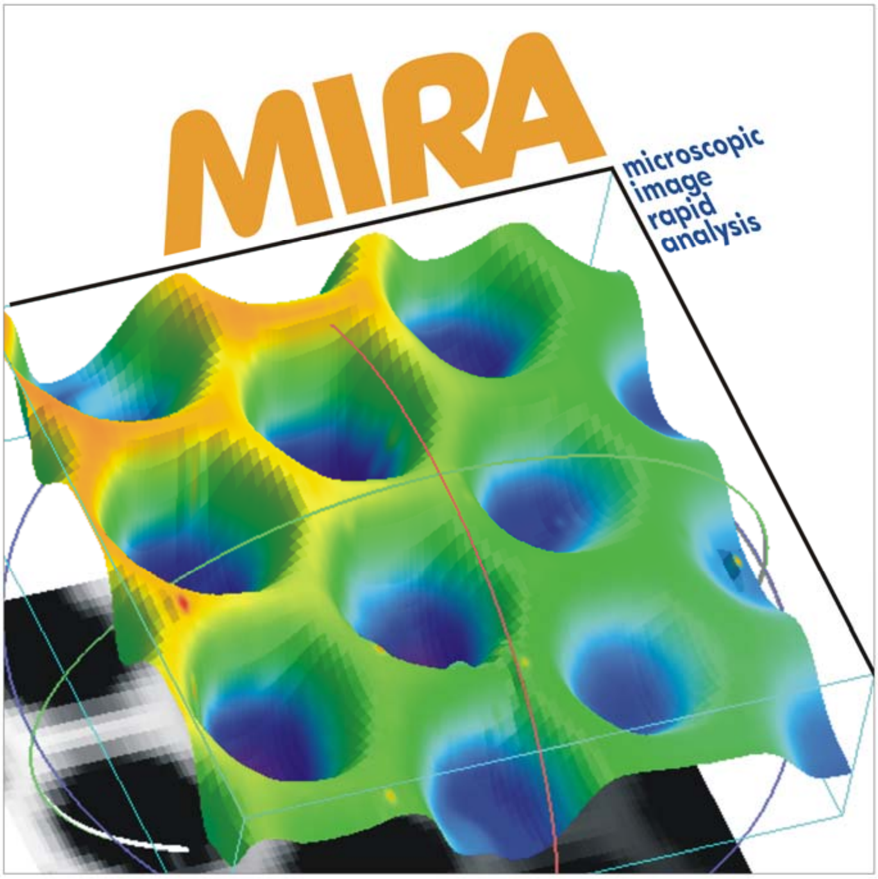
Instructions for the program MIRA



(Microscopic Image Rapid Analysis, span. "Look!")

Last Changes: 16 April 2011

This program is developed for the representation of data from various instruments. The data are processed by unified principles for all data sets, which eases the comparison of data coming from various instruments.

It contains productivity tools that were developed for everyday laboratory routines.

Software requirements: Windows 2000 or Windows XP, running in 24 bit color depth or 256 bit color depth.

1 Installation of MIRA

1.1 How to install MIRA

Start the program

InstallMIRA.exe

which you find on the CD or which you obtained via internet. If your computer allows autorun, the program will be started automatically, if you insert the CD. The following screen appears.

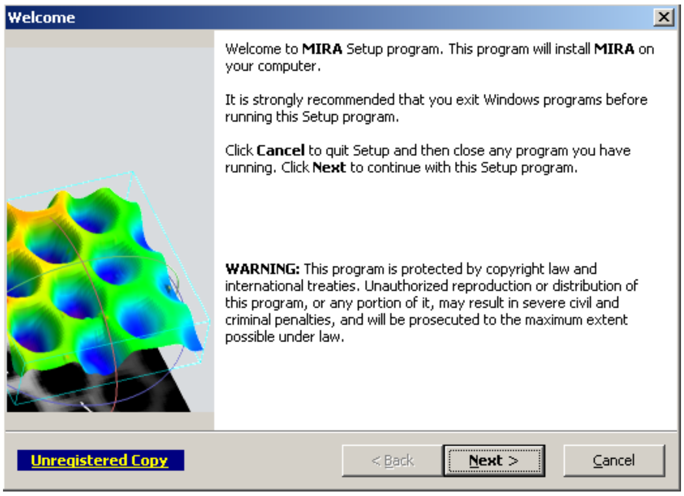


Abb. 1: Screen shot of the MIRA installation program.

In order to run the installation program, you need Administrator rights on the computer.

After continuing with ***<Next>*** you will be asked for the User Information. Please type the Serial Number exactly as received from the supplier. Press <***Next***>.

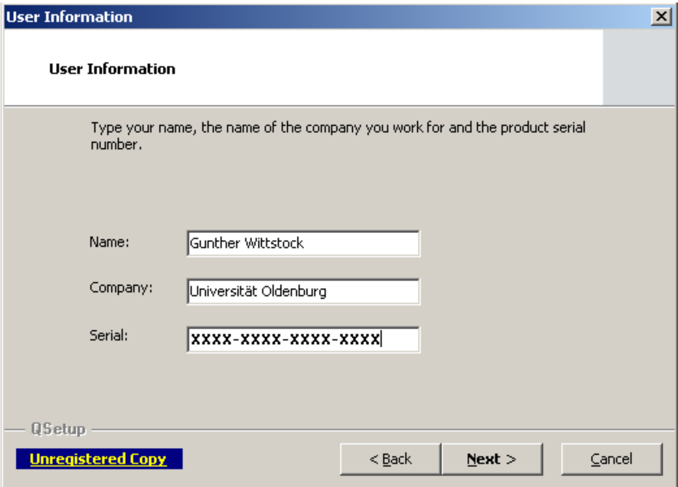


Abb. 2: Dialog for requesting user information.

You are then asked for the folder into which MIRA will be installed. In contrast to previous versions, this installation does not require a previous installation of IDL Runtime. Your are independent of any change in the IDL language. You do not need to contact Research Systems.

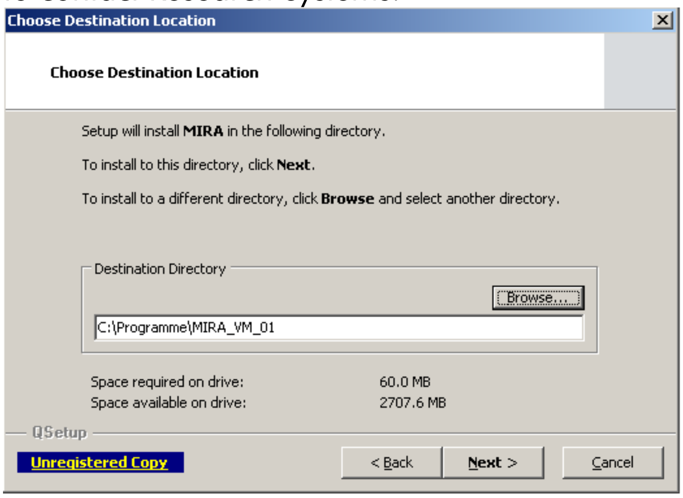


Abb. 3: Dialog for requesting installation path.

The installer will create shortcuts on the desktop and entries into the Quick Launch bar for all users. You can modify the entries.

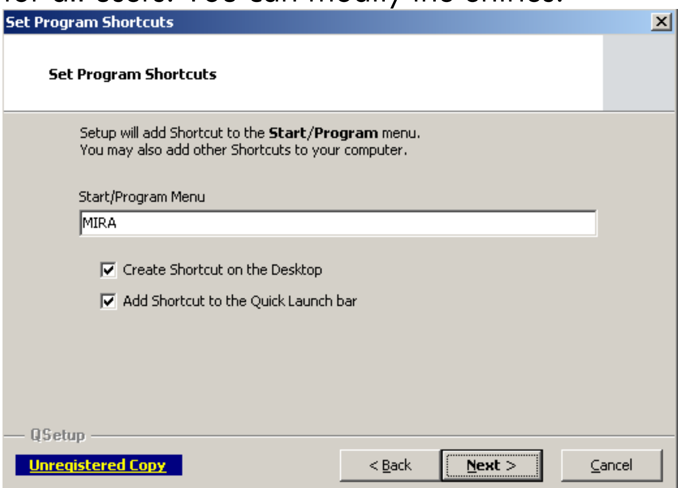


Abb. 4: Dialog for confirming entries in Start/Program menu, desktop icon and Quick Launch bar.

