog box displaying the filter parameter settings for the line subtraction operation (more details can be found in Section 7.1.8), the surface subtraction operation (Section 7.1.9), the matrix operation used by the median image filter (Section 7.1.21), and the average image filter (Section 7.1.22).

Data Analysis

The data analysis function opens a dialog box displaying the parameters used by the cross section (Section 7.1.14) and histogram (Section 7.1.10) data analysis functions.

Export

The export function opens the dialog box represented in Fig. 2.2, Fig. 2.3, and Fig. 2.4. The tab sheet allows the user to select the number of pixels to be used for the bitmap export. The software uses this pixel number to define the larger side of a rectangular image.
If the checkbox Automatic Crop is checked, the plain color around the image is cropped out. For more information concerning bitmap export, see also Section 5.1.

Save Project Settings

All project settings of a project can be saved. A standard Windows® dialog box appears, allowing the user to save the settings in a *.wps file. The current project settings are stored automatically when the program is closed. Upon reopening, the new project settings will be active.

Open Project Settings

To open a stored project setting, the Windows® dialog box allows the user to select from saved *.wps files.

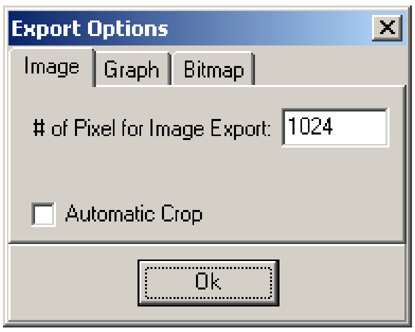


Fig. 2.2: Image export options dialog box.

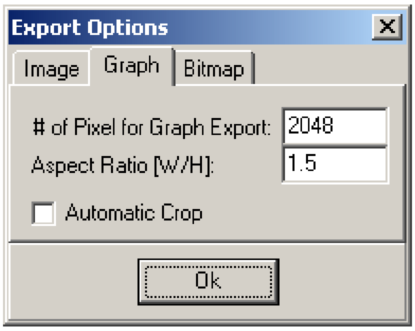


Fig. 2.3: Graph export options dialog box.

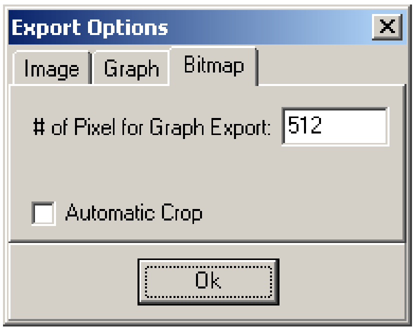


Fig. 2.4: Bitmap export options dialog box.

2.2.5 Help

In this section, the user can find information about the software. If the WITec Project software is embedded in any other data acquisition software, additional information for this software can be found here.

About

The about function opens the splash form. It shows the contact address and the current version of the software.

WITec Project Manual 

This menu item opens the WITec Project Manual inside a PDF viewer. For this function, Adobe Acrobat® Reader™ must be installed. Also, the file extension *.pdf must be associated with the Acrobat® Reader™.

2.3 Status Bar

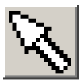
The status bar provides information about the available computer memory (memory status) expressed in percent: PM refers to the free physical memory, PF gives information on the free page file size, and AS refers to the free address space for this program.

Chapter 3

Data Objects

3.1 General Data Properties

All data are stored in data objects. Every kind of data has its own data type. The basic properties of all data types are a caption, an icon, and a unique identification number. The caption and icon can be changed by the user. This change has no effect on the operation of the software. The identification number is for internal use only and cannot be changed. Data objects and viewers are linked by this identification number.
The specialized data objects store their own data, have links to other data objects, and introduce a context menu (e.g. parameter change, data analysis, or export function).
All viewers and data objects of the project are informed by the internal message system about changes in other data objects.

3.2 Cursor 

The cursor can be considered a messenger within a project. If the same cursor is linked to several viewers, the viewers and the project itself can communicate with each other. Every physical quality has its own cursor object (e.g. time, space, spectral position ...). A cursor stores the last position, a reference point to calculate distances, and the most recent state of the mouse and keyboard buttons Shift, Alt, and Ctrl. If the left mouse button is clicked, the current position is used as the new reference point.
The cursor can also transmit information about user-selected areas or regions. To avoid miscommunication within the project, only one target (e.g. viewer, project window for data analysis) listens to the cursor. In this case, the target is in a so-called listen mode. All other possible targets deactivate the listen mode automatically. This protocol avoids unintentional parameter changes elsewhere in the project.

The software can work with different interpretations (see Section 3.4) of the same physical quality (m, cm, mm, ...;h, min, s,...). To avoid miscalculations, all data transfers are performed in standard units (see Section 3.4 and Section 3.3). A target can reinterpret the quantity transmitted in standard units in terms of units used by the sender, because the last interpretation is also available in the cursor object.
In the following section, the different types of cursor are described. All cursors appear as in the project manager. The cursor data type introduces a context menu, which allows the opening of the cursor viewer (see Section 4.7).

3.2.1 Spatial Cursor

This cursor is used for spatial positions. It is a 3-dimensional cursor with the quantities X, Y and Z. Its standard unit is μm. This cursor is used in combination with spatial interpretations (see Section 3.4.1).

3.2.2 Spectral Cursor

The spectral cursor reads out spectral positions within a spectrum. The standard unit is nm. This cursor is used in combination with spectral interpretations (see Section 3.4.2).

3.2.3 Time Cursor

The time cursor can be used to monitor the time coordinate. This cursor works together with the time interpretation (see Section 3.4.3). The standard unit is s.

3.2.4 Z-Cursor

The z-cursor can be used in cases in which the software has no information about a measured quantity. This cursor is used together with the z-interpretation (see Section 3.4.4). In this interpretation, only the unit of the quantity is stored. For every new unit name (z-interpretation), a new z-cursor is created.

3.3 Transformation

Transformation data objects are needed to scale arrays of digital data into terms of real physical positions and distances. Generally, transformations convert pixel indices into a standard unit or vice-versa. These data objects do not contain a context menu.

3.3.1 Spatial Transformation

The spatial transformation data object converts a 3-dimensional pixel array into real space coordinates. This transformation scales the array in all three dimensions and rotates this cuboid. After this operation, the cuboid is shifted to its origin.
This kind of transformation is used for 1-, 2-, and 3-dimensional pixel arrays. It can appear as  or  in the project manager. This object can be linked to image or graph data objects.

3.3.2 Spectral Transformation

The spectral transformation data object is needed for spectral data. It stores the calibration of the spectrograph. The pixel positions of the CCD camera are set to represent the appropriate wavelengths. The standard unit of wavelength is nm. This data object appears as . It is linked to graph data objects.

3.3.3 Linear Transformation

The linear transformation data object is a linear transformation between a 1-dimensional pixel array and a real physical coordinate. These data objects are linked to graph data objects in order to scale e.g. time series and histograms. Therefore, the standard unit depends on usage. It appears as  in the project manager.

3.4 Interpretation

The software operates in so-called standard units. Every physical property has its own standard unit. Interpretations are required to change a standard unit to an equivalent description of this property. The interpretations are used by viewers to give coordinate systems the correct scaling and units. All interpretations introduce a context menu, which allows the user to change between several units.
With the default settings of the project manager, these objects are not visible (see Section 4.2).

HINT Every viewer can have its own unique interpretation. One viewer can scale data in e.g. μm, while another viewer can scale the same data in nm. The software tries to keep the number of interpretations to a minimum. If one type of interpretation already exists, it does not create a new one.

3.4.1 Spatial Interpretation

The standard unit for spatial coordinates is μm. With this interpretation, the user can switch between m, mm, μm, nm, Å and pm. Its data object is represented by the icon in the project manager.

3.4.2 Spectral Interpretation

With the spectral interpretation data object, a user can switch between the units nm (standard unit), μm, $\frac{1}{cm}$, $rel.\frac{1}{cm}$, eV, meV, $rel.eV$ and $rel.meV$. For relative units (rel.), a reference wavelength is required. This parameter is also stored in the data object. Raman measurements use the laser excitation wavelength as the reference wavelength. Every spectrum has its own spectral interpretation to make measurements with different excitation wavelengths comparable.
The object uses the icon in the project manager.

3.4.3 Time Interpretation

A time interpretation data object changes the unit of time scales. The standard unit is s. The user can switch in the context menu between h, min, s, ms, μs, ns, ps, and fs. This object is represented as in the project manager.

3.4.4 Z-Interpretation

Z-interpretations contain only one unit name. Generally this object is used for user-defined qualities. This object has the icon in the project manager.

3.5 Image

An image data object stores a 2-dimensional data array which can be displayed with the image viewer (see Section 4.3). The number of bins in both dimensions can be chosen independently. The maximum size is limited only by the computer memory. The image data object stores a link to the spatial transformation data object (see Section 3.3.1). Via this link, the pixel array is transformed into real space coordinates, which allows the image to be placed in any position (shift, scale, and rotation) in real space. The scaling of the data itself is performed with a link to a z-interpretation data object (see Section 3.4.4). If this link exists, the data is assigned an appropriate unit.
This object also introduces a context menu and allows the user to open a second image viewer, or to save the data as a 2-dimensional ASCII array.
Via drag and drop, the links to the z-interpretation and spatial transformation can be changed. The image object appears as in the project manager.

3.6 Bitmap

A bitmap data object stores any bitmaps which can be displayed with the bitmap viewer (see Section 4.4). The bitmap data object can have a link to the spatial transformation data object (see Section 3.3.1). Via this link, the pixel array of the bitmap is transformed into real space coordinates.
This object also introduces a context menu and allows the user to open a second bitmap viewer, or to copy the bitmap to the graphic export window (see Section 5.1).
The bitmap data object appears as in the project manager.

3.7 Graph

Graph data objects are used to store line graphs such as cross sections, spectra, and histograms. This object can store more than one line graph. The graphs are arranged in a 2-dimensional array. The graph data object is linked to a spatial transformation data object, showing the position of each graph in 3D space. In order to scale the x-coordinate of the line graph, a second transformation from a pixel array to a real physical quality is required. This x-transformation can be a spatial transformation, a spectral transformation, or a linear transformation data object. These values are interpreted by a corresponding interpretation data object. The y-coordinate of a line graph gets its unit by a link to a z-interpretation data object.
The context menu of this data object allows the user to open the line graph in a new graph viewer (see Section 4.5) and to save the data as ASCII text. The y-values of all line graphs are stored in one column. The x-values can be stored in a file with a second function in the context menu.
Via drag and drop, the unit of the y-values and the scaling of the two dimensional array can be changed.
This data object can appear as , , , , , or in the project manager.

3.8 Text

The text data object contains a formatted text. This object can be used to add a user comment to the project (see Section 4.6). In general, each measurement creates its own text object to store all relevant parameters. The object appears as in the project manager.

3.9 Color Profile

Color profile data objects store a color sequence for false color images (see Section 4.3). This object introduces a context menu, which allows the user to choose from among several default color tables and a number of color table cycles. Fig. 3.1 shows a selection of default color tables. The color profile object appears as in the project manager.

3.10 Filter

To reduce a spectrum with 1000 data points to single or multiple data points, filter data objects are required. These objects store all information required to perform a background subtraction and to calculate the desired qualities. The number of input and output parameters depend on the filter type.
The working area of every filter is defined by the limiting values x_{n_1} and x_{n_2}. The corresponding pixel numbers in the spectrum are n_1 and n_2. The unit of these spectral positions changes with the interpretation of the spectrum (see Section 3.4.2 and Section 3.7).

Before calculating images, all filters perform a background subtraction. This background B_i is computed with the measured intensity values I_i' and the spectral positions x_i outside the left and right borders of the working area.

$$I_i = I_i' - B_i \tag{3.1}$$

To avoid additional background noise, it is possible to average over a few data points outside the working area. Fig. 3.2 shows how the background B_i is computed. If the number of averages on both sides is larger than zero ($\Delta n_{lb} > 0$ and $\Delta n_{rb} > 0$), a linear slope is subtracted as the background (red line). If only averaging on one side makes sense, the background is a horizontal line (blue line). If no background subtraction is desired ($B_i = 0$), both numbers can be set to zero.

In addition, every filter stores the identification numbers of the data objects where the result (output parameters) is stored. In the event of a second calculation, it overwrites the old values.

3.10.1 Sum

The sum filter has only one output result (see. Equ. 3.2). The output unit is the same as the z-interpretation of the spectrum, e.g. CCD Counts (see. Section 3.4.2).

$$\text{Sum} = \sum_{i=n_1}^{n_2} I_i \tag{3.2}$$

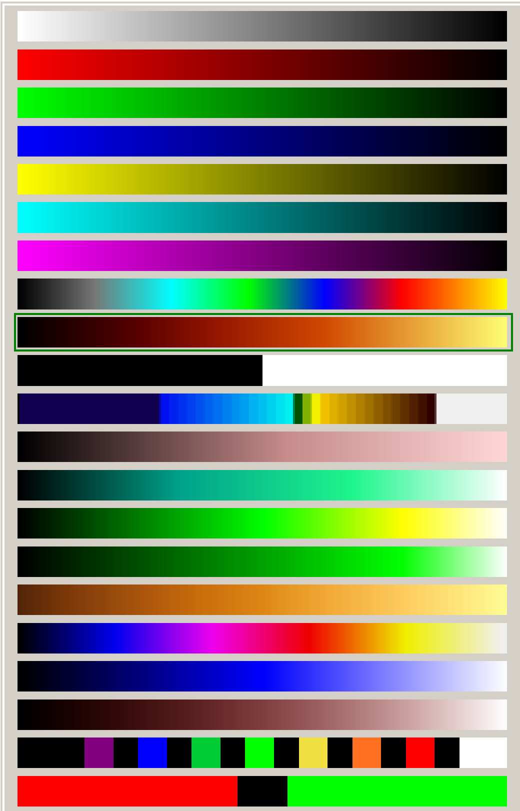


Fig. 3.1: Available color profiles.

3.10.2 Min and Max

The min and max filter can be used to find the extreme values and their spectral positions. The 4 output values of this filter are described in Equ. 3.3. The units of the extreme values are the same as the z-interpretation of the spectrum (see. Section 3.4.2). The units of their position have the same units as the filter's spectral positions.

$$\left.\begin{aligned}
\text{Minimum} &= \min\{I_i : n_1 \leqq i \leqq n_2\} \\
\text{Position of Minimum} &= \min\{x_i : I_i = \text{Minimum}, n_1 \leqq i \leqq n_2\} \\
\text{Maximum} &= \max\{I_i : n_1 \leqq i \leqq n_2\} \\
\text{Position of Maximum} &= \min\{x_i : I_i = \text{Maximum}, n_1 \leqq i \leqq n_2\}
\end{aligned}\right\} \tag{3.3}$$

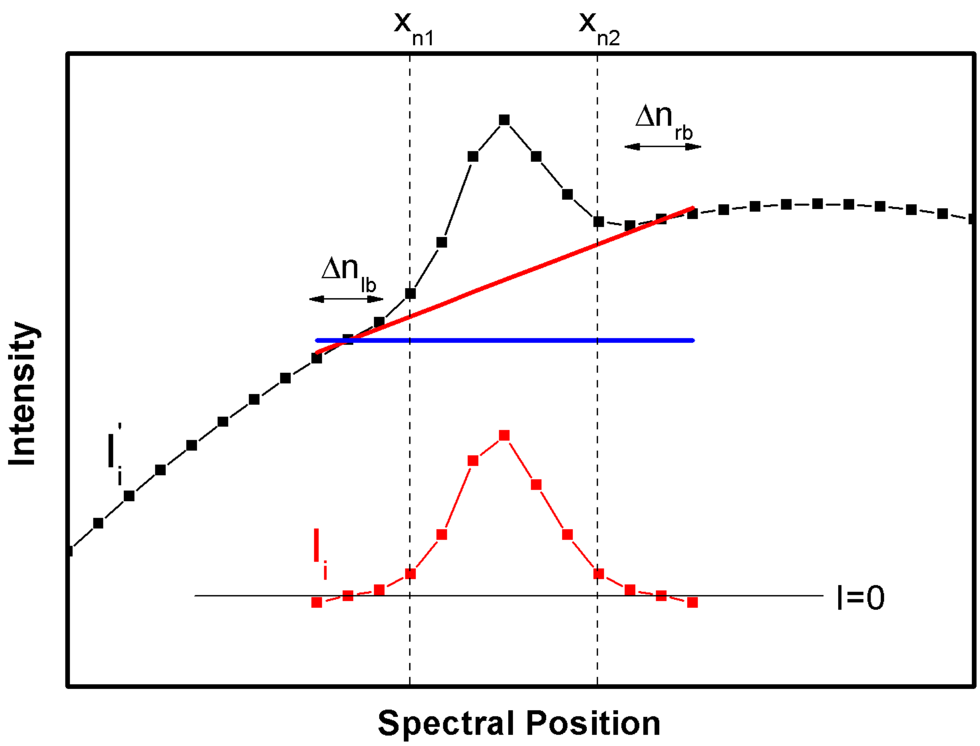


Fig. 3.2: Schematic diagram for background subtraction, black squares: original data $I_i^{'}$, red squares: corrected data I_i, red and blue line: background B_i calculated with ($\Delta n_{lb} = 3$, $\Delta n_{rb} = 3$) and ($\Delta n_{lb} = 3$, $\Delta n_{rb} = 0$).

3.10.3 Center of Mass

The center-of-mass filter calculates the intensity-weighted spectral position (see. Equ. 3.4). The output unit is determined by the spectral interpretation used.

$$\text{Center of Mass} = \frac{\sum_{i=n_1}^{n_2} x_i I_i}{\sum_{i=n_1}^{n_2} I_i} \tag{3.4}$$

3.10.4 Width

The width filter calculates the width of a selected peak. This filter needs an additional input parameter, which can be changed in the filter manager (see. Section 4.8). The parameter tells the algorithm at which level (e.g. 25% of the peak height) the width should be determined. The output parameter of the filter is the width of the selected peak in the units of the spectral position.

3.10.5 Average

This filter calculates the average intensity of a spectral range. The unit is given by the z-interpretation of the spectrum.

$$\text{Average} = \frac{\sum_{i=n_1}^{n_2} I_i}{n_2 - n_1 + 1} \tag{3.5}$$

3.10.6 Parabolic

This filter creates a parabolic fit for the selected peak. Equ. 3.6 is fitted to the data by the least squares method (Equ. 3.7).

$$y(x) = \text{Curvature}(x - \text{Center})^2 + \text{Intensity} \tag{3.6}$$

$$\sum_{i=n_1'}^{n_2'} (I_i - y(x_i))^2 = \min \tag{3.7}$$

The output parameters are curvature, center, intensity, and error (see. Equ. 3.8). The working area, fixed by the limits x_{n_1} and x_{n_2}, is only responsible for background subtraction and for finding the position of maximum intensity. The additional input parameter, width, sets the number of data points used for the fit.

$$\text{Error} = \frac{100\%}{n_2' - n_1' + 1} \sum_{i=n_1'}^{n_2'} \left| \frac{(I_i - y(x_i))}{y(x_i)} \right| \tag{3.8}$$

The width has the unit of the spectral interpretation (e.g. nm or $\frac{1}{cm}$). The pixel numbers n_1' and n_2' in Equ. 3.7 and Equ. 3.8 are calculated from the width and position of the maximum intensity.

Chapter 4

Viewers

Viewers are windows that display the data of the project. A viewer uses one or more data objects to show results. To obtain the desired information from a measurement, the various types of viewers are interconnected.

4.1 Viewer Positions

To organize the viewers in terms of size and position, WITec Project contains a cleanup tool, which can be activated by the Reset Viewers button.
Each viewer has its own rules. These rules can be changed and tested in the viewer positions options dialog. Fig. 4.1 shows this dialog. All changes in the rules will be automatically applied to the viewers. The left side of the dialog contains a list box of all available viewers. The rules of the highlighted viewer are shown and can be changed on the right side of the window. The user can select from among four different types. They are called None, Array, Cascade, and Single Position. Their behavior and parameters are explained in the following section.

None

The viewers remain unchanged. There are no parameters available.

Array

The viewers are sorted as an array. If not all viewers fit inside this array, the cleanup tool will start with a new cascaded array.

The cleanup tool does not check the new viewer positions. If the rules are not properly set, some viewers could be placed outside the desktop area. In this case, they are no longer accessible.

- **Left and Top**
  Left and top are the array start positions on the desktop.

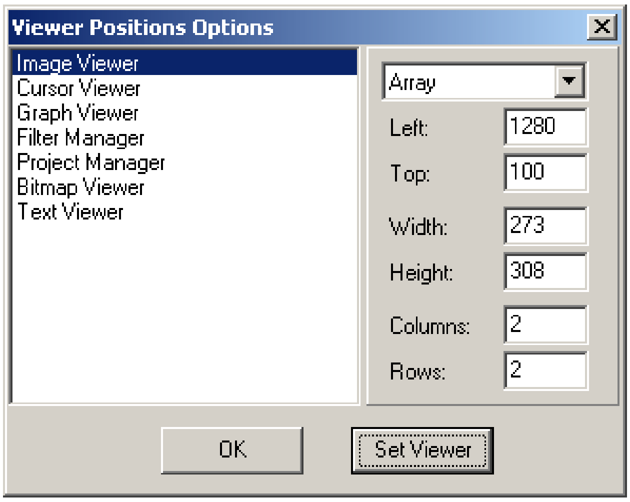


Fig. 4.1: Viewer positions options dialog.

- **Width and Height**
  The viewer's width and height can be changed with these parameters. If these parameters are set to zero, the viewer will maintain its default configuration.

- **Columns and Rows**
  The number of viewers inside the array can be changed with these parameters.

Cascade

The viewers are sorted as a cascade. If not all viewers fit onto the desktop, the cleanup tool will start again at the start position.

- **Left and Top**
  Left and top are the array start positions on the desktop.

- **Width and Height**
  The viewer's width and height can be changed with these parameters. If these parameters are set to zero, the viewer will maintain its default configuration.

- **Step Right and Step Down**
  Step right and step down are the increments of displacement in pixels for performing the cascade.

Single Position

The viewers are all set to the same position.

The cleanup tool does not check the new viewer positions. If the rules are not properly set, some viewers could be placed outside the desktop area. In this case they are no longer accessible.

- **Left and Top**
  Left and top are the array start positions on the desktop.
- **Width and Height**
  The viewer's width and height can be changed with these parameters. If these parameters are set to zero, the viewer will maintain its default configuration.

4.2 Project Manager

At the start of every project, the project manager is automatically added to the project. An additional project manager can be opened manually from the main menu with the function Add (see Section 2.2.2). The project manager displays a list of data objects that belong to the current project (see Chapter 3). The appearance of the project manager for a typical AFM measurement is shown in Fig. 4.2. The listed data objects contain the icon of the data object, followed by a short description of the object (called a caption). The order of the data objects can be changed in various ways. By including or excluding data categories, a selection of the current data objects can be displayed.
The project manager is the starting point for all drag and drop operations.
In Fig. 4.2, the data objects are sorted by categories. Fig. 4.2 (a) shows a default setting and Fig. 4.2(b) shows all data objects. In the project manager, image data objects, text data objects, cursors, and color profiles are listed. A detailed description of all data objects is given in Chapter 3.

4.2.1 Mouse Operations

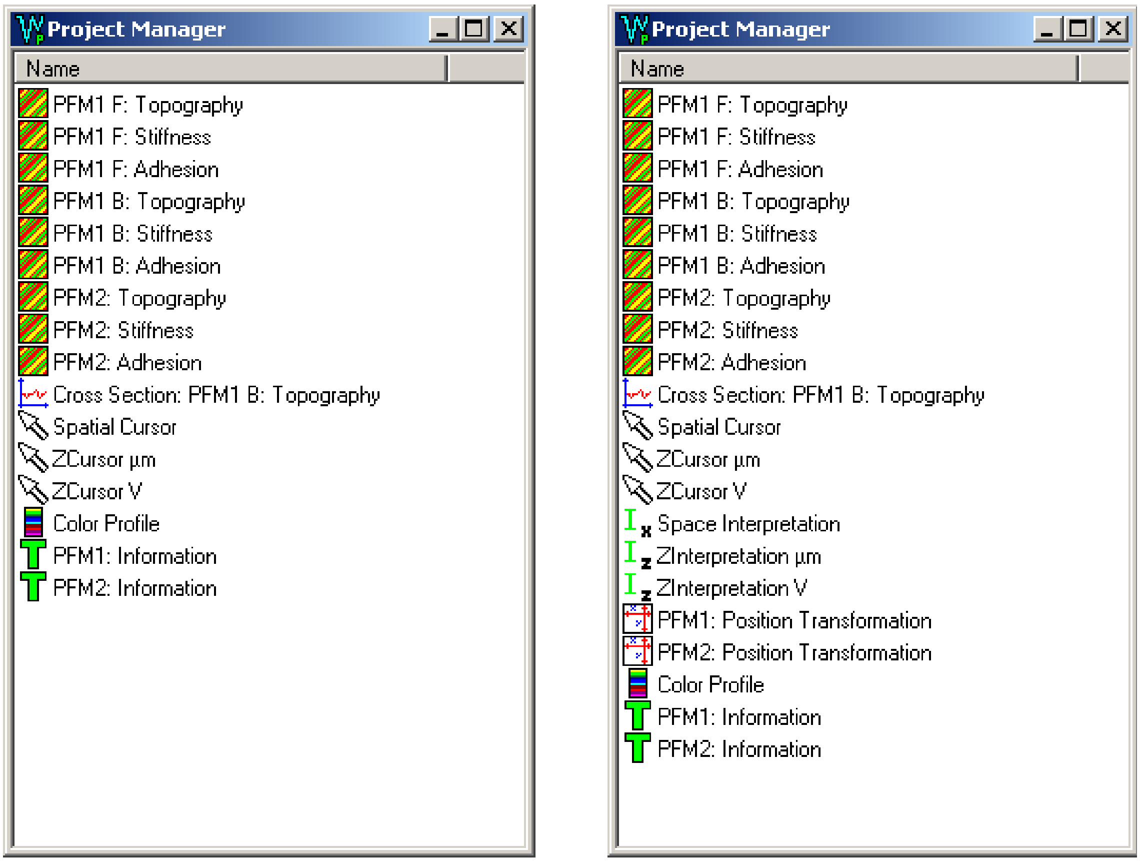
The list view of the project manager supports all standard Windows® mouse interactions.

Hint

Leaving the cursor over a data object for a short time causes a hint to appear, which describes its association with other data objects and viewers. This is a quick way to find out which other data objects and viewers use this data object.

Select

Clicking with the left mouse button on a data object selects a single data object. To select more than one data object press Ctrl on the keyboard and



(a) (b)

Fig. 4.2: Appearance of the project manager for a standard AFM measurement: show default selection of categories (a), show all categories (b).

select other data objects with the left mouse button. To select multiple data objects in a column, click with the left mouse button on the first object, then press the Shift on the keyboard and select the last object in the column. Ctrl and Shift can also be used in combination.

Double Click

Double clicking with the left mouse button on a data object causes the project manager to open the corresponding standard viewer (if available).

Rename Caption

An object is selected with a left mouse click. A second click on the caption will allow the caption name to be changed.

Drag and Drop Action

Select data objects, click on any selected item and keep the left mouse button pressed while dragging the mouse onto the desired drop zone. The appearance of the cursor changes if the selection is accepted by the drop zone. Releasing the mouse button will drop the data objects onto the drop zone, initiating the corresponding data operation.

4.2.2 Context Menu

The way data are displayed in the project manager can be chosen from a context menu. The context menu of the project manager opens by clicking the right mouse button. It contains the functions listed below. This menu can also be found in the main menu of the WITec Project software if the project manager window is activated.

File

The File function allows the user to add data objects to the project and to save a selection of data objects without any viewer.

- **Append Data**
  The Append Data function allows the user to append data objects to the project. The suffix of the data file is *.wid.

- **Save Data**
  The Save Data function allows the user to save selected data objects of a project. In addition, all necessary linked data are added to this data selection. All data objects are saved in a *.wid file.

Copy Data

This function copies the selected data objects and their linked data objects to the standard Windows® clipboard.

Cut Data

This function copies the selected data objects and their linked data to the standard Windows® clipboard and deletes the selected data objects in the current project.

Paste Data

This function copies the data objects from the standard Windows® clipboard to the current project.

If the standard Windows® clipboard contains data objects when the software is closed, it will be cleared. Copying data objects from the clipboard to the current project will change their internal identification numbers.

Delete Data

The Delete data function removes data objects from the project.

Do not delete data objects such as: interpretation, transformation, etc. They are required by image objects, graph objects, etc.

Show

The Show function enables the user to select which data objects are represented in the project manager.

▶ **Show All**
All categories are selected, therefore all data objects are shown in the list view of the project manager.

▶ **Hide All**
No categories are selected, all data objects are hidden.

▶ **Show Default**
Selects the default categories and displays only a selection of data objects in the project manager. Only data objects of primary interest are displayed.

▶ **Category**
Allows the user to make a selection of data object categories visible in the project manager. The data object categories are:

- Image ✓
- Filter
- Cross Section ✓
- Spectrum ✓
- Histogram ✓
- Cursor ✓
- Interpretation
- Transformation
- Cross Section Info ✓
- Look and Feel ✓
- Text ✓

The checked categories are selected by default. In Fig. 4.2, two representations of the project manager are displayed: (a) shows the project manager with Show Default setting and (b) shows the project manager with Show All setting.

Sort

This function changes the sorting of the data objects in the project manager.

- **by Name**
  All data objects are sorted in alphabetical order.
- **by Index**
  Data objects are sorted by their internal identification numbers. The most recently created data object will be the last in the list.
- **by Category**
  The data objects are arranged by categories as listed above. The example shown in Fig. 4.2 lists the data objects as sorted by categories.

Bring To Front

This function brings all viewers which are using the selected data object to the front. For a quick search of the selected data object, this function helps the user to see the desired window, which may have been hidden behind another window.

Data Object Specific Context Menu

If only one data object is selected, the data-specific object menu is linked to the context menu. This function contains operations specific to the data object (see Chapter 3), e.g. ASCII export and change of parameters.

4.3 Image Viewer

The image viewer allows the user to display image data objects with a false color profile. It is possible to change between a top view and a pseudo-3D representation of image data. To display an image, several data objects are required: image data object , color profile , spatial cursor , spatial interpretation , and their linked data objects (see Section 3). The image viewer window (an example is shown in Fig. 4.3) opens by double clicking with the left mouse button on an image data object in the project manager (see Section 4.2).
As an option, the user can link a bitmap data object to the viewer. This bitmap can be used as a color texture for the pseudo-3D representation.