The installer then copies all files to the new application folder. The following directory structure is created.

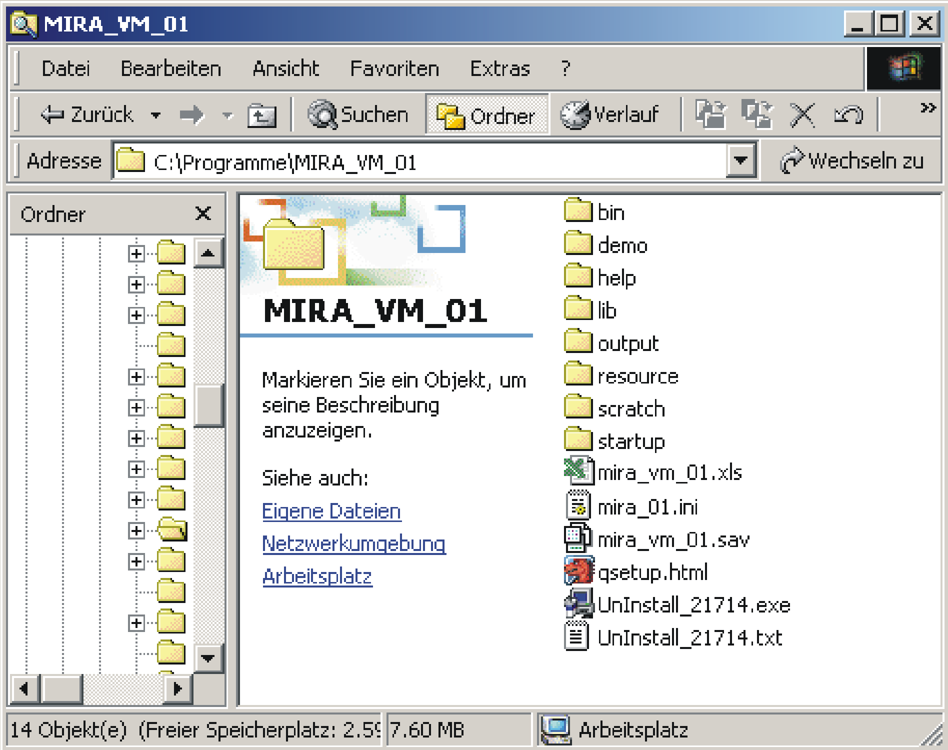


Abb. 5: Directory structure of the MIRA VM installation.

Three files will be copied to the ~\winnt\system32 folder:
mfc70.dll
msvcp70.dll
msvcr70.dll
if the DLL is newer than any possible DLL of the same name already in the folder

After completing copying all files, the program should be started from the following screen.

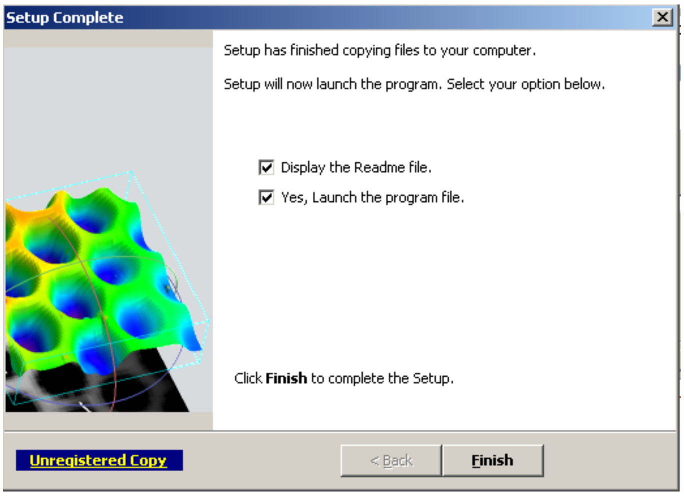


Abb. 6: Dialog for starting MIRA for the first time.

It is necessary that MIRA is started now, because information is transferred form ini-files to the registry entries on the machine. Please confirm the following query (Fig. 7).

It might be that this dialog appears *behind* other windows. In such case move other windows away to find the file. After that, the installation process is completed. From now on MIRA should start as described in the next chapter.

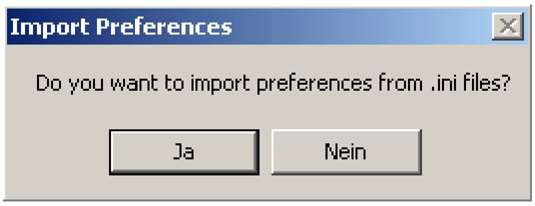


Abb. 7: Dialog for importing preferences, press<***Yes***> or <***Ja***>.

1.2 How to uninstall MIRA

Start *Uninstall MIRA* from the *Start/Program/Mira* group. All files will be removed, EXCEPT: mfc70.dll, msvcp70.dll, msvcr70.dll because they might be used by another program. Also the path ~*output* will not be removed if it contains user data. If it is empty, it will be removed.

2 First look at MIRA

2.1 Launch MIRA

Right after the installation MIRA should start automatically if the settings of Fig. 6 were confirmed. Later, you can start MIRA by a double click on the icon on the desktop.

The following window appears, click on it to proceed. The program is based on IDL (Interactive Data Language, vers. 6.0 by Research Systems Inc., Boulder Colorado)

Fig. 8: Startup window of the IDL data processing machine.

A window as in Fig. 9 opens and you can select between two startup configurations: *Multiplot* and *Single Plot* and various <*.ini*>-files that contain user-specific preferences.

Multiplot means that you can load many data sets into one form. Processing can be toggled quickly between these data. The configuration *Single Plot* stands for the opposite: Only one data set is processed.

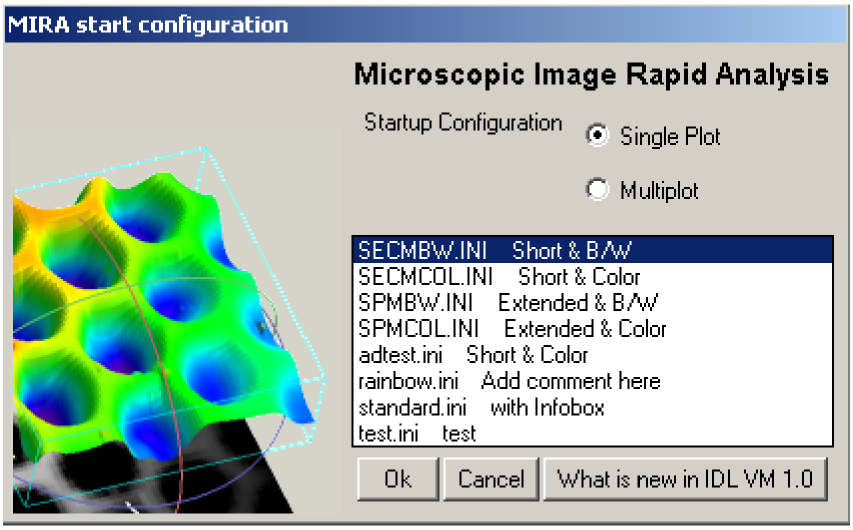


Fig. 9: Select Startup Configuration

These two versions can be started with a number of user-defined startup settings. They are stored and can be retrieved from <*.*ini*> files. Among others the startup values determine the appearance of the first window. A standard initialization is given. Other startup values can be created by saving current settings. A startup file is given below. It can of course also be edited by a text editor. After choosing the configuration and the default value you can start with ***<Ok>***. Alternatively you can double click on an <*.*ini*> files to start the application.