This window is divided into three parts:

Title

The image window title contains the image symbol followed by the image description (data caption). Every change to the image data object will show up automatically in the image viewer. On the right side of the image window, the standard Windows® buttons are available: minimize, maximize, and close window. Closing the image viewer window will not delete the image data.

Image

The image displays an array of image data in false colors. In Fig. 4.3 the to-

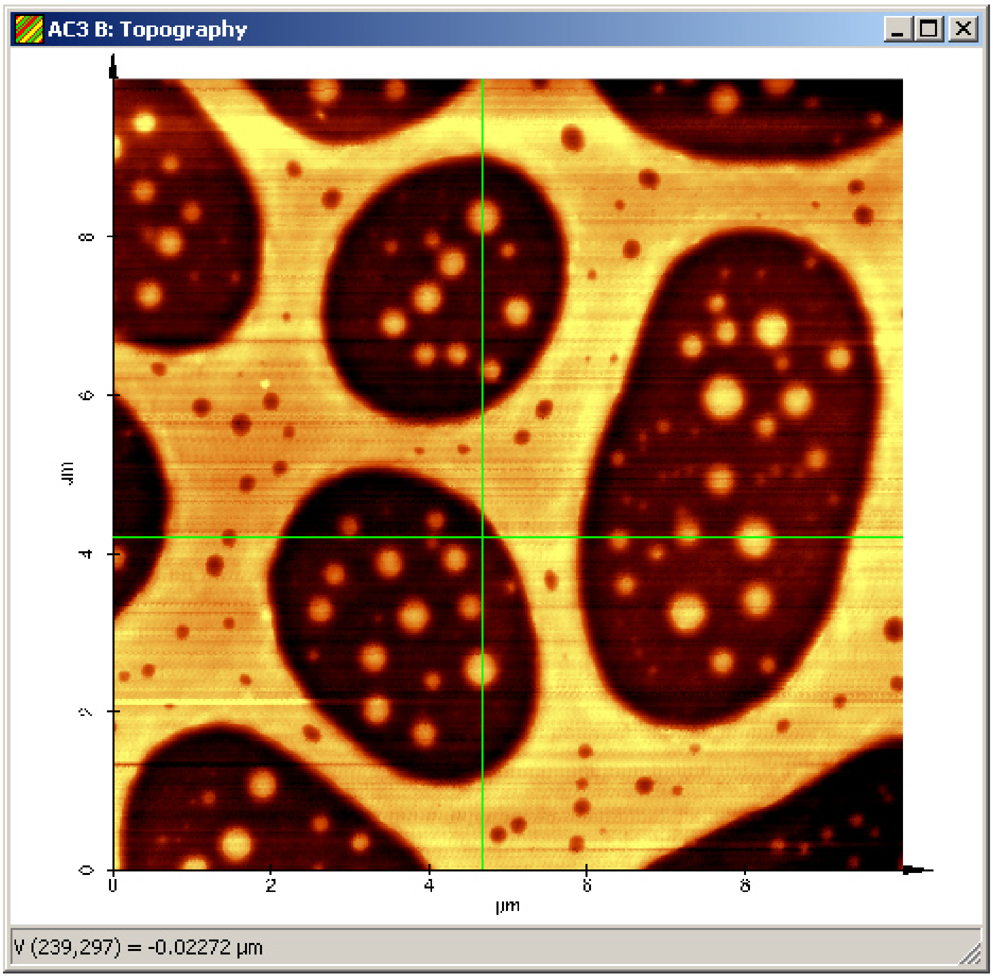


Fig. 4.3: Image viewer window.

pography of a polymer film is displayed, with bright colors representing high topographic features and dark colors representing low topographic features. The position of the mouse in the image is shown by green crosshairs.

Status Bar

The status bar at the bottom of the window shows the actual value of the third dimension at the center of the crosshairs. The third dimension can be height, as shown in Fig. 4.3, or any data stored in the z-interpretation data object linked to this image data object.

4.3.1 Context Menu

Clicking with the right mouse button inside the image viewer opens a context menu. It contains the functions listed below. This menu can also be found in the main menu of the WITec Project software (Action and Data). The context menu is split into two parts. The upper part refers to functionalities of the image viewer, whereas the bottom part refers to the used data objects. In this part, the context menu of each data object can be found. The upper part contains the following functions:

Export

The export function allows the image to be exported as a bitmap file.

▶ **Bitmap to File**
Saves the display of the image viewer as a bitmap file. A standard file dialog window opens to store the bitmap on the hard disk. A large variety of bitmap file versions are available (Section 5.1).

HINT Bitmap file storage is only possible if a correct extension is added to the file name (e.g. *.jpg for JPEG file or *.png for Portable Network Graphic file). For the export of images, the *.png file format is recommended. This format compresses the bitmap without any loss of data. If data loss is acceptable, the *.jpg file format is also a good choice.

▶ **Bitmap to Preview**
Copies the image to the graphic export window, where the bitmap can be changed before saving. A detailed description of the graphic export window is given in Section 5.1.

Make Texture Bitmap

This function creates a bitmap data object, which contains a bitmap of the currently set false color image. The size of the bitmap and the link to the spatial transformation data object are equal to that of the image data object. The bitmap data object is added to the current project.

Line Correction

The line correction function allows the represented image to be changed without changing the original data. The filters are only applied to the image viewer. The sub average and sub line filters apply to topography images, whereas the div average filter is used mainly for light intensity measurements. An overview of the line subtraction filters is shown in Fig. 4.4.

▶ **None**
Displays the raw image without line correction. In this case, many surface features might be hidden if the sample is not parallel with respect to the scan stage (Fig. 4.4(a)).

▶ **Sub Average**
Before determining the color and the 3D parameters for the displayed image, the average of each horizontal line is subtracted from the original data.

To preserve the characteristic value of the data, the total average of the image is added (Fig. 4.4(b)).

▶ **Div Average**
Before determining the color and the 3D parameters for the displayed image, the original data points are divided by the average of each line. To preserve the characteristic value of the data, the total average of the image is multiplied (Fig. 4.4(c)).

▶ **Sub Line**
Before determining the color and the 3D parameters for the displayed image, a linear slope, calculated from the current line by linear regression, is subtracted from the original data points. To preserve the characteristic value of the data, the total average of the image is added (Fig. 4.4(d)).

HINT Raw data is not changed when line corrections are applied. Line correction is only active in the image viewer. Other image viewers linked to the same data object can use a different line correction type.

Draw Field

An empty boolean overlay, called a draw field, is present on top of each displayed image. Using draw tools, it is possible to draw in this overlay. The overlay has the same pixel size as the image data. If a pixel of the overlay is set, the color of the image is inverted. Fig. 4.5 (a) shows an example of draw options in the draw field of an image. For a more detailed description of the draw tools, refer to the mouse mode descripton in this section. The draw field submenu contains the following functions:

▶ **Clear**
The Clear function clears the draw field.

▶ **Invert**
The Invert function inverts the draw field.

▶ **Make Image**
The Make Image function creates a logical image based on the draw field (as shown in Fig. 4.5 (b)). This image can be used as an inclusion area for data analysis (Section 7.1).

Mouse Mode

The mouse mode lists a selection of operations that can be performed with the mouse. A quick selection of mouse modes is possible in the toolbar of the image tools window (Section 4.3.4).

The following mouse operations are available:

▶ **Move**
If this mode is active, the mouse moves the crosshairs across the image. In

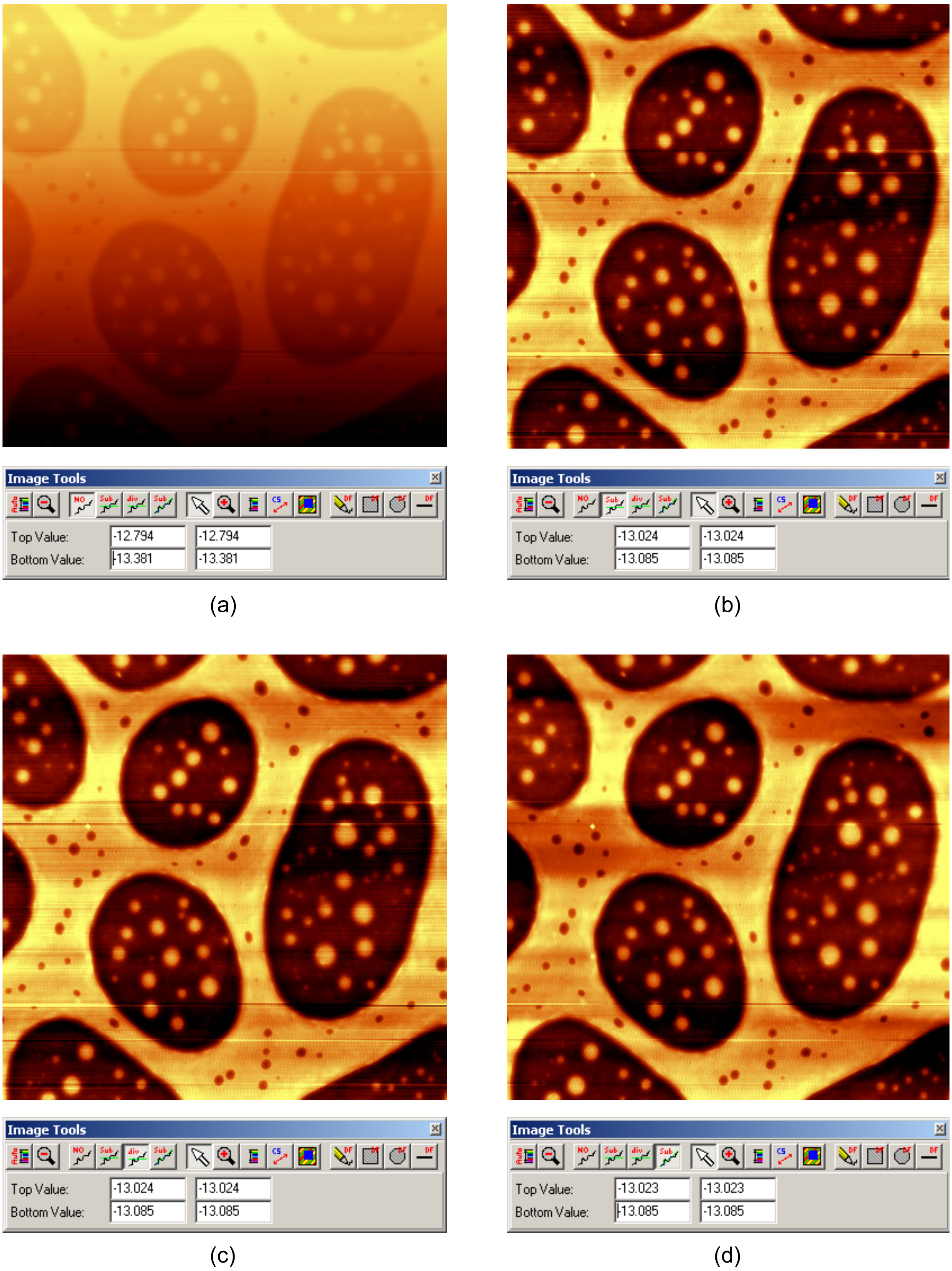


Fig. 4.4: Examples of line correction filters: no subtraction (a), average subtraction (b), average division (c), and line subtraction (d).

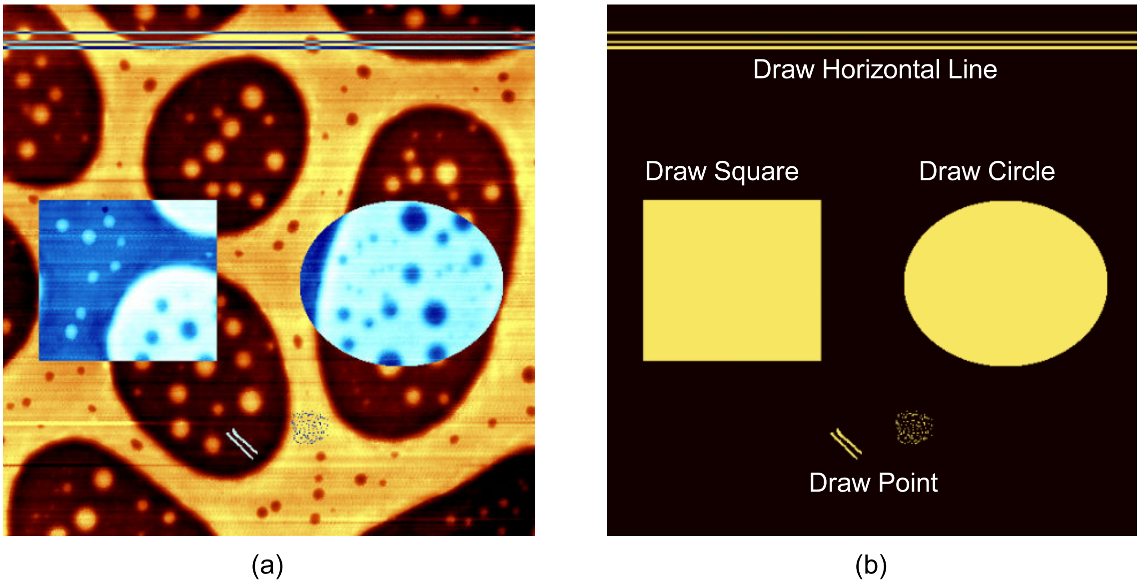


Fig. 4.5: Draw field operations (a) draw objects with the draw field mouse functions, (b) make a logical image (draw field image) using the objects drawn in (a).

the status bar, the value at the current data position is displayed in units of the z-interpretation.

- **Zoom**
  The zoom mode enables the user to enlarge areas of the image. If this mode is active, the mouse can be dragged over the image as in the move mode. However, as soon as the left mouse button is pressed, a square opens, showing the area to be zoomed in. Releasing the mouse button will automatically display the enlarged area in the image viewer with the appropriate image scaling. For a precise zoom, the size of the zoom box can be monitored in the cursor viewer (Section 4.7).

- **Draw Point**
  Draw point allows the user to select points in the draw field of an image as shown in Fig. 4.5 (a). If this mouse mode is active, every left mouse click will draw a point on the image.

HINT All draw field mouse operations can be inverted by pressing the Shift key.

- **Draw Square**
  Draw square allows the user to draw squares in the draw field of an image as shown in Fig. 4.5 (a). Move the mouse to the upper left corner of the square, press and hold the left mouse button and move the cursor to the lower right corner. The square becomes active upon releasing the mouse button. More than one square can be drawn on an image.

- **Draw Circle**
  Draw circle allows the user to draw circles or elliptical forms on the image as shown in Fig. 4.5 (a).

- **Draw Horizontal Line**
  Draw horizontal line allows the user to draw horizontal lines in the image as shown in Fig. 4.5 (a). If this mouse function is active, every click with the left mouse button draws a horizontal line on the image. To remove a horizontal line, press Shift on the keyboard and click on the line with the left mouse button.

- **Define Cross Section**
  The define cross section mouse mode allows the user to define which line in the image is to be analyzed. The starting point of the line is defined by pressing the left mouse button, while releasing it defines the end point. A cross section data object with the symbol is created and added to the project. For more details on cross sectional analysis see Section 7.1.14.