[MIRA USER DEFAULTS]	Section header
FOLLOWING LINES = 12	Number of the following lines
COMMENT = Standard	Comment which is shown in the menu selection
INFOBOX = True	If true displays in the Single Plot and Multiplot windows a status bar.
LAYOUT = EXTENDED	Type of layout. The program differs between extended and minimal widget. → *Single Plot*
COLORTABLE = 39	There is a selection of 40 predefined color tables (0–39)
SHADE TOP = 254	Color shade scale from 0 till 254 That means that there are 255 different shades. The upper bound is modifiable. From the indes 255 is the color used for axis or labels.
STANDARD 3D PLOT = Image	Standard graphic mode for 3D datasets
STANDARD 2D PLOT = Single 2D	Standard mode for 2D datasets
STANDARD MULTI-2D PLOT = Multiple 2D	Standard mode for multiple 2D datasets
STANDARD DATA INPUT PATH = D:\Dateien\Mira\Input	Standard path where data were read out off.
STANDARD OUTPUT PATH\= D:\Dateien\Mira\Output\	Standard path for print files.
STANDARD FORMAT FILE PATH = D:\Dateien\Mira\SPM\	Standard path for formatting files.
STANDARD PRINTER = Color encapsulated PS	Standard graphic format

2.2 Customizing IDL

After installation the data input path is the path with demo data supplied with the installation. The output path is an empty folder within the application folder. It is strongly recommended that each user of the machine makes its input and output path OUTSIDE the MIRA application path and save the preferences to an ini-file such as *gunther.ini*, *felix.ini* and *alena.ini*. We made good experiences with an arrangement, where each user has an own data input path and a data output path. **It is strongly recommended that data output path is NEVER the same as the data input path.** Otherwise, there is a risk that input data are overwritten although MIRA will query before doing so (new in this version). This will not be a problem if the output path is used exclusively to receive output from MIRA.

You can change the path setting (and others) by starting the menu *Options + ?/Save INI file*. Use the <***Select***> button besides the text fields to select a new path in your folder tree. After set confirm and select a file name. In order to make the ini file your current preference, load it with *Options + ?/Load INI* file.

For a more detailed description see the description of the menu *Option + ?/Save INI file*.

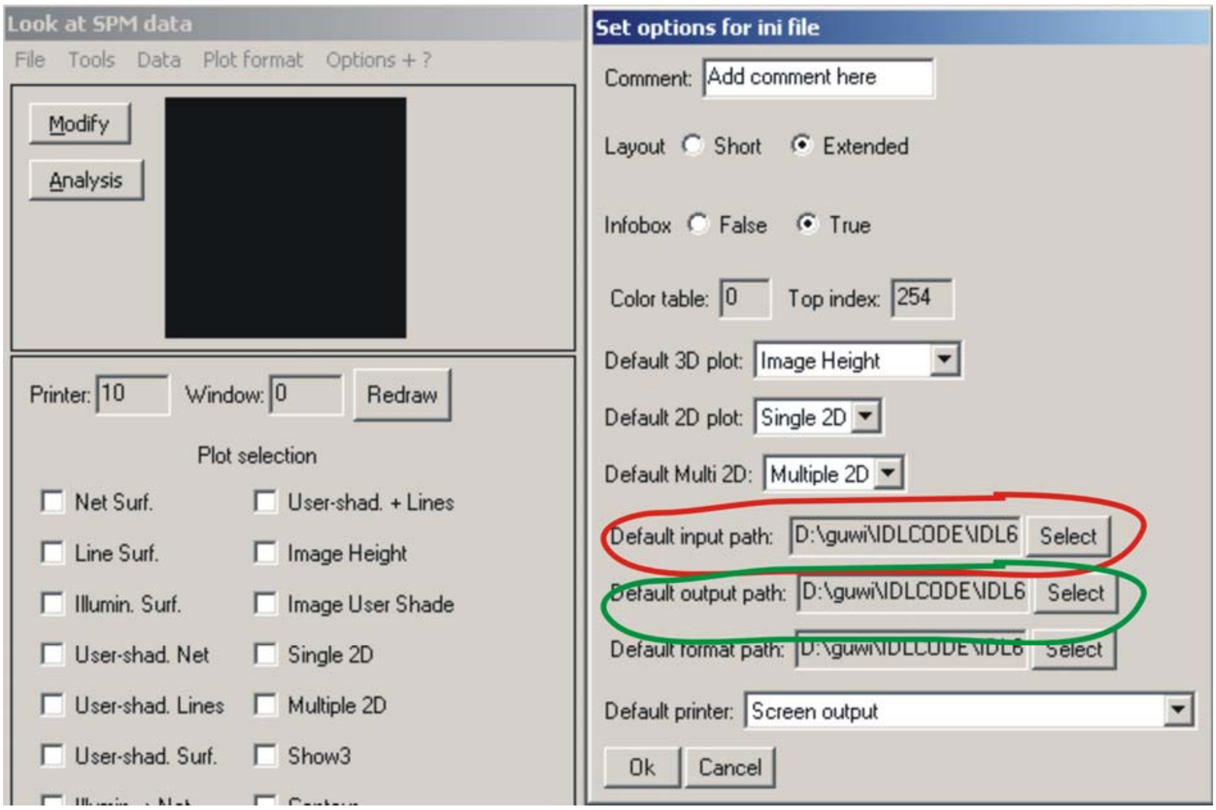


Abb. 10: Dialog for making user-specific initializations. The input path and the output path should be changed for each user.

3 Single Plot

This configuration can be used with two settings:
Extended widget and *Minimal widget* and Info box True/False.

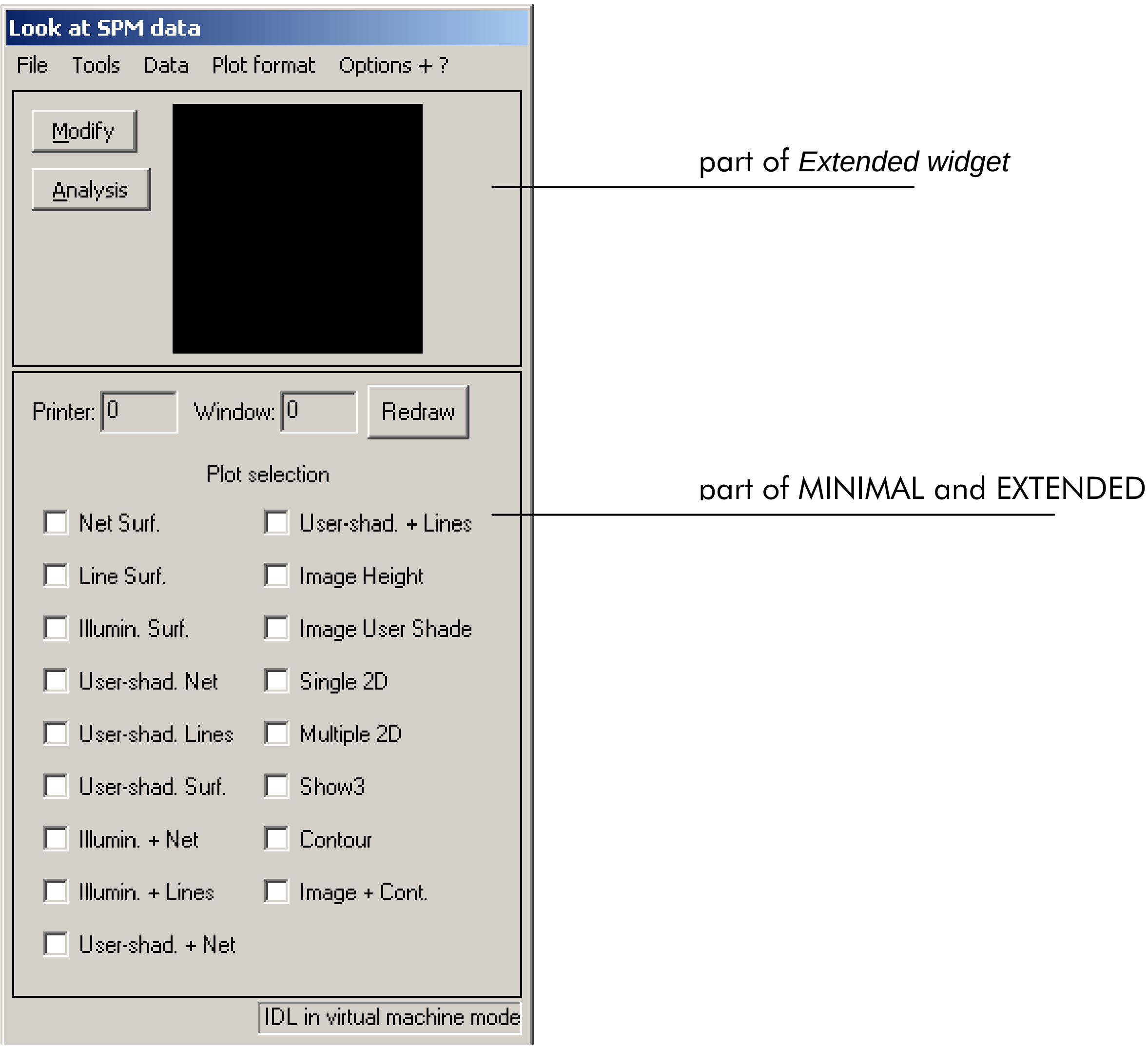


Fig. 11: Extended Widget

As you can see at Fig. 11 *Extended* means that a preview of the marked plot is included in the widget. If your screen is small a minimal widget might be more practical as you can see the entire form. Choose *Options* to select a display mode.

This preference can be saved in ***<name.ini>***.

In the following section the menu items are explained.

3.1 File

3.1.1 Open File

An existing file can be opened. Every file type, MIRA has an import filter for is detected automatically. If the program does not detect your file type, please get in touch with Gunther.Wittstock@Uni-Oldenburg.de
Till now files of the following commercial apparatuses are recognized:

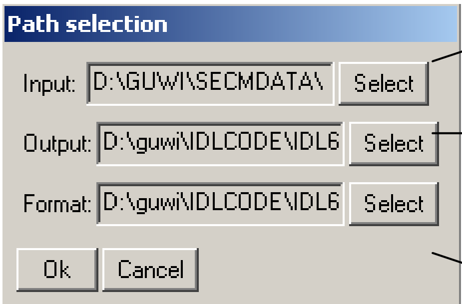
AUTOLAB	potentiostat
CHI	potentiostat
DME	scanning probe microscope
NANOSCOPE	scanning probe microscope
VG	electron microscope
MOLECULAR IMAGING	scanning probe microscope

and diverse home-build apparatuses of several groups

If the inner structure of the files is known, other import filter for other instruments can be made on demand.

3.1.2 Change default paths

You can choose the defaults path for Data input Graphic output and formatting input/output. Please note that when loading files, the input path for this loading procedure can be changed in a dialog. However, for data safety input and output path should never be identical. To change the path setting click on select and use the standard path navigator dialog to select a path.



The folder where the *File/Open* window starts when data are to be read out of.

Folder where the output graphics will be stored were automatically saved.

Folder where formating information is stored and retrieved. The folder where the *File/Save Formating* or *File/Load Formating* window starts when data are to be read out of.

Fig. 12: Path Selection

3.1.3 Save/Load formatting

Select a file to save the formatting information in it. This menu should be chosen if your file is finished and you only want to archive the result. Further MIRA versions will read the file without any problems if the basic structure of MIRA is still unchanged.
Further you can load an existing formatting file to be applied to the data (*Load as current hardware setup*) or to define a new standard for subsequent data sets (*Load as session default*).
Press select to choose a file of which you want to load the information. Finish your selection by pressing ***<OK>***. Up to this moment it is also possible to cancel loading.

3.1.4 Save to/Load from IDL (Interactive Data Language) binary

IDL is a commercial array-oriented language with numerical analysis and display features. It supports interactive reduction, analysis, and visualization of scientific data.
Save a file together with the formatting information in a compressed file format. It allows to save the working state including the processing, axis formatting etc. for later reprocessing. WARNING: Old *IDL* binary file might be not readable in future MIRA versions. This option should be used only for short term storage of work in progress. For long-term archiving saving the original data together with a record on all operation performed with MIRA is suited best.

3.1.5 Import form ASCII

ASCII file can be imported into IDL. They must have on out of three formats. Empty lines are ignored. Comments can be present if preceded by a comment identifier character sequence.

Format type 1: columns of equal length for x,y,z as used by Origin etc.). There can be 2 or 3 columns.

x_0	y_0
x_1	y_1
x_2	y_2
…	…
x_n	y_n

x_0	y_0	$z_{0,0}$
x_1	y_0	$z_{1,0}$
x_2	y_0	$z_{2,0}$
…	…	…
x_0	y_1	$z_{0,1}$
x_1	y_1	$z_{1,1}$
…	…	…
x_0	y_n	$z_{0,n}$
…	…	…
x_m	y_n	$z_{n,m}$

Format type 2: A matrix with x and y values surrounding the z values

--	y_0	y_1	y_2	…	y_n
x_0	$z_{0,0}$	$z_{0,1}$	$z_{0,2}$	…	$z_{0,0}$
x_1	$z_{1,0}$	$z_{1,1}$	$z_{1,2}$	…	$z_{1,0}$
x_2	$z_{2,0}$	$z_{2,1}$	$z_{2,2}$	…	$z_{2,0}$
…	…	…	…	…	…
x_m	$z_{n,0}$	$z_{n,1}$	$z_{n,2}$	…	$z_{n,0}$

Format type 3: A matrix with only z values. x and y values will be integers numbering the columns and rows. The can be transformed to real values using *Data/Arithmetics/X-axis* or *~/Y-Axis*.

$z_{0,0}$	$z_{0,1}$	$z_{0,2}$	…	$z_{0,0}$
$z_{1,0}$	$z_{1,1}$	$z_{1,2}$	…	$z_{1,0}$
$z_{2,0}$	$z_{2,1}$	$z_{2,2}$	…	$z_{2,0}$
…	…	…	…	…
$z_{n,0}$	$z_{n,1}$	$z_{n,2}$	…	$z_{n,0}$

After selecting the menu item the following window appear.

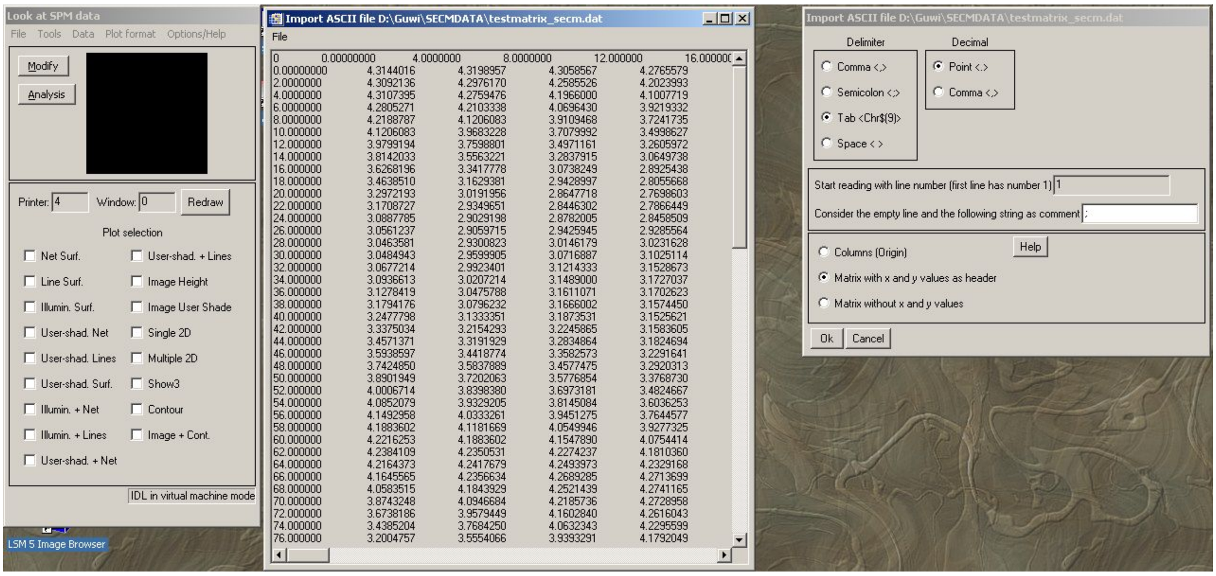


Fig. 13: Windows for importing ASCII data. The file is displayed (middle) to help setting the proper option in the right window.