- **Scale Color**
  If the scale color mode is active, a click on the image with the left mouse button will set the top value for color scaling (see Section 4.3.4), while the same action together with the Shift key sets the bottom value.

- **Marker**
  In this mouse mode, information from a selected area can be sent to all data objects and viewers. This is helpful if a new scan area must be defined.

Show

The show function allows the user to select how the image is to be displayed. The default setting shows the images as 2D top view images with false color coding and x-y axes. The sub menu with the following settings is available:

- **Coordinate System**
  Determines whether the coordinate system is displayed or not.

- **Z Axis**
  Determines whether the z-axis is displayed or not.

- **As 3D Image**
  If this function is checked, the image appears as a 3D image.

- **Use Bitmap Color**
  Uses the linked bitmap data object as a color texture instead of calculating the color from the image data using the scaling parameters and the color profile.

Automatic Color Scale

The top and bottom values for color scaling and 3D scaling are set to appropriate values by clicking with the left mouse on the scale color function.

Zoom Out 

Clicking this button will zoom out to show all data of the image data object.

Camera

In the camera submenu, the properties of the camera can be changed. The following menu items are available:

- **Camera Top View**
  The camera top view displays the image as seen from above.
- **Camera Side View**
  The camera side view displays the image as seen from a standard side view. To change the view angle of the camera, please read the details of key operations (see Section 4.3.2).
- **Projection**
  The projection function allows the user to display the image in either orthogonal or perspective projection.

4.3.2 Key Operations

This section lists keyboard operations associated with the image viewer.

Page Up and Page Down

Image data objects from the project are toggled in the image viewer. The displayed images change along with the image viewer window title. Any existing link to a bitmap data object will be cleared.

Arrows Up and Arrows Down

Tilts the image in the image viewer from top view to side view.

Arrows Left and Arrows Right

Rotates the image in the image viewer.

4.3.3 Drop Operations

Changes to the linked data objects can be performed by following the drag and drop procedure described in Section 4.2.1. The drop zone for the image viewer is the image area. The following data objects can be dropped onto the image viewer:

Image Data Object

Performing this drop operation will display the new image in the image viewer. This procedure deletes the draw field.

Spatial Cursor Data Object

Performing this drop operation will switch between cursors.

HINT This operation is primarily for advanced users and only necessary if working with more than one spatial cursor in the same project.

Spatial Interpretation Data Object

Performing this drop operation will exchange the spatial interpretation.

Color Profile Data Object

Performing this drop operation will change the color profile in the selected image viewer.

Bitmap

Performing this drop operation will change or set the link to a bitmap data object. The bitmap data object must have the same size and the same link to the spatial transformation object as the currently set image data object. Otherwise, the bitmap data object will be rejected.

4.3.4 Image Tools

The image tools enable the user to change the display of image data in the image viewer. The original data remain unchanged. The image tools window can be opened from the main menu of the WITec Project software as described in Section 2.2.3. The image tools window is shown in Fig. 4.6.

The toolbar provides quick access to line corrections, mouse operations, and automatic scaling functions as described in the context menu of the image viewer (Section 4.3.1).

Fig. 4.6: Image tools window.

The panel below the toolbar contains a user interface, required to modify the top and bottom values for the color scale, and the 3D scale. These values refer to the last active image viewer.

The left column of edit boxes refers to the color scaling of the image. All image data values larger than the top value are represented with the last color in the color profile. All values below the bottom value are represented with the first color in the color profile. Image data values in between the limits are colored via a linear model.

The right column of edit boxes refers to the 3D representation of the image. The height of the 3D representation can be changed by varying the top and bottom values.

4.4 Bitmap Viewer

The bitmap viewer allows the user to display bitmap data objects. If the linked bitmap data object is a scaled bitmap and has a link to a spatial transformation data object, this viewer can be used to transfer positions or regions to the project via a spatial cursor data object. Therefore, the viewer also has a link to a spatial cursor data object. Every change of the bitmap data object will show up automatically in the bitmap viewer.
The bitmap viewer window (an example is shown in Fig. 4.7) opens by double clicking with the left mouse button on a bitmap data object in the project manager (see Section 4.2).

This window is divided into three parts:

Title

The bitmap viewer title contains the bitmap symbol  followed by the bitmap description (data caption). On the upper right side of the bitmap window, the standard Windows® buttons are available: minimize, maximize, and close window. Closing the bitmap viewer window will not delete the bitmap data.

Bitmap

The bitmap is shown in the center of the windows. It automatically expands to the maximum size of the window. The position of the mouse in the bitmap is shown by green crosshairs. If the bitmap is scaled the viewer shows a scale bar in the lower left corner.

Status Bar

The status bar at the bottom of the window shows the pixel position at the center of the crosshairs.

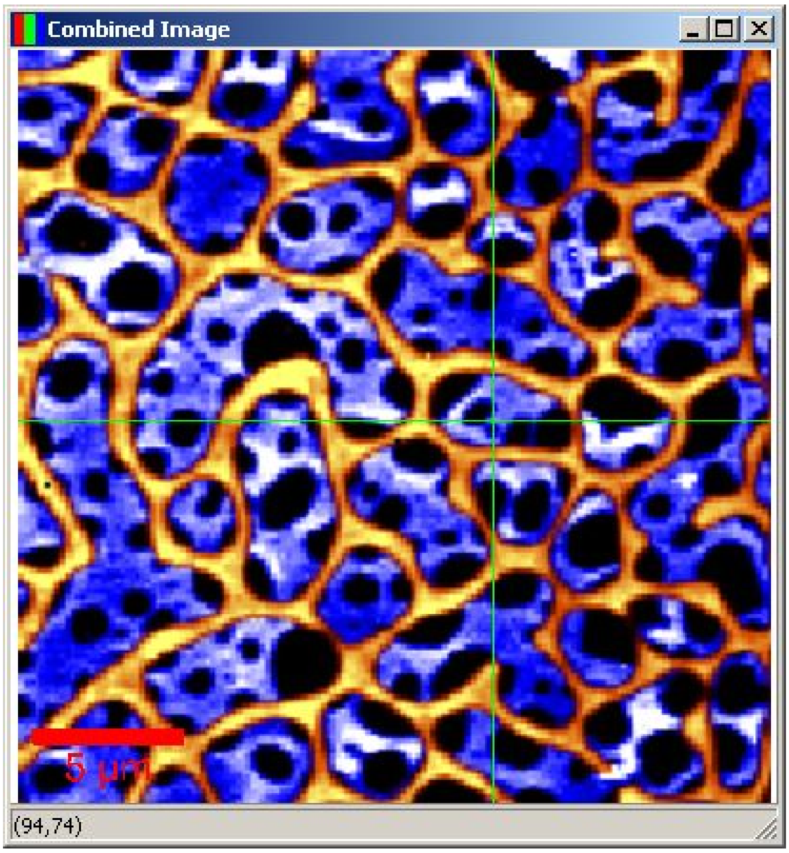


Fig. 4.7: Bitmap viewer window.

4.4.1 Context Menu

Clicking with the right mouse button inside the bitmap viewer opens a context menu. It contains the functions listed below. This menu can also be found in the main menu of the WITec Project software (Action and Data). The context menu is split into two parts. The upper part refers to functionalities of the image viewer, whereas the lower part refers to the used data objects. In this part, the context menu of each data object can be found. The upper part contains the following functions:

Export

The export function allows the display to be exported as a bitmap.

- **Bitmap to File**
  Saves the display of the bitmap viewer as a bitmap file. A standard file dialog window opens to store the bitmap on the hard disk. A large variety of bitmap file versions are available (Section 5.1).

HINT Bitmap file storage is only possible if a correct extension is added to the file name (e.g. *.jpg for JPEG file or *.png for Portable Network Graphic file). For the export of images the *.png file format is recommended. This format compresses the bitmap without any loss of data. If data loss is acceptable, the *.jpg file format is also a good choice.

- **Bitmap to Preview**
  Copies the display of the bitmap viewer to the graphic export window, where the bitmap can be changed before saving. A detailed description of the graphic export window is given in Section 5.1.

Mouse Mode

The mouse mode lists a selection of operations that can be performed with the mouse. The following mouse operations are available:

- **Move**
  If this mode is active, the mouse moves the crosshairs across the display. In the status bar, the current pixel position is displayed.
- **Marker**
  In this mouse mode, information from a selected area can be sent to all data objects and viewers. This is helpful if a new scan area must be defined.

Show

The show function allows the user to select how the image is to be displayed. The sub menu with the following settings is available:

- **Scale Bar**
  Determines whether the scale bar is displayed or not.

Change Scale Bar Color

This function allows the user to change the color of the scale bar.

4.4.2 Drop Operations

Changes to the linked data objects can be performed by following the drag and drop procedure described in Section 4.2.1. The drop zone for the bitmap viewer is the display area. The following data objects can be dropped onto the bitmap viewer:

Bitmap Data Object

Performing this drop operation will display the new bitmap in the bitmap viewer.

Spatial Cursor Data Object

Performing this drop operation will switch between cursors.

HINT This operation is primarily for advanced users and only necessary if working with more than one spatial cursor in the same project.

4.5 Graph Viewer

The graph viewer allows the user to display graph data objects such as cross sections, spectra, and histograms. The expression graph will be used for a function of type $y = f(x)$. A graph data object can contain more than one graph belonging to various positions or different times. To display a sequence of graphs, the graph viewer stores the graph data object, an x-interpretation, an x-cursor, a sequence cursor, and their linked data objects. The x-interpretation contains the unit of the x-coordinate. The x-cursor is used to move along the x-axis. To display the various graphs along a sequence, the sequence cursor is used.

The graph viewer opens by double clicking with the left mouse button on a graph data object in the project manager (see Section 4.2). The link to the additional data objects, as described above, is automatically performed. A graph viewer can display more than one graph data object. The active graph data object can be selected from the graph tools window (described later in this chapter).

The graph viewer is shown in Fig. 4.8. The window is divided into three parts:

Title

The graph window title contains the icon followed by the active graph description (data caption). Every change to the graph data object will show up automatically in the graph viewer. On the upper right side of the graph window, the standard Windows® buttons are available: minimize, maximize, and close window. Closing the graph viewer window will not delete the graph data.

Display

The display shows an x-y coordinate system in which the graph data object is represented as a line graph. If the graph data object contains a sequence of graphs, the last graph defined by the sequence cursor is displayed. The y-axis has the unit of the active graph data object.

The position of the mouse in the graph viewer is shown by green crosshairs. This position is copied to the x-cursors.

Status Bar

The status bar at the bottom of the window shows the actual y-value at the center of the crosshairs in the units of the active graph data object.

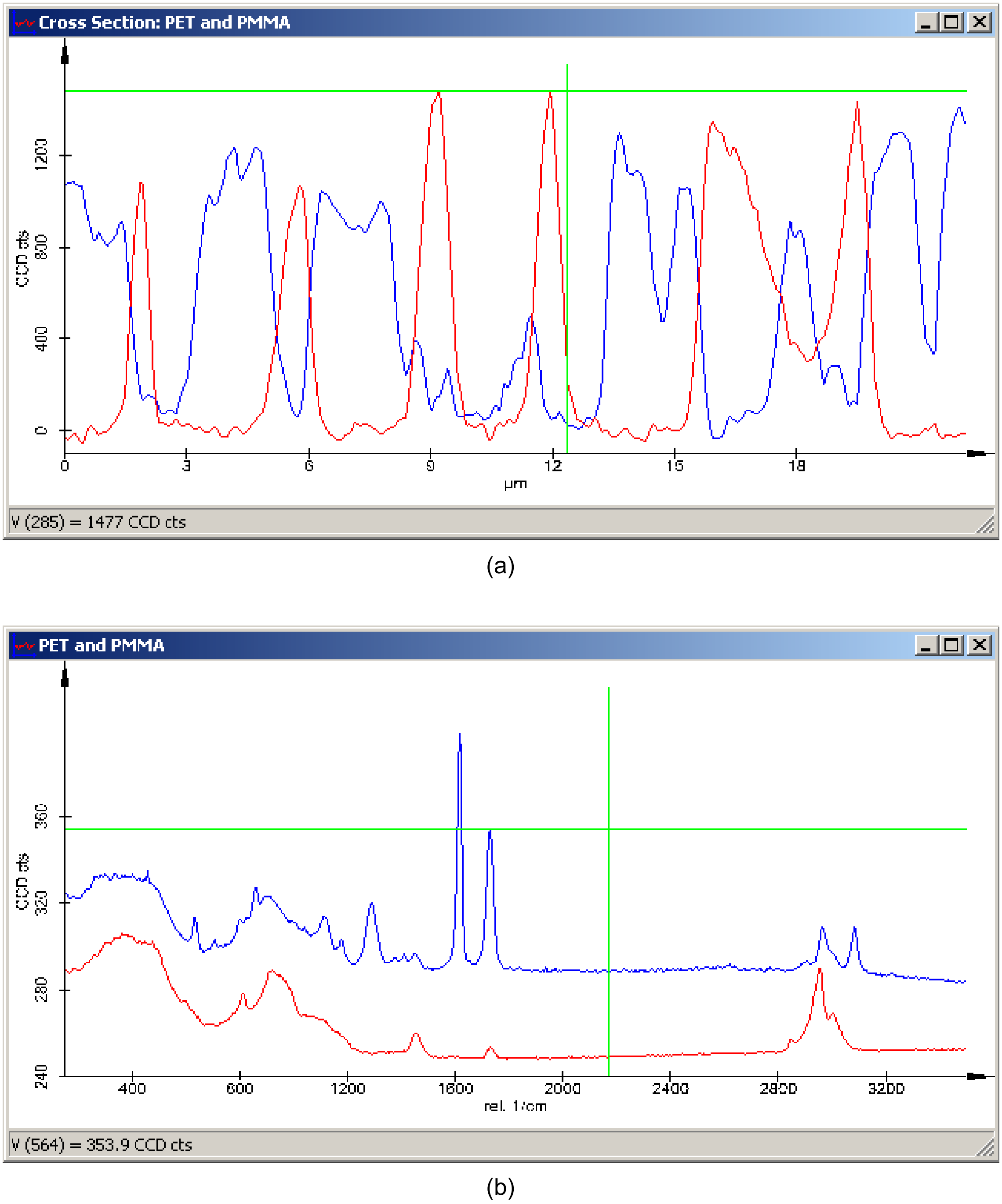


Fig. 4.8: Appearance of the graph viewer for: a cross section (a) and a spectrum (b).

4.5.1 Context Menu

Clicking the right mouse button inside the graph viewer opens a context menu. It contains the functions listed below. This menu can also be found in the main menu of the WITec Project software (Action and Data). The context menu is split into two parts, the upper part refers to functionalities of the image viewer (Action), whereas the lower part refers to the used data objects (Data). In this part, the context menu of each used data object can be found.

The upper part of the context menu contains the following functions:

Export

The export function refers to the export of the represented graph in the graph viewer.

▶ **Bitmap to File**
Saves the display of the graph viewer in a bitmap file. A standard file dialog window opens to store the bitmap on the hard disk. A large variety of bitmap file versions are available (Section 5.1).

HINT Bitmap file storage is only possible if a correct extension is added to the file name (e.g. *.jpg for JPEG file or *.png for Portable Network Graphic file). For the export of graphs, the *.png file format is recommended. This format compresses the bitmap without any loss of data.

▶ **Bitmap to Preview**
Copies the display of the graph viewer to the graphic export window, where the bitmap can be changed before saving. A detailed description of the graphic export window is given in Section 5.1.

▶ **ASCII to File**
With this function, the represented graph of the active sequence can be saved in ASCII format on the hard disk.

▶ **ASCII to Clipboard**
Saves the represented graph of the active sequence in ASCII format to the clipboard.

Mouse Mode

The mouse mode lists a selection of operations which can be performed with the mouse. The following mouse operations are available:

▶ **Move** 
If this mode is active, the mouse moves the crosshairs over the graph. In the status bar, the current value of data is displayed with the unit defined by the linked z-interpretation of the active graph.

- **Zoom**
  The zoom mode enables the user to enlarge areas of the graph. If this mode is active, the mouse can be dragged over the graph as in the move mode. However, as soon as the left mouse button is held pressed, a square opens, showing the area to be zoomed in. Releasing the mouse button will automatically display the enlarged area in the graph viewer with the appropriate graph scaling.
- **Marker**
  The marker function will select a range of data in the graph viewer.

Zoom

The zoom function lists a selection of zoom out operations. The following zoom out functions are available:

- **Zoom out**
  The zoom out fits the graph with its full x-y range to the graph window.
- **Zoom out X**
  Zoom out X keeps the y-axis as is and fits the graph to the full range of the x-axis.
- **Zoom out Y**
  Zoom out Y keeps the x-axis as is and fits the graph to the full range of the y-axis.

Change Graph Color

This function allows the user to change the color of the active graph data object. A standard Windows® color dialog will be opened.

Only one Y Scale

If this function is active, all graph data objects connected to the graph viewer use the same y-scale.

4.5.2 Key Operations

If the graph viewer contains a graph data object with a sequence of graphs, the arrows up/down and left/right move along the sequence.

4.5.3 Drop Operations

Changes to the linked data objects can be performed by following the drag and drop procedure described in Section 4.2.1. The drop zones for the graph viewer are the title and the display area. The following data objects can be dropped onto the graph viewer:

Cursors

Performing this drop operation will switch between cursors.

HINT This operation is primarily for advanced users and only necessary if working with more than one cursor of the same kind in the same project.

X-Interpretation

Performing this drop operation will exchange the x-interpretation.

Graph Data Object

Performing this drop operation will add a graph to the viewer.

HINT The unit of the x-coordinate of the graph determines whether or not the cursors, interpretations, and additional graphs can be accepted for the drop operation.

4.5.4 Graph Tools

The graph tools enable the user to change the display of graph data in the graph viewer. The original data remain unchanged. The graph tools window can be opened from the main menu of the WITec Project software as described in Section 2.2.3. The appearance of the graph tools window is shown in Fig. 4.9.

The toolbar provides quick access to zoom out and mouse operations as described in the context menu of the graph viewer.

The panel below the toolbar contains a user interface to change the top and bottom values for the x- and y-axes. These values refer to the last active graph viewer. In the right column, all graph data objects linked to the viewer are listed. The active graph data object is highlighted. By clicking with the mouse, the active graph data object can be changed.

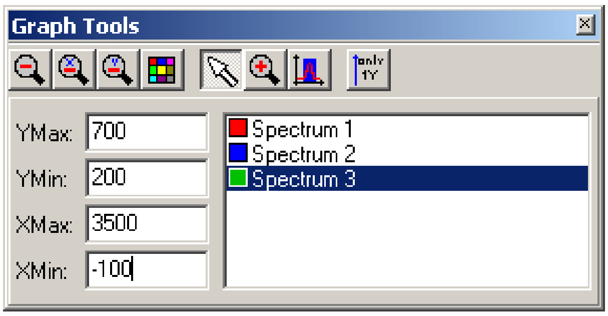


Fig. 4.9: Graph tools window.

4.6 Text Viewer

The text viewer displays the text data objects of a project and can be used to add text information to a project. Double clicking with the mouse on a text data object in the project manager will open the text viewer window. In general, every measurement creates a text data object containing all measurement-specific parameters. An additional text data object together with the corresponding text viewer window can be opened from the main menu with the function Add (see Section 2.2.2).

The text viewer window is shown in Fig. 4.10. It is divided into three parts:

Title

The text window title contains the text symbol followed by the text description (data caption). Every change to the text data object will show up automatically in the text viewer. On the upper right side of the image window, the standard Windows® buttons are available: minimize, maximize, and close window. Closing the text viewer window will not delete the text data.

Toolbar

The toolbar contains standard text formatting functions:

- **Bold fonts**
  Allows the user to use bold fonts for the text.
- **Italic fonts**
  Allows the user to use italic fonts for the text.
- **Underlined fonts**
  Allows the user to use underlined fonts for the text.
- **Align left**
  Aligns the text along the left border.
- **Align center**
  Centers the text.
- **Align right**
  Aligns the text along the right border.
- **Select fonts**
  Displays a selection of fonts.
- **Select font size**
  Allows the user to select the font size.
- **Format fonts**
  Opens the standard Windows® text formatting window, allowing the user to select the font type, format, size, and color.

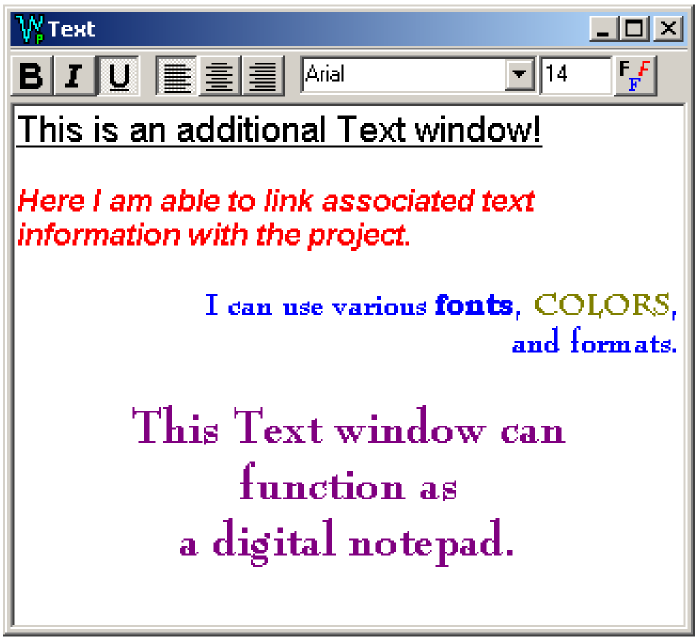


Fig. 4.10: Appearance of the text viewer window displaying a new text data object.

Text

The text field displays text messages and allows the user to edit additional text. Fig. 4.10 shows an example of text editing and formatting.

HINT Selecting the paragraph and using the keys Ctrl + C will copy the paragraph to the clipboard. Using Ctrl + V in word processing programs will paste the paragraph along with format settings.

4.7 Cursor Viewer

Cursor viewers are required to display the position of a measured data point and to measure differences between two data points. Cursor viewers can be opened by double clicking on a cursor data object in the project manager. Fig. 4.11 shows the appearance of cursor viewers, a spatial cursor viewer (a), and a z cursor viewer (b).

Each measured quantity has its own cursor data object  (see Section 3.2). Other viewers such as image viewer and graph viewer change the current position of the cursor data objects. This change is automatically displayed in the cursor viewer. Clicking the left mouse button sets a reference point, which is used to calculate the difference to the current cursor position.

The cursor viewer uses the local interpretation of the sender (image viewer, graph viewer, etc.) to display the units. For internal communication, the program uses standard units (e.g. time: seconds, space: μm). This avoids errors when different interpretations are used (Section 3.4).

The cursor viewer window contains two parts:

Title

The title of the cursor viewer displays the cursor icon followed by the cursor description (data caption). On the upper right side of the image window, the standard close window button is available. Closing the cursor window will not delete the cursor data objects.

Data Panel

The data panel contains data in two columns.
The left column displays the current quantity. The right column displays the difference between a reference point and the current position. Multidimensional cursors display the radial distance between data points in the last row as shown in Fig. 4.11(a) for the spatial cursor viewer.

HINT With a left mouse click, a position in the image or graph viewer is marked as a reference point. This will set the data in the right column of the cursor viewer to zero. Moving the mouse inside an image or graph viewer will display the difference between the actual mouse position and the reference point.

4.7.1 Drop Operations

Following the drag and drop procedure described in Section 4.2.1, changes to the linked data objects can be made. The drop zone for the cursor viewer is the title area. Cursor data objects can be dropped onto the cursor viewer, producing a new display of the cursor viewer.

(a) (b)

Fig. 4.11: Appearance of the cursor viewer displaying: a spatial cursor viewer (a) and a z cursor viewer (b).

4.8 Filter Manager

The filter manager organizes a collection of filter data objects. If these are applied to a sequence of a graph data object, the information in the graphs is reduced to a few values. These values can be represented as images or line graphs. The filter manager has a link to the graph data object to be evaluated. In addition, a cursor and a list of filters are linked to the filter manager.
The filter manager is created at the beginning of a measurement. If the filter manager is closed, a new or an additional filter manager can be opened from the main menu with the function Add (see Section 2.2.2).
Filter data objects can be added to the collection of the filter manager. The working area and the parameters of the filters can be modified. The collection of filters can be saved to the file system. Saved collections of filters can be appended to a project and linked to the filter manager.
The filter manager is shown in Fig. 4.12. The filter manager displays a list of filter data objects linked to the sequence of a graph data object (see Chapter 3.10). The filter manager window is divided into four parts:

Title

The title contains the data caption of the used graph data object. On the upper right side of the filter manager window, the standard Windows® buttons are available: minimize, maximize, and close window. Closing the filter manager window will not delete the data, however, the links between the data objects are lost.

Toolbar

The toolbar provides quick access to the functions of the context menu.

Filter List and Filter Parameters

The filter data objects are listed in the filter manager. The first column contains the icon of the filter data object, followed by the name of the filter. The following two columns display the start and end positions of the filters. Depending on the type of filter, additional parameters are listed in the panel on the right (see Section 3.10).

Lock Filter

An active filter can be changed only if this box is unchecked.

Start and Stop Position

The edit boxes for the start and stop positions (working area) of the filter can be changed manually or by using the marker mouse mode of a graph viewer (see Section 4.5). Above the edit boxes, the name of the active filter is displayed.

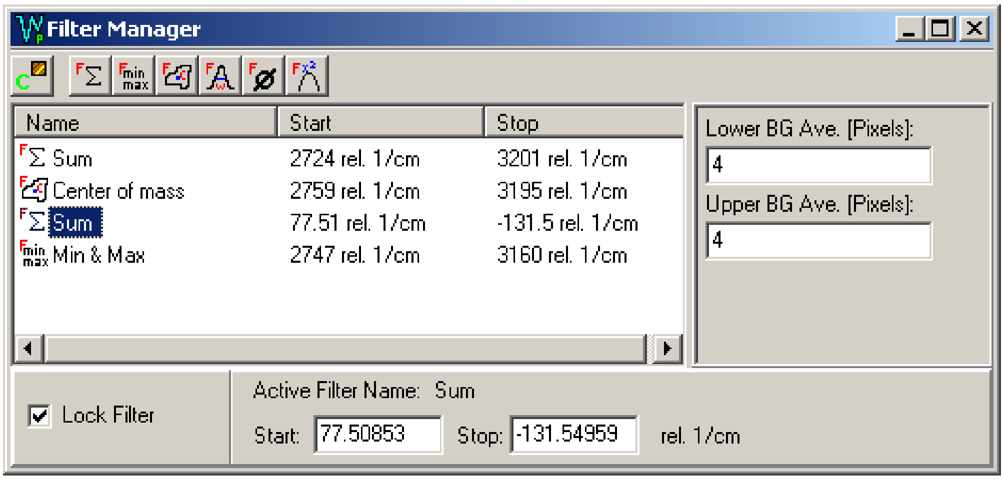


Fig. 4.12: Appearance of the filter manager.

4.8.1 Context Menu

Clicking the right mouse button inside the list view of the filter manager opens a context menu, which contains the functions listed below. This menu can also be found in the main menu of the WITec Project software (Action and Data). The context menu is split into two parts, the upper part refers to functionalities of the filter manager (Action), whereas the lower part refers to the used data objects (Data). In this part, the context menu of each used data object can be found.

Calculation

Recalculates all data.

Add Filter

In the submenu Add Filter the following filter data objects are available and can be added to the filter manager: Sum , Minimum Maximum , Center of Mass , Width , Average , and Parabolic . A detailed description of the filter data objects can be found in Section 3.10.

File

Allows the user to append filters to the filter manager and to save the collection of filters. The file format is *.wid.

4.8.2 Drop Operations

The filter manager contains two drop zones: the title bar and the calculation button in the toolbar.

Dropping a spectrum data object or a cursor data object onto the title bar will change the link to the data objects. Dropping filter data objects onto the title will add the filter to the filter manager.

To perform a calculation without changing the link of the graph data object, another graph data object can be dropped onto the calculation button in the toolbar.

Chapter 5

Export

In this chapter, the export of data from the WITec Project software is described. The first section covers the export of data bitmap files, whereas the second section deals with ASCII export.
At various places in the WITec Project software, bitmaps can be exported to files or displayed in a preview. Both functions copy the bitmap to the graphic export window. The function Bitmap to File will automatically start the save process of the graphic export window. Bitmap to Preview will show the graphic export window.

5.1 Graphic Export

The graphic export window shown in Fig. 5.1 is a preview for bitmaps that provides some additional tools. In addition, the graphic export can load and save bitmaps from the file system or clipboard.
The size of the graphic export window can be changed using the standard Windows® mouse functions.

The graphic export window is divided into four parts:

Title

The window title contains the logo followed by the description of the window. On the left side, the standard Windows® functions for minimize, maximize, and exit are available. Closing the graphic export window will not delete the bitmap.

Toolbar

The toolbar of the graphic export window provides access to the functions listed below (from left to right).

- **Save File**
  Saves the bitmap from the graphic export window to the file system. The following file formats are available: JPEG file (*.jpg and *.jpeg), BITMAP file (*.bmp), TIFF file (*.tif and *.tiff), and Portable Network Graphic file (*.png).

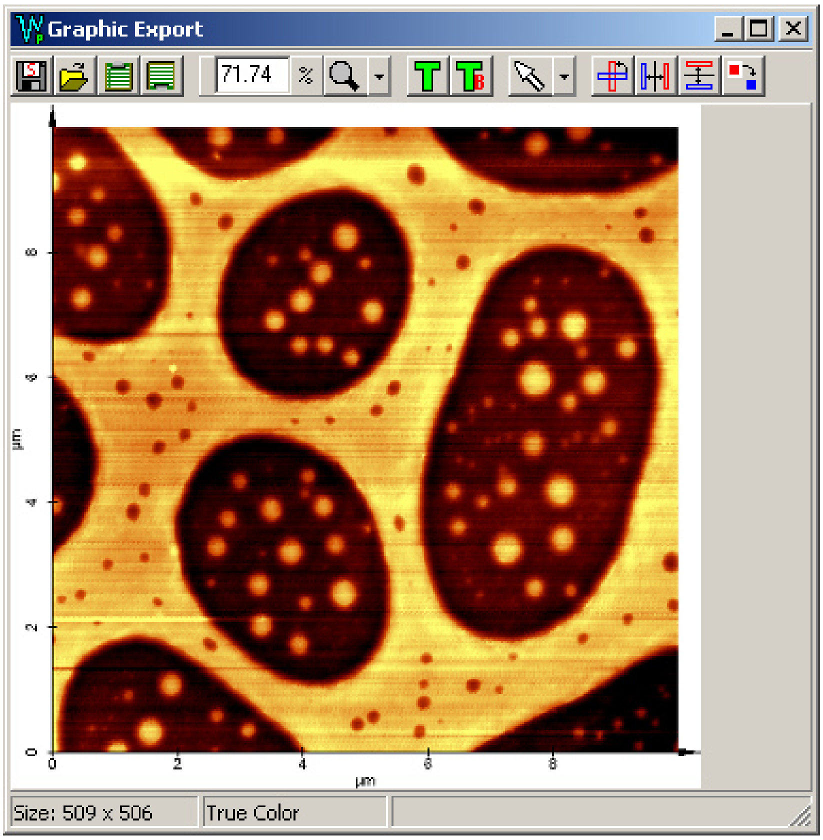


Fig. 5.1: Appearance of the graphic export preview window.