The options regarding delimiter, decimal point and data arrangements can be adjusted according to the displayed file in the middle. You can specify one or more characters that identify a line within the file as a comment. The content of comments will not be read into variables. Many data files contain header, start marks etc. that can be skipped in this way. A specified numbers of lines can be treated as header. If an error occurs during reading the routine should exit quietly.

3.1.6 Export to ASCII

Export the present file to the *ASCII* format. Various options are available to make the exported file processable by spread sheet programs like *EXCEL*™ and *ORIGIN*™.
ASCII is a standard character set, which transfers every information to an eight-bit character. This code is readable for nearly every computer.

Fig. 14: Export To ASCII

Figure 14 shows the different options of presentation the numerical order of and between the codes.

3.1.7 Selection of graphic format

There are different kinds of graphic output options:

Screen output	Choosing screen output you will get a printout of the complete screen.
B/W postscript	PostScript commands do not drive the printer directly. They are language statements in ASCII text that are translated into the printer's machine language by a PostScript interpreter built into the printer.
Color postscript	→ *B/W postscript*
B/W encapsulated PS	Encapsulated PostScript (EPS) is a subset of PostScript used to exchange a single graphic image in the PostScript format.
Color encapsulated PS	→ *B/W encapsulated PS*
HPGL	Hewlett-Packard Graphics Language A vector graphics file format from HP that is developed as a standard plotter language. Most plotters support the *HPGL* and *DMPL* standards.
PCL	Printer Control Language The page description language for HP LaserJet printers. It has become a de facto standard used in many printers and typesetters.
CGM	Computer Graphics Metafile A standard format for interchanging graphics images. *CGM* stores images primarily in vector graphics, but also provides a raster format. Earlier GDM and VDM formats have been merged into CGM. There are many non-standard varieties of *CGM* in use.
GIFF/GIF	Graphics Interchange File Format Bitmap-Graphic-Format
Bitmap	A binary representation in which a bit or set of bits corresponds to some part of an object such as an image or font.
TIFF	Tagged Image File Format A widely used bitmapped graphics file format that handles monochrome, grey scale, 8-and 24-bit colour.
JPEG	Joint Photographic Experts Group. Compressed files with acceptable quality. The quality is goood for shaded images. It is often unacceptable for line drawings.
Windows system printer	Currently selected standard printer.
Draw widget	Graphic setting for little windows inside the MIRA program

On the right sight of the window you can adapt the output format of the selected printer.
The Parameters:

Left margin contribution	The margin is composed of two contributions: The plot type and the type of output file. Here you can change the output file contribution for the left margin. For plot type depending margin look at *Plot format/Plot-dep, margin*.
Right margin contribution	→ *Left margin contribution*
Bottom margin contribution	→ *Left margin contribution*
Top margin contribution	→ *Left margin contribution*
Horizontal size	Change the horizontal size of the graphic. The number of pixels is given.
Vertical size	Change the horizontal size.
Character size factor	Choose a dimensionless factor for the size of the graphic.
Character thickness factor	To change the thickness of the labelling of the axis enter the favored factor. To change only the character thickness of one of the axis → *Plot format/Axis format*
Line thickness factor	Choose a dimensionless factor for the line thickness.
Tick length ratio	According to the parallel axis percentage tick length of another axis can be selected.
Color ability of printer	Only two values are available: 0 for a non-color printer and 1 for a color printer.
Foreground color	Change the color of the axis and the labels. To get the information about the color-number-affiliations look at *Tools/XPalette.*
Background color	Choose a color for the background. Depending on the printer a start up value is given. Changing the color might be important if your graphic contents a similar palette of colors than the background.
Bits per pixel	To change the resolution by putting in the number of binary digits per pixel. If you want to print a cutout of your graphic increasing the resolution will give you a proper look.
Plot file extension	Every type of printer has its own extension to make the file readable. If you want to use a printer for more than one plot, you have to change the extension. In case you do not the existing plot will be transcribed by the new one.
Orientation	For your printout you can select either *Portrait* (vertical) or *Landscape* (horizontal) orientation.
Connection to the printer	It is possible to copy the file to the printer.

If you are not pleased with your selection you can go back to the startup values.

3.1.8 System printer setup

Choose an installed printer for your printout. If it is necessary change the features by pressing the button.

3.1.9 Print

Click on print to print out the present graphic. **Caution:** a name will be automatically generated and **without query** the file will be printed. If you want to print several versions of one data set in a graphic format, they will overwrite each other and you will find only the file from the last print command. Rename the files after printing to prevent this effect. This algorithm was introduced to accelerate routine processes and avoid annoying queries by the computer.

3.1.10 Start MULTIPLT

If you want to change from *Single plot* to *Multiplot*, you can do that without starting the program once again. The appearing window is shown in figure 15.

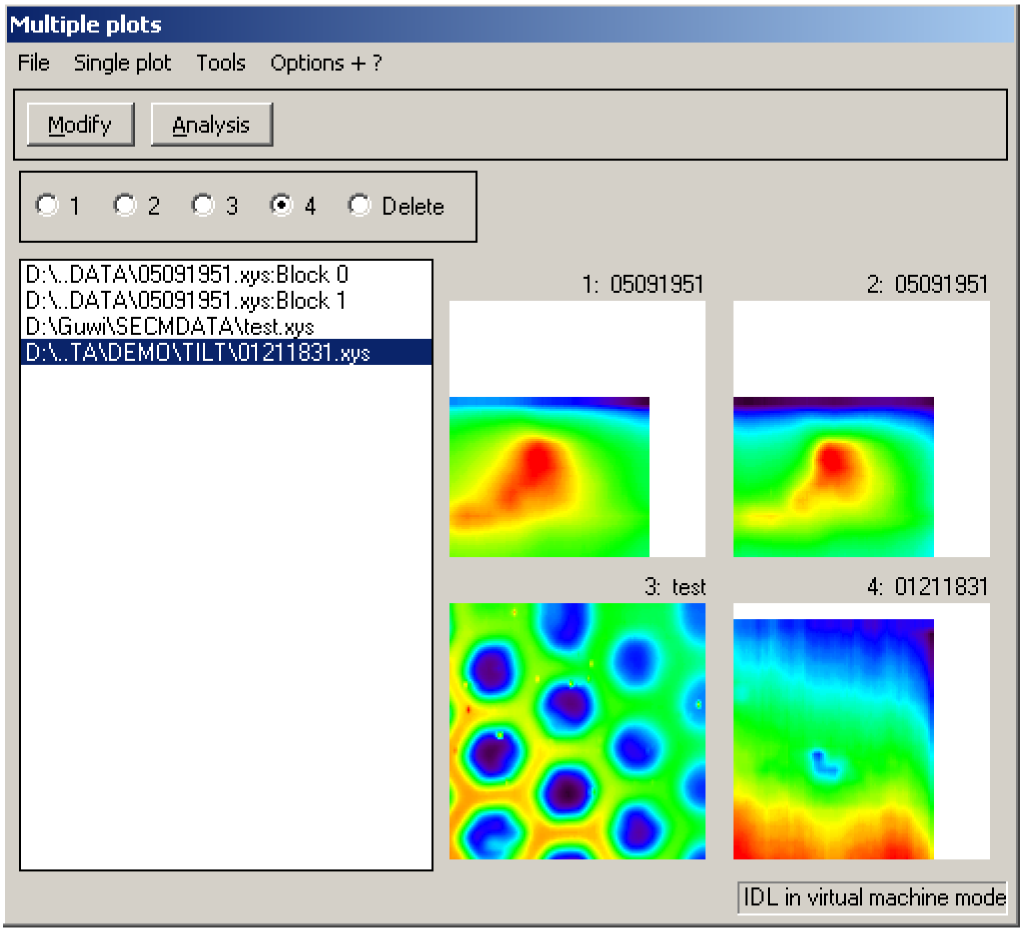


Fig.15: Multiplot Main Window.