▶ **Open File**
Loads a bitmap file from the file system into the graphic export window.

▶ **Clipboard**
Saves the displayed bitmap to the clipboard. If an area of the bitmap is selected, only this area is copied to the clipboard.

▶ **From Clipboard**
Loads a graphic from the clipboard to the graphic export window.

▶ **Preview image size**
Allows the user to change the displayed size of the image in the graphic export window.

▶ **Image size**
Allows the user to change the size of the displayed image. Clicking this option will open a drop window with the following options:

Full Page
Displays the full graphic in the graphic export window.

Original size

Displays the graphic in its original size in the graphic export window.

Fit Width

Fits the width of the graphic to the size of the graphic export window.

Fit Height

Fits the height of the graphic to the size of the graphic export window.

▶ **Add Text**

This function allows the user to add a text to the displayed graphic. The functionalities of this text field are described below.

Mouse Operations

Clicking with the left mouse button in the text field will mark the text field. A second left mouse click in the text field allows the user to drag the text field over the graphic area. Releasing the mouse button will set the text field to that position. Clicking with the right mouse button on the text field will open a context menu.

Context Menu

The context menu refers to the text field format. It contains two functions:

Properties

Allows the user to format the text and opens the window shown in Fig. 5.2. This window offers the possibility to change the actual position and size of the text field. It also allows the user to select the color represented as the transparent color in the text field.
The text format features are represented in the lower part of the window.

Delete

Deletes the text field.

▶ **Burn Text**

This function saves the text field to the bitmap. After performing this operation, the text can no longer be moved across the bitmap and will be saved with the bitmap.

▶ **Cursor**

This cursor allows the user to change the functionalities of the mouse operations for the text field.

▶ **Rotate Graphic**

Rotates the graph in steps of 90 degrees.

▶ **Flip Graphic Horizontal**

Flips the graph horizontally.

▶ **Flip Graphic Vertical**

Flips the graph vertically.

▶ **Auto Crop Graphic**

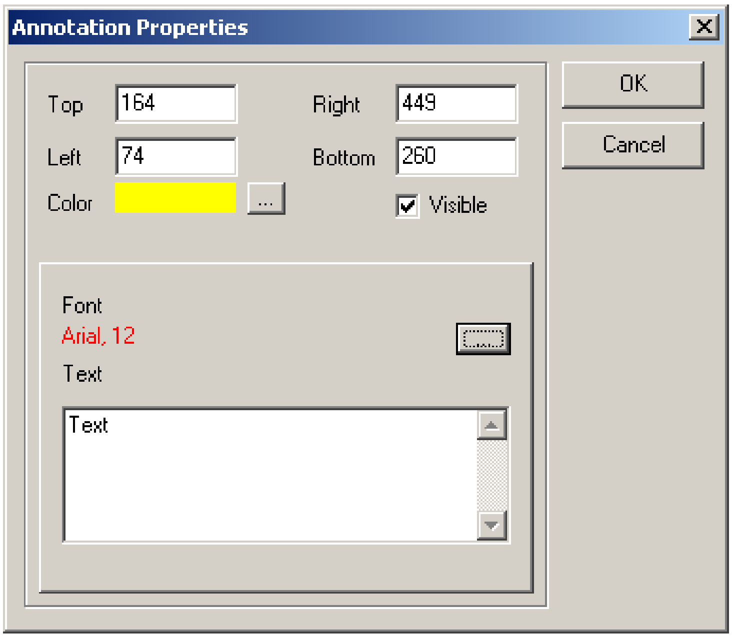


Fig. 5.2: Text formatting in the bitmap export window.

Crops a uniform border around the graphic.

Status Bar

The status bar displays the size of the graphic (in pixels) followed by the color type of the bitmap.

Chapter 6

Import

This chapter describes how to import other file formats into the WITec Project software. All import functions append the data to the current project. To start with an empty project, use the New Project function before importing (see Section 2.2).

6.1 ScanCtrl and DPFM Images

This function allows the user to import *.wit files, which have been created with ScanCtrl or PFMControl software. The *.wit file can be selected in a standard Windows® open-dialog.
All images of the *.wit file are imported, along with their lateral scaling and their z-unit. For each image, a separate image data object with a link to a spatial transformation and z-interpretation data object is created. All other information in the file is ignored (e.g. note book).

6.2 WinSpec

The WinSpec import function can read WinSpec files with the extension *.spe. These files can be a single spectrum or multi-spectra files. In the *.spe file format, all spectra are sorted in a 1-dimensional array. In order to import these spectra as a 2-dimensional array, the user will be asked about the array size. If this array size does not match the number of spectra, the import is aborted. All spectra are stored in one graph data object.
The import function also reads the calibration for these spectra. This calibration is stored in a spectral transformation data object. The wavelength of the excitation laser is stored in a spectral interpretation data object. All other information in the file is ignored.
In this import function, the graph data object is not linked to a position transformation data object, which converts the 2-dimensional array into physical qualities. A spatial transformation data object can be linked to this graph data object via drag

and drop (see Section 3.7). It is possible to use the spatial transformation data object from the ScanCtrl import function(see Section 6.1).

6.3 ScanCtrl and WinSpec

This function imports a ScanCtrl file and a WinSpec file at the same time. The scaling parameters for the WinSpec file are taken from the ScanCtrl structure. In this case, no user input for the 2-dimensional array size is needed. The graph data object gets the same link to the spatial transformation data object as the image data objects (see Section 6.1 and Section 6.2).

Chapter 7

Data Analysis

This chapter describes how to process, filter, and analyze data. Most of these routines are started by taking data objects from the project manager and dropping them onto an icon in the drop action window.

7.1 Drop Action

The drop action window shown in Fig. 7.1 can be opened from the main menu of the WITec Project software (see Section 2.2.3). It contains buttons for various data analysis operations. These buttons are drop zones for drag and drop operations. Clicking on a button opens a dialog for parameter settings. A detailed description of each function is provided below.

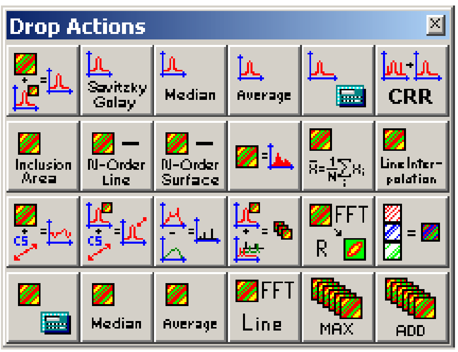
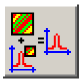


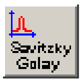
Fig. 7.1: Drop action window.

7.1.1 Average Spectrum 

Average spectrum calculates a weighted spectrum. The drop zone accepts a single graph data object or a single graph data object and an image data object. The image data object and the graph data object must have the same link to a spatial transformation data object, otherwise the drop zone will not accept these data objects. After dropping the data, calculation of the average spectrum begins.
The graph data object contains a $N \times M$ array of spectra $\vec{S}_{i,j}$. The image data object must contain a 2-dimensional array of the same size. These single values $I_{i,j}$ are used to weight or mask the spectra. In the absence of an image, all $I_{i,j}$ are set to one. The routine adds the average spectrum $\vec{S}_{ave}$ to the current project. Equ. 7.1 is the mathematical description of this average spectrum function.

$$\vec{S}_{ave} = \frac{\sum_{j=0}^{M-1} \sum_{i=0}^{N-1} I_{i,j} \vec{S}_{i,j}}{\sum_{j=0}^{M-1} \sum_{i=0}^{N-1} I_{i,j}} \tag{7.1}$$

HINT The software offers many ways to create the desired weighted or masked image. One possibility is to use the draw field of an image viewer as described in Section 4.3. This allows the manual selection of interesting spectra.
Another possibility is the image calculator (see Section 7.1.20). The weighted image can be set by several input images and a mathematical expression. The calculator accepts boolean operators to create a mask image using limit values.

7.1.2 Savitzky-Golay Graph Filter 

The Savitzky-Golay filter is a linear filter to smooth data. This filter is useful for spectra in which the peak widths are comparable in size. A detailed description of this filter can be found in [1].
This drop zone accepts a single graph data object. All line graphs in the graph data object are filtered by the Savitzky-Golay algorithm. The filtered data is copied to a new graph data object, which is added to the current project.
Like all smoothing filters, this filter uses the values that surround a data point to calculate a new value. In principle, this filter fits a polynomial of the Nth-order through the data points of the surrounding values. The filter also allows the differentiation of the polynomial at the same time. The new data point is given by this fit function or the differentiated fit function.
Fig. 7.2 shows the parameters of this filter. Press  in the drop action window to open this dialog. The parameters left and right are used to define the range of the surrounding values. The parameter order changes the order of the polynomial and the parameter derivative sets the order of derivative. The order of the derivative

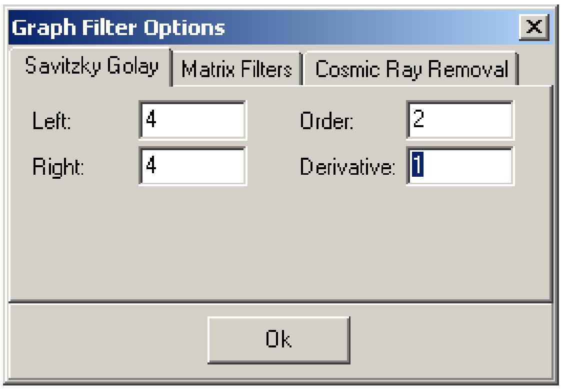
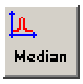
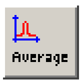


Fig. 7.2: Savitzky-Golay filter options.

must be less than or equal to the order of the polynomial used.

7.1.3 Median Graph Filter 

The median graph filter is a smoothing filter for graph data objects. This filter is a good choice for removing spikes in a line graph without rounding edges.
The drop zone accepts a single graph data object. All line graphs in the graph data object are filtered by the median value of the surrounding values. The filtered data is copied to a new graph data object, which is added to the current project. The parameter median filter size in Fig. 7.3 defines the range of the surrounding values. A filter size of 4 sets the range to $2 \cdot 4 + 1 = 9$.

7.1.4 Average Graph Filter 

The average graph filter is a smoothing filter for graph data objects. The drop zone accepts a single graph data object. All line graphs in the graph data object are filtered by the binomial average of the surrounding values. The filtered data is copied to a new graph data object, which is added to the current project. The parameter average filter size in Fig. 7.3 defines the range of the surrounding values. Tab. 7.1 shows the filter matrices which are used to calculate the weighted average from the surrounding values. The filter coefficients are calculated by binomial distribution.

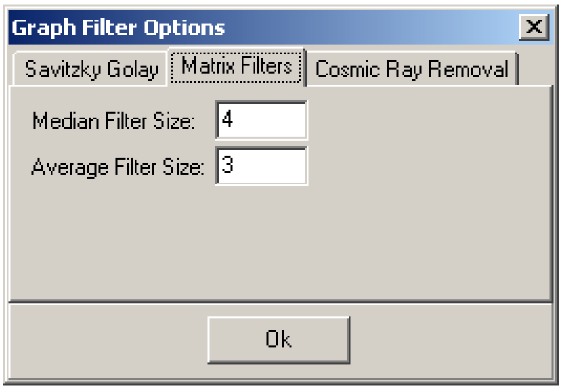
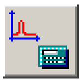


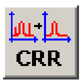
Fig. 7.3: Parameters for the median and average matrix filter.

Filter Size	Range	Filter Coefficients
1	3	$\frac{1}{4}(1,2,1)$
2	5	$\frac{1}{16}(1,4,6,4,1)$
3	7	$\frac{1}{64}(1,6,15,20,15,6,1)$
4	9	$\frac{1}{256}(1,8,28,56,70,56,28,8,1)$
5	11	$\frac{1}{1024}(1,10,45,120,210,252,210,120,45,10,1)$

Table 7.1: Matrices for the graph average filter

7.1.5 Graph Calculator 

The graph calculator is a calculator for graph data objects. The drop zone accepts any number of graph data objects with only one line graph (spectrum). All graph data objects must have the same array size (number of data points). The result of the user-defined formula is stored in a new graph data object, which is added to the current project.
For a detailed description of the calculator's functionality, see Section 7.2.

7.1.6 Cosmic Ray Removal 

The cosmic ray removal drop action allows the user to remove cosmic ray-like features from spectral data. The drop zone accepts a single graph data object. All spectra in the graph data object are filtered. Clicking on the drop action button will show a dialog which allows the user to change the parameters of the cosmic ray removal filter. Fig. 7.4 shows this dialog.
The filter algorithm is divided into two parts. The first part marks the cosmic ray-like features by comparing each data point with its spectral region. The range of the surrounding values is defined by the parameter filter size. The smallest value of the

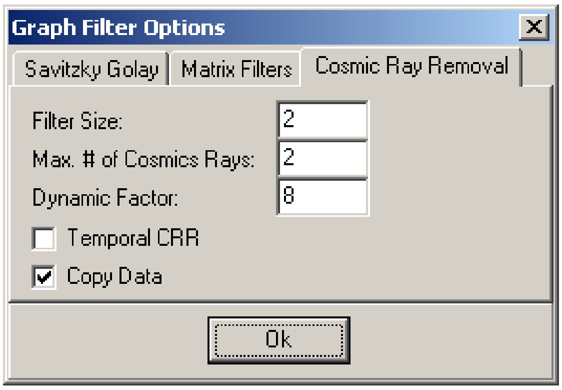


Fig. 7.4: Parameters for cosmic ray removal filter.

surrounding values is used as a base level. If the difference between the data point and base level is larger than the difference between the largest reliable value inside the range of surrounding values and the base level multiplied by the dynamic factor, then the data point will be removed. To find the largest reliable value, the surrounding values are sorted in ascending order. Cosmic ray-like features add a positive value to the signal, so all data points which include cosmic ray signals will be placed in the upper part of the sorted array. The maximum number of cosmic rays determines the position of the largest reliable value inside the sorted array.
The marked cosmic ray-like features can be removed by two methods. If the Temporal CCR checkbox is checked, the cosmic ray-like features will be replaced by the median values of the previous, the current, and the next spectrum. This strategy is useful for spectral time series. In all other cases, the Temporal CCR checkbox should be unchecked. In this case, the cosmic ray-like features will be replaced by interpolating from the surrounding values.
If the Copy Data checkbox is checked, the filtered data is copied to a new graph data object. Otherwise, the original data will be overwritten.