→ *Multiplot*

3.1.11 Add to MULTIPLT

Add a the currently processed data set from *Single Plot* to the file list in *Multiplot*. That file will be written down in the list in the left part of the window. How to work with *Multiplot* → *Multiplot*

3.1.12 Exit

Click on *File/Exit* to finish the program.
Note: Do not exit *MIRA* while *iTools* are still active. First close *iTools* then close *MIRA*.

3.2 Tools

3.2.1 XLoadct

Choose a color palette out of forty predefined color tables. To change the brightness it is possible to vary the top and the bottom of color shade (Fig 16).

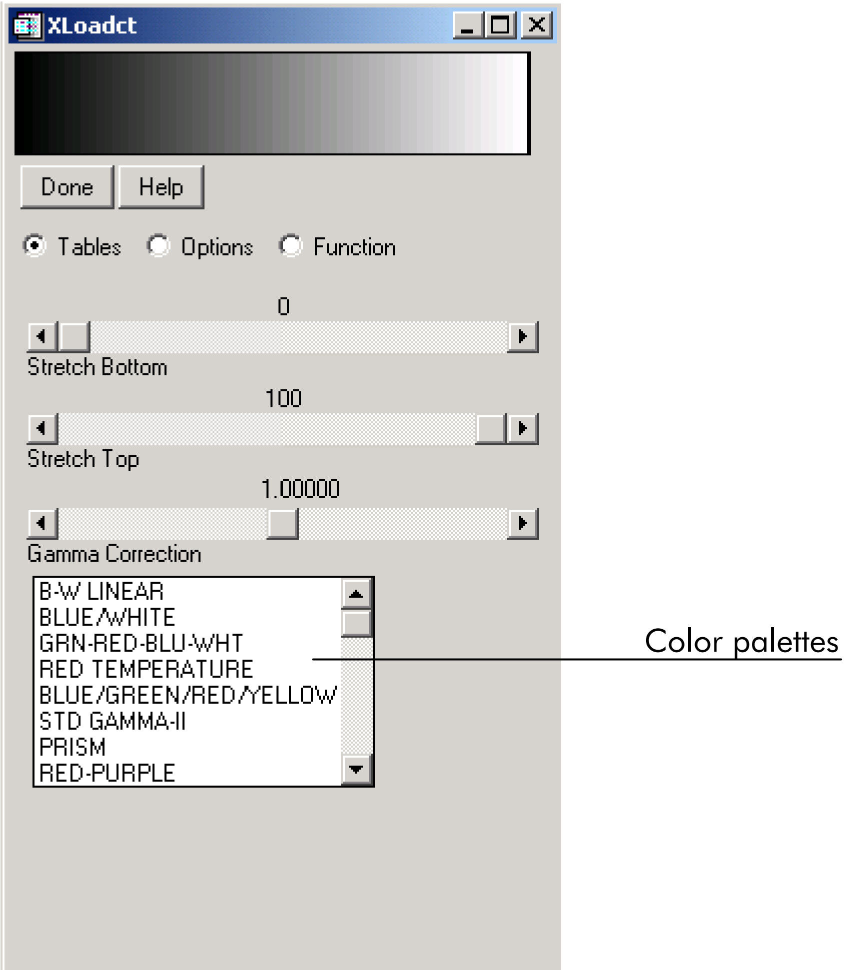


Fig. 16: Xloadct, main screen.

3.2.2 XPalette

For editing the palette a separate tool XPalette is available. Figure 17 shows the main screen of the palette of functions.

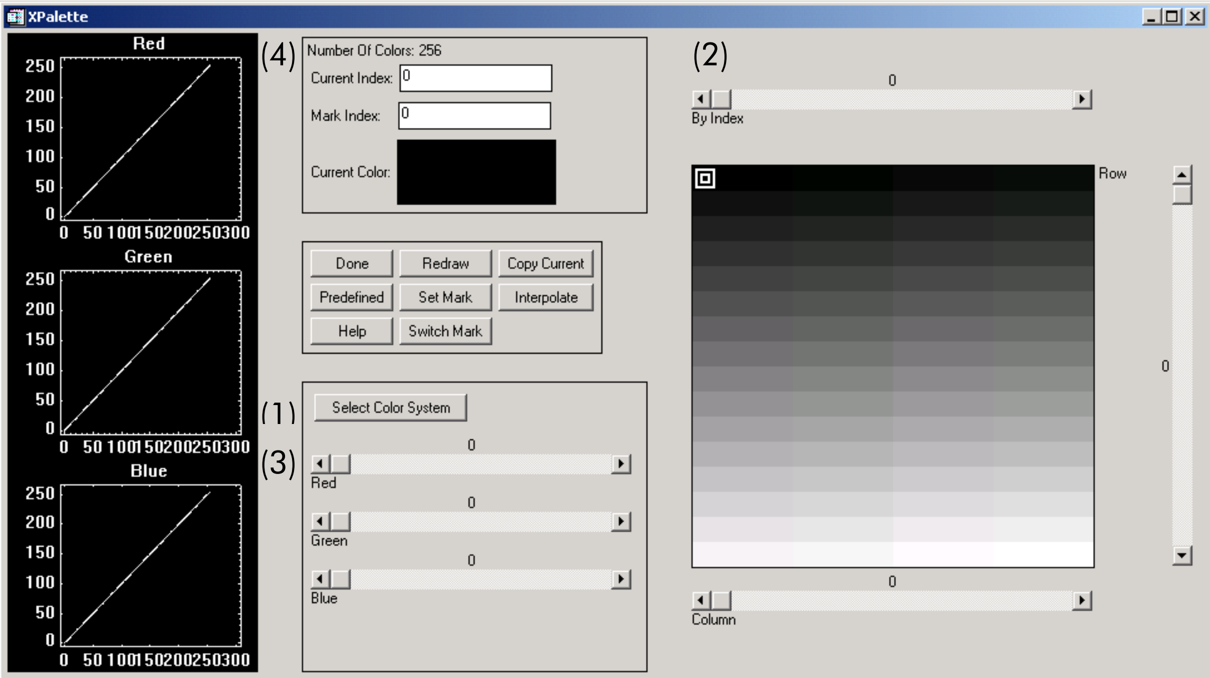


Fig. 17: XPalette, main screen.

At first you should select a color system (1) with which you want to work.

RGB (Red/Green/Blue)
CMY (Cyan/Magenta/Yellow)
HSV (Hue/Saturation/Value)
HLS (Hue/Lightness/Saturation)

By marking a field (2) you can vary the ratio of the different colors (3). To find a special number of one of the 256 colors it is also possible to write down (4). The three diagrams on the left show the amount of red green and blue for each color index.

There are some supporting and executive options in the middle of the window:

Done

Press ***<Done>*** if you want to close the window. All changing will be saved for the following applications.

Redraw

After every changing you have to press ***<Redraw>*** in order to verify.

Copy Current

If you want to get the same color for a row of fields mark the first field of which should assume the color specified by Set Mark. View the result by with ***<Redraw>***.

Predefined

Predefined allows to change the color palette. The window *XLoadct* will appear. After your selection press ***<Done>*** to go back to *XPalette*. To view the change press ***<Redraw>***.

Set Mark

Press this button to give the border for one of the functions *copy current*, *interpolate* or *switch mark*.

Interpolate

To interpolate a color shade between to borders you at first have to mark one border and press ***<Set mark>***. After making the other border press ***<Interpolate>*** and verify with ***<Redraw>***. The result will be a smoothed transition from one color to the other.

Help
To get some help by the program press ***<Help>***.
Switch Mark
If you have worked with *Copy Current* and you want to take the color for the row not from the first marked but from the second marked field press ***<Switch Mark>*** after marking once again the border. So the number of color gets interchanged between *Current Index* and the *Mark Index*. To verify this process press ***<Redraw>***.

3.2.3 Show header

Here you will find the measuring conditions registered by the measure device.
For example, a simple *Show header* form is shown in Figure18.

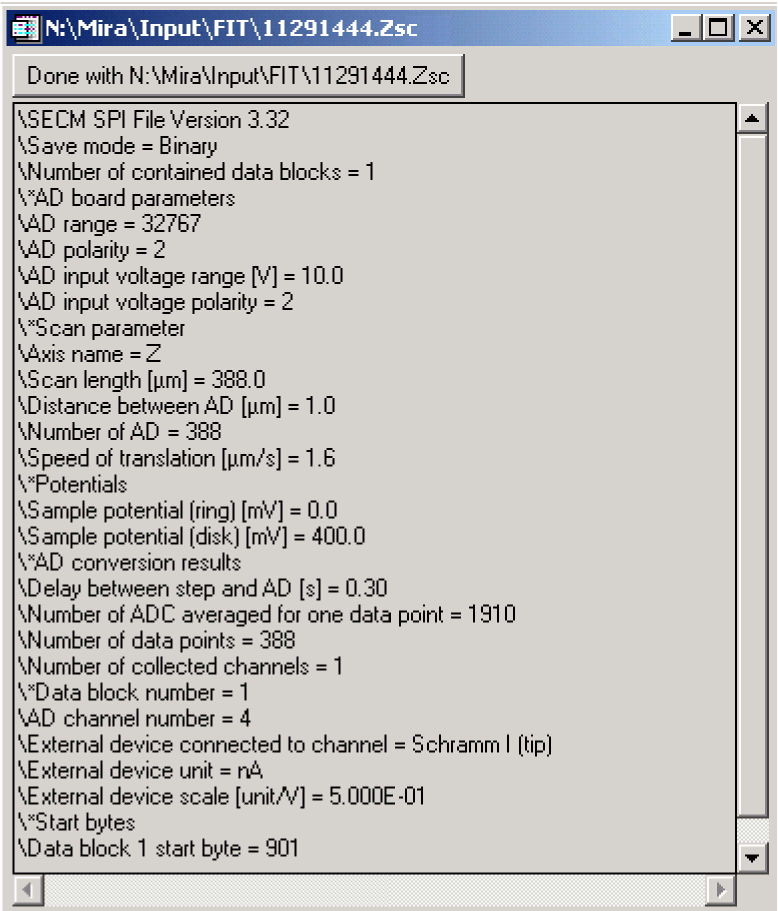


Fig. 18: Example of a header.

3.2.4 iSurface

Starting with this version of MIRA, access is provided to the iTools coming from RSI. This is a family of user interface tools that is programmed by RSI. It shall indicate the future development of the IDL language. It uses an object-oriented approach to graphics whereas MIRA in its traditional form provides direct graphics. In short direct graphics seems to be more efficient for repeating graph applications like encountered in SPM applications. iTools add more to flexibility. However, they are not nearly as efficient for preparing graphs for a lot of measurements obtained on one day. The author recommends to use direct graphics of MIRA for creating plots for notebooks and to use iTools only for those tasks where MIRA does not offer a function. Examples are changing font types and combining different data sets in one graph, making transparent surface plots etc. iTools come with an own set of import and export options. A complete description how to use iTools is beyond the scope of this manual. There is an own manual by RSI which you can call from *Option/Help/RSI Manual about iTools*. Here the general functionality is explained and the data transfer to MIRA is explained. This is the same for all iTools and will not be repeated with the other iTools. If iTools are called with no data sets loaded an empty iTools will be created. You may use that to import some standard data formats supported by RSI. Data formats of specialized instrumentation that are automatically recognized by MIRA will not be loaded.

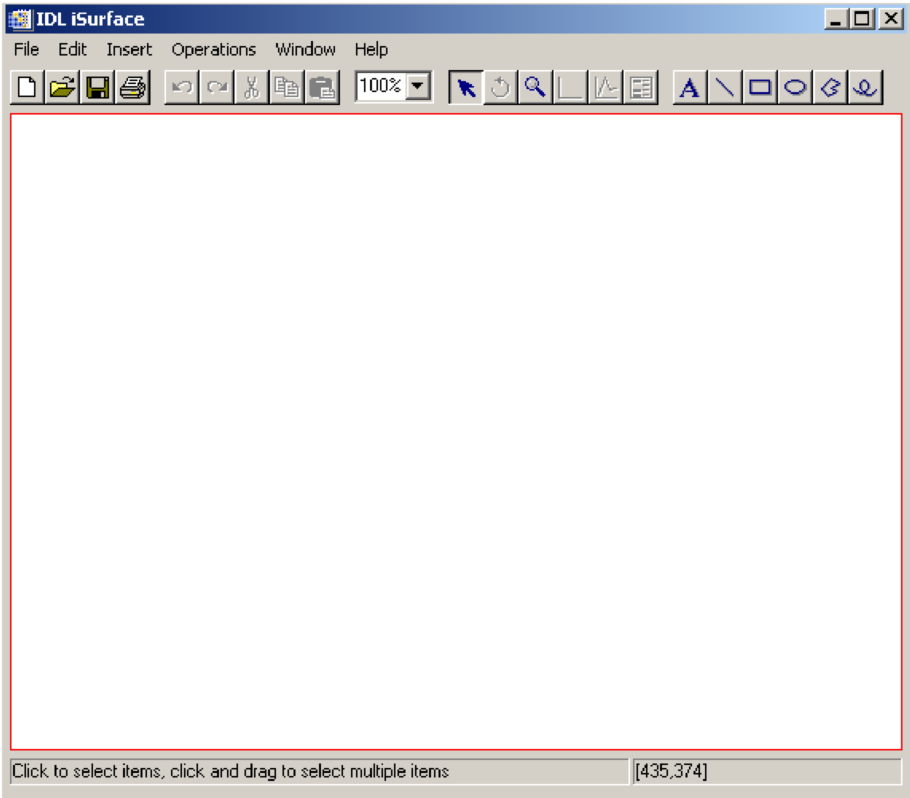


Fig. 19: Empty iSurface tool.

If a 3D data set is loaded, iSurface, iContour, iImage are started with this data set.

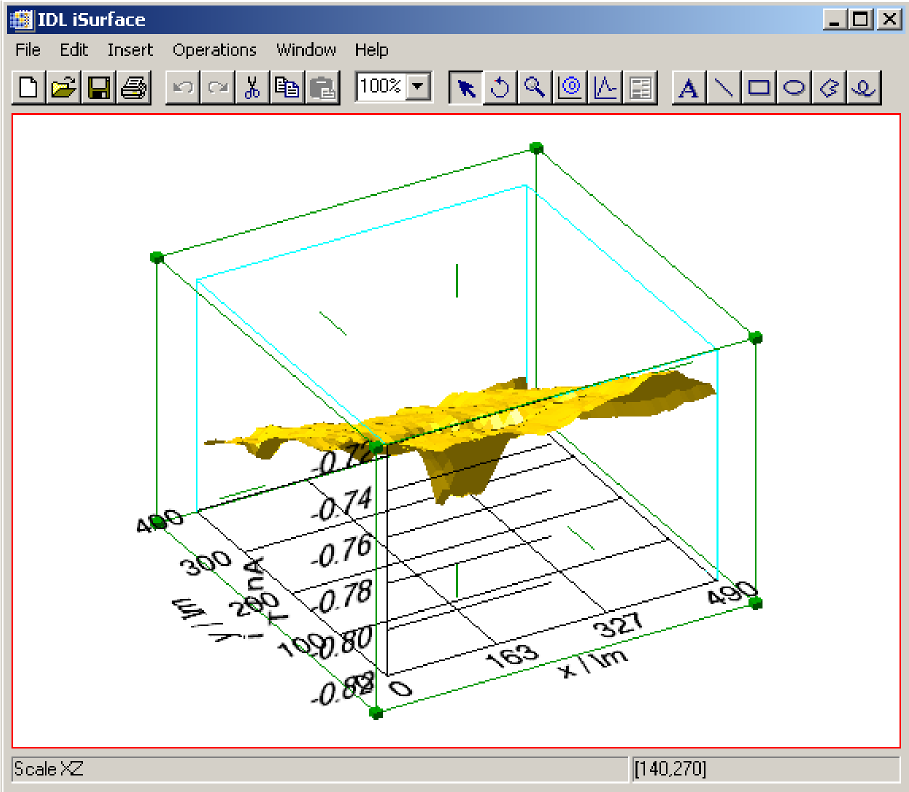


Fig. 20: ISurface with data set.