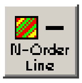
7.1.7 Inclusion Area 

With the inclusion area function, certain areas of an image can be selected. Only these areas are used in subsequent image operations. The inclusion area can be used in combination with:

- N-Order Line Subtraction (Section 7.1.8)
- N-Order Surface Subtraction (Section 7.1.9)
- Image Histogram (Section 7.1.10)
- Image Statistics (Section 7.1.11)

- Line Interpolation Filter (Section 7.1.12)

After marking some points, lines, and areas in an image and creating a draw field image (see Section 4.3), this image can be taken and dropped onto the inclusion area button.
Only areas not equal to zero are then used for the subsequent image operation. The software stores this data object until the user clicks on the inclusion area button or deletes the image data object.
The inclusion area image data object and the image to be processed must have the same 2D array size and the same link to the spatial transformation object.

7.1.8 N-Order Line Subtraction 

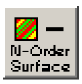
The N-order line subtraction is a data correction routine for AFM and SNOM images. It subtracts an Nth-order polynomial from each line. This polynomial is fitted to the data of the same line with the least squares method. This routine can work together with an inclusion area (see Section 7.1.7). Only data points which are set in the inclusion area are taken into account for fitting. If no inclusion area is set, all data points are used for the fit. Equ. 7.2 and Equ. 7.3 are the mathematical descriptions of this routine.

$$I'_{i,j} = I_{i,j} - P_j(i) \tag{7.2}$$

$$P_j(i) = \sum_{k=0}^{N} a_k i^k \tag{7.3}$$

$I_{i,j}$ are the original data points of the image and $I'_{i,j}$ are the corrected values. These values are copied to a new image data object.
The order N of the polynomial $P_j(i)$ can be changed by clicking on the N-order line subtraction button.
The drop zone accepts all image data objects. See Section 7.1.7 for restrictions, if an inclusion area is used.

If an inclusion area is used, each line must have enough data points to fit a polynomial. The line will be cleared if the number of data points is insufficient. An error message will be displayed.

7.1.9 N-Order Surface Subtraction 

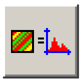
The N-order surface subtraction is a data correction routine for AFM and SNOM images that is particularly useful for topographical images. The routine subtracts an Nth-order 2-dimensional polynomial from the image data. This polynomial is fitted to the data of the image with the least squares method. This routine can work with an inclusion area (see Section 7.1.7). Only data points which are set in the inclusion area are taken into account for fitting the polynomial. If no inclusion area is set, all data points are used for the fit. Equ. 7.4 and Equ. 7.5 are the mathematical descriptions of this routine.

$$I'_{i,j} = I_{i,j} - P(i,j) \tag{7.4}$$

$$P(i,j) = \sum_{l=0}^{N} \sum_{k=0}^{N} a_{k,l} i^k j^l \tag{7.5}$$

$I_{i,j}$ are the original data points of the image and $I'_{i,j}$ are the corrected values. These values are copied to a new image data object.
The order N of the polynomial $P(i,j)$ can be changed by clicking on the N-order surface subtraction button.
The drop zone accepts all image data objects. If an inclusion area is used, see Section 7.1.7 for restrictions.

The number of data points in the inclusion area should be much larger than N^2 and they should be distributed over a large area. Otherwise, the resulting image might be useless.

7.1.10 Image Histogram 

The image histogram drop action creates a histogram from an image data object. This drop action can be combined with an inclusion area (Section 7.1.7). All data points marked in the inclusion area are used to create the histogram. If no inclusion area is set, all data points are used. The drop zone accepts all image data objects. See Section 7.1.7 for restrictions if an inclusion area is used. The histogram data is stored in a new graph data object and a linear transformation data object for the x-scaling. Both objects will be added to the current project.
The histogram routine has some user-adjustable parameters that control its output. With a left mouse click on the button, these parameters can be changed. Fig. 7.5 shows the dialog used to change these parameters.
The software calculates the size and the first bin position. All data points are sorted by their value in a 1D-array. The upper and lower level values can be found in this array. These levels can be changed by their percentage position in the array (see Fig. 7.5). The parameter range in the dialog expands the interval between these two levels to an initial position and a final position for the histogram. This range is divided into the number of bins. The software then stores the number of data falling into the appropriate bin in a graph data object.

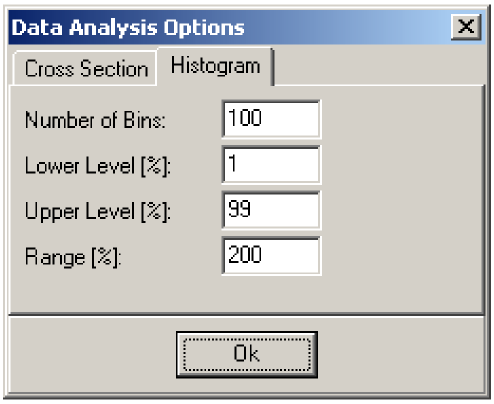
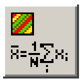


Fig. 7.5: Parameters used to control the output of the image histogram routine.

HINT The parameters in Fig. 7.5 are standard values and can be used for most images. If the histogram is too noisy, decreasing the number of bins may produce a smoother histogram.

7.1.11 Image Statistics 

The image statistics drop action calculates some statistical values from the image intensities $I_{i,j}$. This drop action can be combined with an inclusion area (Section 7.1.7). All data points marked in the inclusion area are used for the statistic. If no inclusion area is set, all data points are used. The drop zone accepts all image data objects. See Section 7.1.7 for restrictions if an inclusion area is used. The statistical values are stored in a text data object, which is added to the current project.
In the following mathematical description $\epsilon_{i,j} = 1$ if the pixel i, j is set in the inclusion area, and $\epsilon_{i,j} = 0$ if not. The size of the pixel array, stored in the image data object, is $M \times N$. The number of pixels and the average is given by:

$$\text{Number of Pixels} = \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} \tag{7.6}$$

$$\text{Average} = \frac{1}{\text{Number of Pixels}} \sum_{j=1}^{N} \sum_{i=1}^{M} I_{i,j}\epsilon_{i,j} \tag{7.7}$$

The variance and the standard deviation is calculated by the formula:

$$\text{Variance} = \frac{1}{\text{Number of Pixels}} \left(\sum_{j=1}^{N} \sum_{i=1}^{M} I_{i,j}^2 \epsilon_{i,j} \right) - \text{Average}^2 \tag{7.8}$$

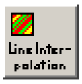
$$\text{Standard Deviation} = \sqrt{\text{Variance}} \tag{7.9}$$

The extreme values are defined by:

$$\text{Maximum} = \max\{I_{i,j} : 1 \leqq i \leqq M, 1 \leqq j \leqq N, \epsilon_{i,j} = 1\} \tag{7.10}$$

$$\text{Minimum} = \min\{I_{i,j} : 1 \leqq i \leqq M, 1 \leqq j \leqq N, \epsilon_{i,j} = 1\} \tag{7.11}$$

If the image data object has a link to a z-interpretation data object, all values are displayed in its units. Otherwise $a.u.$ (arbitrary units) are used.

7.1.12 Line Interpolation Filter 

The line interpolation filter can be used to remove bad pixels and lines in image data objects. The drop zone accepts all image data objects. All bad pixels should be marked in the inclusion area. Without an inclusion area, the filter routine has no effect (see Section 7.1.7).
The filter routine replaces all bad pixel values with interpolated values. These values are calculated by a linear interpolation of a reference line above and below the discarded line.
This filter stores the result in a new image data object, which is added to the current project.

HINT Selecting several lines in a row can lead to strange results in the filtered image. Use of this filter is recommended only for one or two bad lines in a row.

7.1.13 Roughness 

The image roughness drop action calculates roughness parameter from the image topography values $z(x_i, y_j)$.

HINT Roughness analysis is mainly used for topography image data objects. These data objects have a link to a z-interpretation which contains either μm or nm as unit. All other image data objects can be analyzed with the roughness drop action, nevertheless the meaning of the results is questionable.

This drop action can be combined with an inclusion area (Section 7.1.7). All data points marked in the inclusion area are used for the evaluation of the roughness

parameter. If no inclusion area is set, all data points are used. The drop zone accepts all image data objects. See Section 7.1.7 for restrictions if an inclusion area is used. The roughness values are stored in a text data object, which is added to the current project.
In the following mathematical description $\epsilon_{i,j} = 1$ if the pixel i, j is set in the inclusion area, and $\epsilon_{i,j} = 0$ if not. The size of the pixel array, stored in the image data object, is $M \times N$. The number of pixels and the analyzed surface area is given by:

$$< MN >= \text{Number of Pixels} = \sum_{j=1}^{N}\sum_{i=1}^{M} \epsilon_{i,j} \tag{7.12}$$

$$\text{Area} = \sum_{j=1}^{N}\sum_{i=1}^{M} \Delta x_{i,j} \Delta y_{i,j} \epsilon_{i,j} =< MN > \Delta x \Delta y \tag{7.13}$$

The roughness average, SA, is defined as:

$$\text{SA} = \frac{1}{< MN >} \sum_{j=1}^{N}\sum_{i=1}^{M} \epsilon_{i,j} |z(x_i, y_j) - \bar{z}| \tag{7.14}$$

with $\bar{z}$ representing the mean hight.

$$\bar{z} = \frac{1}{< MN >} \sum_{j=1}^{N}\sum_{i=1}^{M} \epsilon_{i,j} z(x_i, y_j) \tag{7.15}$$

HINT A proper plane correction is recommended before a roughness analysis is performed

The root mean square SQ is defined as:

$$\text{SQ} = \sqrt{\frac{1}{< MN >} \sum_{j=1}^{N}\sum_{i=1}^{M} \epsilon_{i,j} [z(x_i, y_j) - \bar{z}]^2} \tag{7.16}$$

The surface skewness SKK, describes the asymmetry of the height distribution histogram and is defined as:

$$\text{SSK} = \frac{1}{< MN > \text{SQ}^3} \sum_{j=1}^{N}\sum_{i=1}^{M} \epsilon_{i,j} [z(x_i, y_j) - \bar{z}]^3 \tag{7.17}$$

If SSK $= 0$, a symmetric height distribution is indicated, e.g. a Gaussian like.

If SSK < 0, it can be a bearing surface with holes and if 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:

$$\mathsf{SKU} = \frac{1}{< MN > \mathsf{SQ}^4} \sum_{j=1}^{N} \sum_{i=1}^{M} \epsilon_{i,j} [z(x_i, y_j) - \bar{z}]^4 \tag{7.18}$$

For Gaussian height distributions SKU approaches 3.0 when increasing the number of pixels. Smaller values indicate broader height distributions.

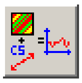
The extreme values are defined by:

$$\mathsf{Max} = \max\{z(x_i, y_j) : 1 \leqq i \leqq M, 1 \leqq j \leqq N, \epsilon_{i,j} = 1\} \tag{7.19}$$

$$\mathsf{Min} = \min\{z(x_i, y_j) : 1 \leqq i \leqq M, 1 \leqq j \leqq N, \epsilon_{i,j} = 1\} \tag{7.20}$$

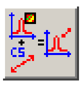
The peak-peak parameter is defined as:

$$\mathsf{Peak\text{-}Peak} = |\mathsf{Max} - \mathsf{Min}| \tag{7.21}$$

7.1.14 Image Cross Section 

The image cross section drop action creates a cross section from image data objects. The drop zone requires a cross section (spatial transformation data object) and one or more image data objects. The cross section consists of a start point ($X1$,$Y1$,$Z1$) and an end point ($X2$,$Y2$,$Z2$), and can be created by using the image viewer (see Section 4.3). Only images which lie parallel to the cross section produce a cross section graph. All other images will be ignored. An image data object will also be ignored if no intersection between cross section and image exists.
Each valid image data object creates a graph data object which stores the cross section data. The spatial transformation data object (cross section) is linked to these graph data objects. In addition, the routine displays all cross sections in a graph viewer (see Section 4.5).
In order to perform a cross section of various images with different overlaps, positions, and scaling, the algorithm requires the number of sampling points for the cross section. This number of sampling points can be changed by clicking on the image cross section button. Fig. 7.6 shows the dialog for this parameter.

HINT If only one part of the cross section lies inside the image area, the first or the last valid value will be copied to the graph data object when no other data is available.

7.1.15 Image Spectrum Cross Section 

The image spectrum cross section drop action creates a cross section from a 2-dimensional graph data object. The drop zone requires a cross section (spatial

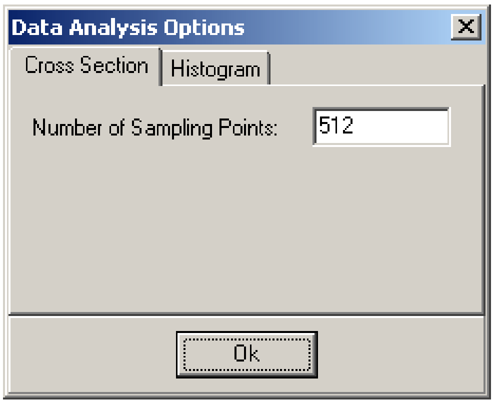
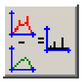


Fig. 7.6: Parameters for image cross section.

transformation data object) and one graph data object. The cross section consists of a start point ($X1$,$Y1$,$Z1$) and an end point ($X2$,$Y2$,$Z2$), and can be created by using the image viewer (see Section 4.3). Only graph data objects which lie parallel to the cross section can produce a graph cross section. Start and end points must lie inside the 2-dimensional array of the graph data object. The number of sampling points can be changed by clicking on the image spectrum cross section button. Fig. 7.6 shows the dialog for this parameter.

7.1.16 Background Subtraction 

The background subtraction drop action allows the subtraction of a background signal from any graph data object. The background is determined by a polynomial of the order N, which is fitted to a user-definable region of the data.
This drop zone accepts a single graph data object with a 1-dimensional x-transformation data object. All line graphs in the graph data object are background subtracted by their own polynomial fit. The background subtracted data is copied to a new graph data object, which is added to the current project.
After dropping a graph data object onto the background subtraction button, an interactive dialog window opens (see Fig. 7.7). In addition to this dialog, a fit preview windows opens, which shows the result of the background estimation. The dialog interacts with two cursor data objects. One cursor data object allows the user to select the regions to which the polynomial should be fitted. The other cursor allows the line graph in the fit preview window to be changed.
The user can change two masks which control the outcome of this dialog. Both masks are completely set after starting the dialog. The so-called fit mask defines the pixels which should be used for the fit. The change mask defines the pixels which should be background corrected. The mask can be changed by setting the start and stop values and pressing the Set or Clear buttons. The corresponding

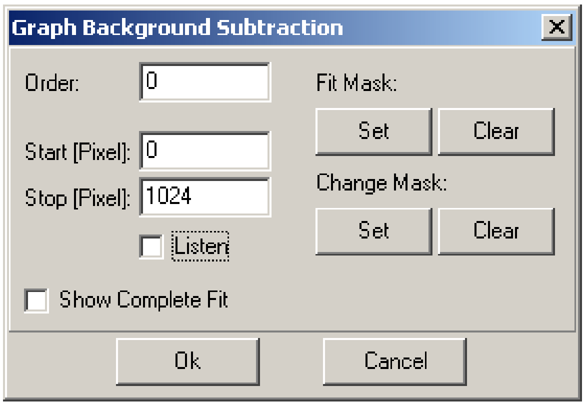


Fig. 7.7: Background subtraction dialog.

mask will be set or cleared within this range. If the Listen checkbox is checked, the start and stop values can be changed via the cursor data object by selecting a region inside the fit preview window or any other graph data viewer which is using the same cursor.
If the Show Complete Fit checkbox is checked, the complete polynomial fit is shown in the fit preview window. Otherwise, only the part of the fit included in the fit mask is shown.
After pressing the Ok button, each line graph of the graph data object is background subtracted using the same fit mask and change mask. Pixels in which the change mask is not set are set to zero.

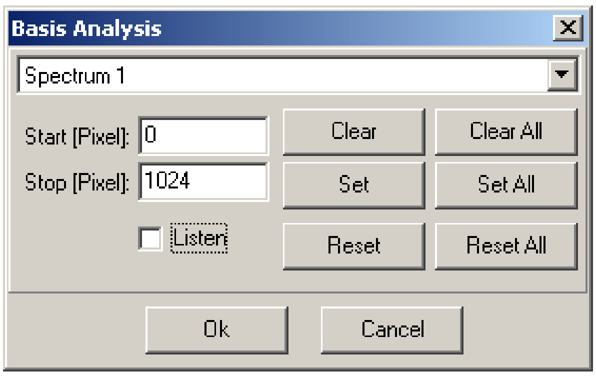
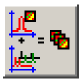


Fig. 7.8: Basis analysis dialog.

7.1.17 Basis Analysis 

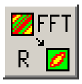
The basis analysis drop action is used mainly for Raman spectroscopy data sets. Each material has a unique Raman spectrum $\vec{B_k}$. The Raman spectra $\vec{B_k}$ are called basis spectra. A sample which consists of N different materials shows a linear superposition $\vec{S}$ of all its basis spectra.

$$\vec{S} = \sum_{k=1}^{N} a_k \vec{B}_k \tag{7.22}$$

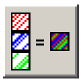
If the basis spectra $\vec{B_k}$ of the pure materials are known, it is possible to estimate the weighting factor a_k by the least squares fit. The weighting factor is proportional to the quantity of the material.
To start this dialog, the user must drop one graph data object with a 2-dimensional array of spectra and at least one graph data object which contains a single Raman spectrum of the pure material onto the basis analysis button. The number N of the basis spectra is unlimited. For clear results, keep the number of basis spectra as low as possible. All spectra must be free of any background or offset. Background subtraction is described in Section 7.1.16.
After the spectra have been dropped onto the button, the basis analysis dialog window appears (see Fig. 7.8). In addition to this dialog, two graph viewers appear. One viewer shows a fit preview and the other shows the normalized basis spectra.
The dialog interacts with two cursor data objects. One cursor data object allows the user to select the spectral regions in order to include or exclude regions of the basis spectra. The other cursor allows the user to change the spectrum in the fit preview window.
Each basis spectrum has its own inclusion mask. The inclusion mask defines the regions of the basis spectra that should be used for the least squares fit. The mask can be changed by setting the start and stop values and pressing the Set or Clear buttons. The inclusion mask of the current spectrum (see drop down list on top of the dialog) will be set or cleared within this range. The Set All or Clear All buttons can be used to change all inclusion masks at the same time. If the Listen checkbox is checked, the start and stop values can be changed via the cursor data object by selecting a region inside the fit preview window or any other graph data viewer which is using the same cursor.
After pressing the Ok button, each spectrum of the 2-dimensional graph data object is fitted by a linear combination of the basis spectra using the least squares method. The weighting factors are stored in an image data object. The weighting factor is the area below the spectrum, which is needed to produce the best fit. In addition to the weighting factor images, an error image is generated. The error is calculated by the following formula:

$$\text{Error} = \sqrt{\frac{1}{\sum\limits_{Inc.}} \sum_{Inc.} (\vec{S} - \sum_{k=1}^{N} a_k \vec{B}_k)^2} \tag{7.23}$$

HINT Spectral regions that are not proportional to any signal or are represented in more than one basis spectrum must be excluded before fitting. In particular, the region of the laser excitation and spectral regions in which the substrate shows Raman peaks must be excluded.

7.1.18 Image FFT 

This part of the software is under construction. Make sure that the project is stored on the hard disk before using this function.

7.1.19 Image Color Combination 

The image color combination drop action creates a false color bitmap from image data objects. Each image data object will create a single false color bitmap in which the transparent regions can be set by level. All bitmaps are combined into one composite bitmap.
This drop action accepts one or more image data objects. All image data objects must have the same array size and the same link to a spatial transformation object. After the images have been dropped onto the button, the image color combination dialog window appears (see Fig. 7.9). In addition to this dialog, an image viewer and a bitmap viewer appear. The image viewer shows the currently active image data object as a false color image. The transparent regions are displayed as inverted colors. Each image data object uses a different color profile. The color profile can be changed via the context menu of the image viewer preview. The bitmap viewer shows the result of the image combination. All changes in the dialog are automatically shown in this preview window.
The names of all image data objects are listed in a list box in the dialog. The highlighted item is the currently active image data object. Clicking on another item will change the currently active image data object. By pressing the $\boxed{\text{Up}}$ and $\boxed{\text{Dn}}$ buttons, the user can change the order of the image stack.
In the lower part of the dialog, the top and bottom values for the color scale and the transparency can be changed. All settings displayed in the lower part belong to the currently active image data object. The top and bottom values of the first column are used for the color scale. The levels of the second and third columns are used to set the transparency. The transparency above the top value and below the bottom value can be turned on or off by the checked boxes on the right. If the

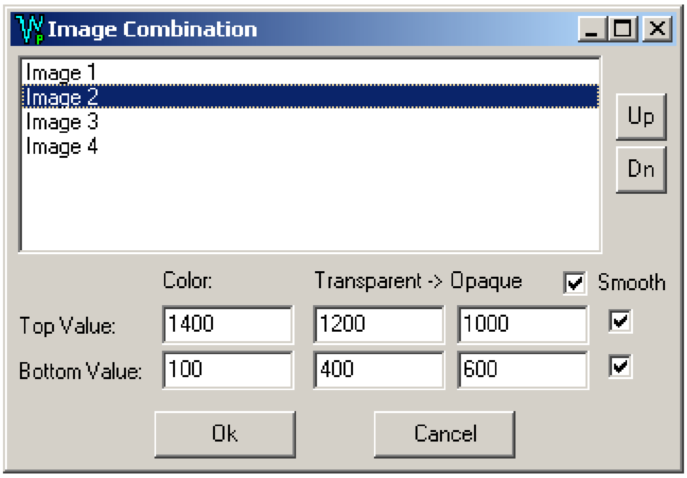
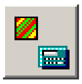


Fig. 7.9: Image color combination dialog.

Smooth check box is unchecked, the transparency will be entirely on or off. Otherwise, the transparency will vary continuously between the transparent and opaque levels. After all parameters are adjusted, the user can create a bitmap data object by pressing Ok. This bitmap data object is added to the current project and contains the combined image. The bitmap data object uses the same link to the spatial transformation object as the image data objects.

7.1.20 Image Calculator 

The image calculator is a powerful tool used to create new images by a user-defined mathematical description and one or more images as input parameters. The drop zone accepts any number of image data objects. All image data objects must have the same array size and the same link to a spatial transformation data object. Each image is an input variable X_k for the user-defined formula. The result of this formula is stored in a new image data object (I_{result}). This object is added to the current project.
For a detailed description of the calculator's functionality, see Section 7.2.

7.1.21 Median Image Filter 

The median image filter is a smoothing filter for image data objects. This filter is used to remove spikes in an image without rounding edges.
The drop zone accepts a single image data object. The image data is filtered by the median value of the surrounding values. The filtered data is copied to a new image data object, which is added to the current project. The parameter median filter

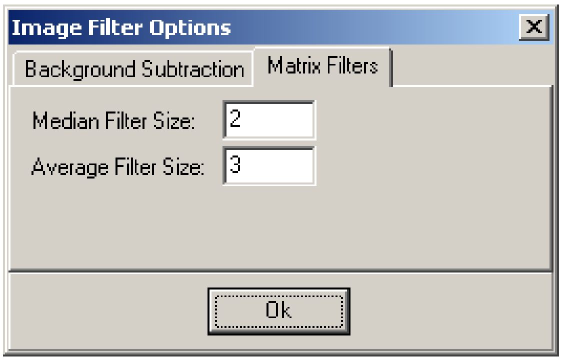
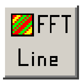


Fig. 7.10: Parameters for the median and average matrix filters.

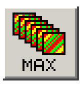
size in Fig. 7.10 defines the range of the surrounding values. A filter size of 4 sets the range to $2 \cdot 4 + 1 = 9$.

7.1.22 Average Image Filter 

The average image filter is a smoothing filter for image data objects. The drop zone accepts a single image data object. The image data is replaced by the binomial average value of the surrounding values. The filtered image is copied to a new image data object, which is added to the current project. The parameter average filter size in Fig. 7.10 defines the range of the surrounding values. Tab. 7.2 shows the filter matrices which are used to calculate the weighted average from the surrounding values.
The filter coefficients are calculated by binomial distribution.

7.1.23 Line Fourier Image Filter 

This part of the software is under construction. Make sure that the project is stored on the hard disk before using this function.

7.1.24 Auto Focus 

This drop action accepts a stack of image data objects. All images in the stack must have the same array size $M \times N$. The intensities $I_{i,j,k}$ of the 3-dimensional stack are reduced to the maximum $I_{i,j}^{Max}$ and the position of the maximum $P_{i,j}^{max}$ of the stack. This data is stored in two image data objects. The parameter k is the image index.

Filter Size	Range	Filter Coefficients
1	3×3	$\frac{1}{16}\begin{pmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{pmatrix}$
2	5×5	$\frac{1}{256}\begin{pmatrix} 1 & 4 & 6 & 4 & 1 \\ 4 & 16 & 24 & 16 & 4 \\ 6 & 24 & 36 & 24 & 6 \\ 4 & 16 & 24 & 16 & 4 \\ 1 & 4 & 6 & 4 & 1 \end{pmatrix}$
3	7×7	$\frac{1}{4096}\begin{pmatrix} 1 & 6 & 15 & 20 & 15 & 6 & 1 \\ 6 & 36 & 90 & 120 & 90 & 36 & 6 \\ 15 & 90 & 225 & 300 & 225 & 90 & 15 \\ 20 & 120 & 300 & 400 & 300 & 120 & 20 \\ 15 & 90 & 225 & 300 & 225 & 90 & 15 \\ 6 & 36 & 90 & 120 & 90 & 36 & 6 \\ 1 & 6 & 15 & 20 & 15 & 6 & 1 \end{pmatrix}$

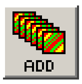
Table 7.2: Matrices for the image average filter

The maximum value for k is the number of images O in the stack.

$$I_{i,j}^{max} = \max\{I_{i,j,k} : 1 \leqq k \leqq O\} \tag{7.24}$$

$$P_{i,j}^{max} = \min\{P_{i,j,k} : I_{i,j,k} = I_{i,j}^{max}, 1 \leqq k \leqq O\} \tag{7.25}$$

This routine is usually used for confocal image stacks.

7.1.25 Extended Focus 

The extended focus drop action accepts a stack of image data objects. All images in the stack must have the same array size $M \times N$. The images with the intensities $I_{i,j,k}$ are accumulated and stored in a new image data object. Equ. 7.26 gives a mathematical description of this routine. The parameter k is the image index. The maximum value for k is the number of images O in the stack.

$$I_{i,j}^{acc} = \sum_{k=1}^{O} I_{i,j,k} \tag{7.26}$$

This routine is usually used for confocal image stacks.

7.2 Calculator

7.2.1 Calculator Dialog

The calculator dialog is the user interface for the formula parser (see Section 7.2.2). Fig. 7.11 shows the dialog. In the listbox at the top, all valid input parameters ($X1$, $X2$, and $X3$) and their corresponding data object names are given. The edit boxes below can be filled in by the user. The box on the left is used for the name of the data object that stores the result. The edit box in the middle is for the formula expression. Valid operators and functions are described in Section 7.2.2. If the formula has a syntax error, it is displayed in red characters. The right edit box defines the unit name of the result. If necessary, a z-interpretation data object is created for this unit name.

7.2.2 Formula Parser

The formula parser converts an algebraic expression (text) into a stack of operations understandable by the computer. This formula parser can deal with several mathematical operators and functions.
Tab. 7.3 shows all valid operators. 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:

$$\text{Boolean}(x) = \begin{cases} \text{true} & \text{for} \quad x <> 0 \\ \text{false} & \text{for} \quad x = 0 \end{cases} \tag{7.27}$$

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 valid functions of the formula parser are given in Tab. 7.3. All functions have at least 10 significant decimal points, other than the besselj1() and the airysqr() function, which deal with only 7 significant decimal points.
Depending on the usage, the formula parser accepts a fixed number N of input variables. These variables are addressed by $X1$, $X2$ ... X_n.

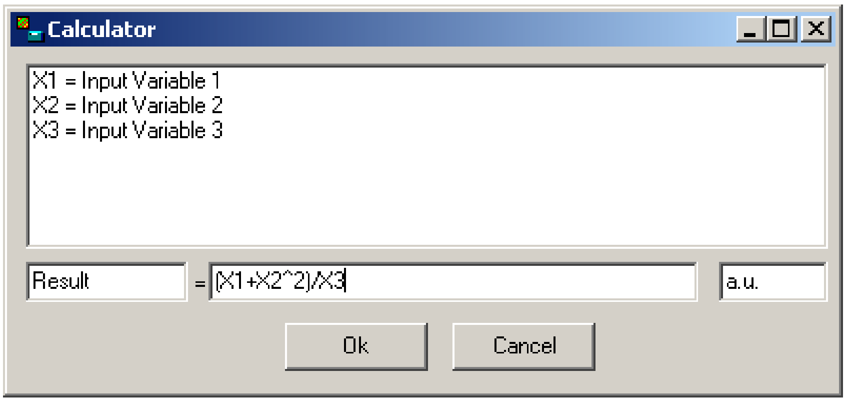


Fig. 7.11: Calculator dialog.

Priority	**Operators**	**Description**
1	| or (boolean)	
2	& and (boolean)	
3	!	invert (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)

Table 7.3: Calculator operators and priorities

Function	Description
sin()	sine (argument in radian)
asin()	arc sine in radian
cos()	cosine (argument in radian)
acos()	arc cosine in radian
tan()	tangent (argument in radian)
atan()	arc tangent in radian
cotan()	cotangent (argument in 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 the base 10
log2()	logarithm of the base 2
exp()	exponential
abs()	absolute
sqrt()	square root
sinc()	sinc$(x) = \frac{\sin(x)}{x}$ (argument in radian)
sincsqr()	sincsqr$(x) = \left(\frac{\sin(x)}{x}\right)^2$ (argument in radian)
heavyside()	heavyside$(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 0.5 & \text{for} \quad x = 0 \\ 1 & \text{for} \quad x > 0 \end{cases}$
sign()	sign$(x) = \begin{cases} -1 & \text{for} \quad x < 0 \\ 0 & \text{for} \quad x = 1 \\ 1 & \text{for} \quad x > 0 \end{cases}$
besselj1()	besselj1$(x) = J_1(x)$ bessel function of first kind
airysqr()	airysqr$(x) = \left(\frac{2J_1(x)}{x}\right)^2$

Table 7.4: Calculator functions

Bibliography

[1] William H. Press, Saul A. Teukolsky, Wiliam T. Vetterling and Brian P. Flannery. Numerical Recipes in C, Kap. Savitzky-Golay Smoothing Filters, S. 650–655. The Press Syndicate of the University of Cambridge, 2. Aufl., 1999.