Changes to the appearance of the plot are made by clicking on the object (e.g. an axis), pressing the right mouse button and calling *Properties*.

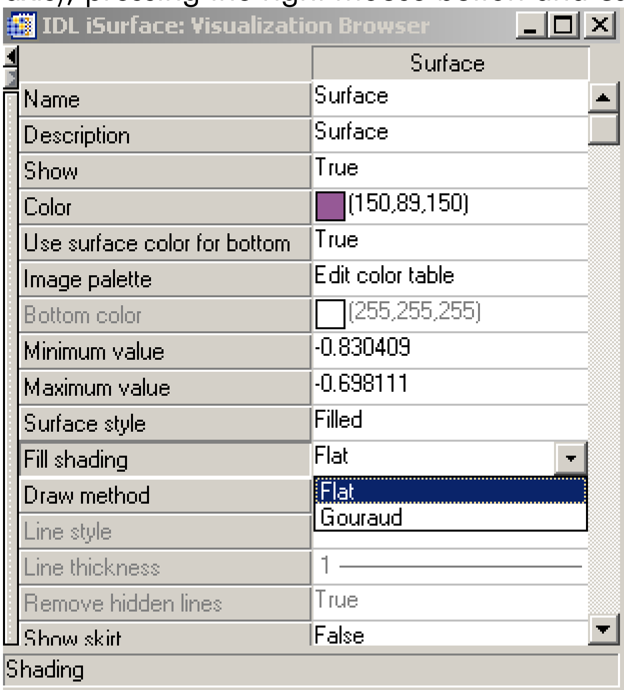


Fig. 21: iSurface property sheet for controlling the properties of the shaded surface. To get the quality you are used to from MIRA you have to set *Fill shading* on Gouraud.

One of the potential application of iTools is the creation of combined plots of two images, e.g. from combined topographic and reactivity imaging from SECM and AFM. Load first the topography data into the *Single Plot* (it works for *Multiplot* the same way). Start iSurface. The data are transferred to the iTool Data manager. Now load the reactivity data. Start iSurface again. You get a second iSurface window with the current data sets. The data do NOT overwrite each other in the iTools. Now you select *Insert/Visualization* in the iTools. You can select a data set (topography) to be plotted as surface and another for the Texture (that is the shading). The export of data from iTools back to MIRA is possible only via Exporting a file from the iTools and reading that into MIRA. This feature has not been tested. It is expected that iTools will develop very fast. Further updates and bug corrections depends on the availability of new IDL versions to the developer of MIRA. No promise can be made at this points. The author would welcome your wish list without returning a warranty that all wishes can be realized.

In general, in the status line at the button of the iTools, the selected object is shown and the possible operations are explained.

3.2.5 iSurface (Shaded)

For a description see iSurface above.

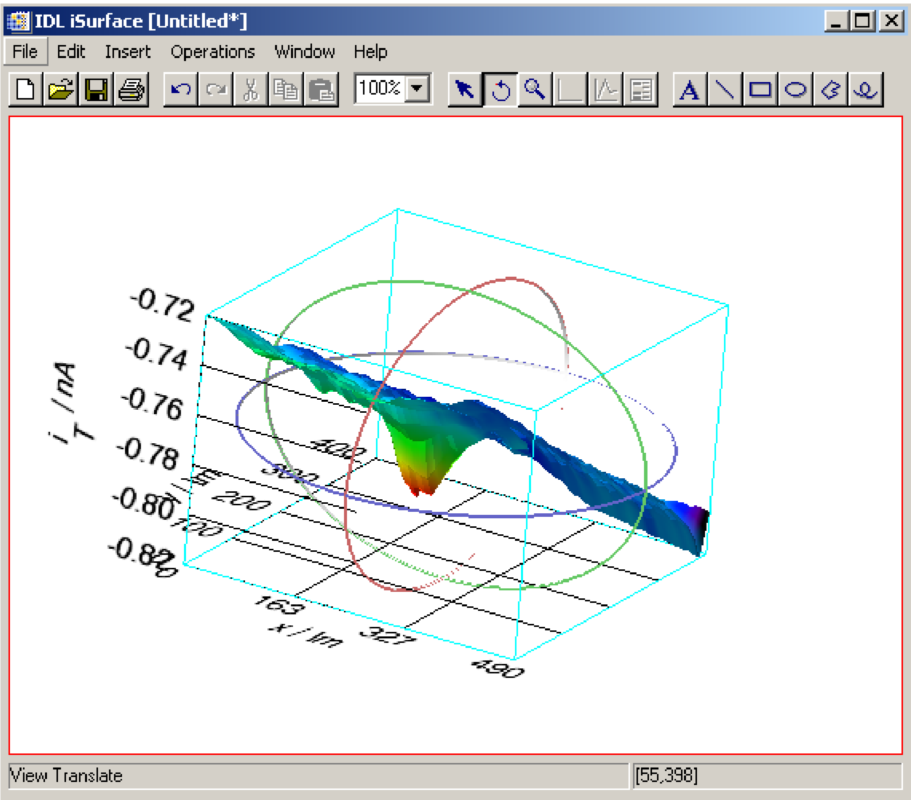
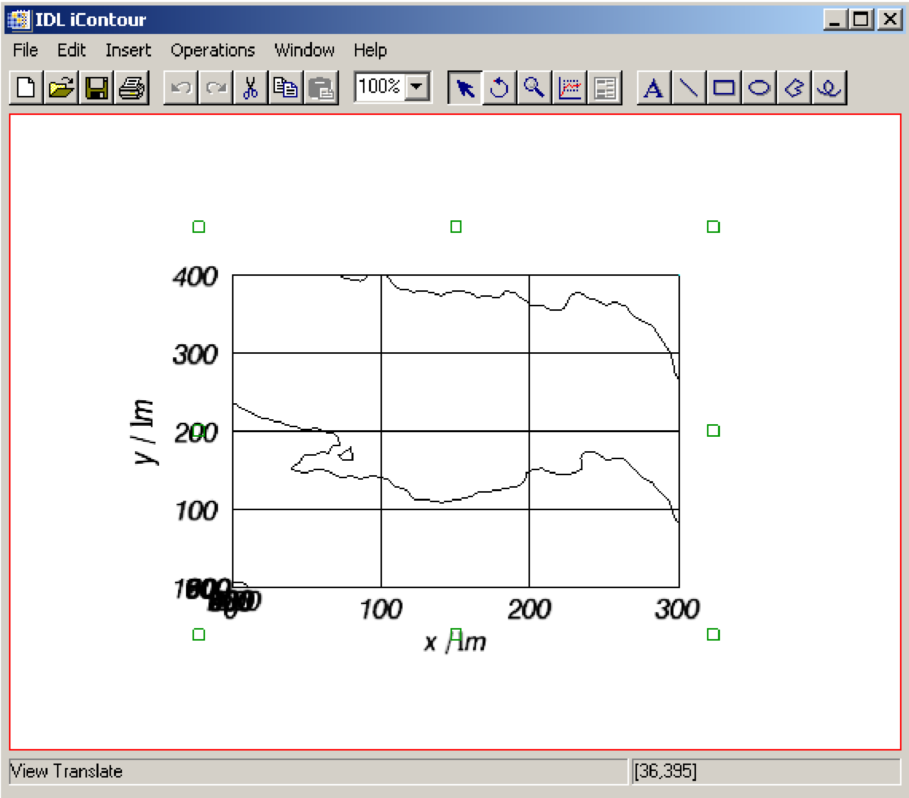


Fig. 22: This is a *iSurface (Shaded)* plot with the rotation tools in action. To get a smooth surface, click on the surface (right) select *Properties* and change *Fill shading* to Gouraud.

3.2.6 iContour

For a description see iSurface above.



Screenshot of iContour after startup.

3.2.7 iImage

For a description see iSurface above.

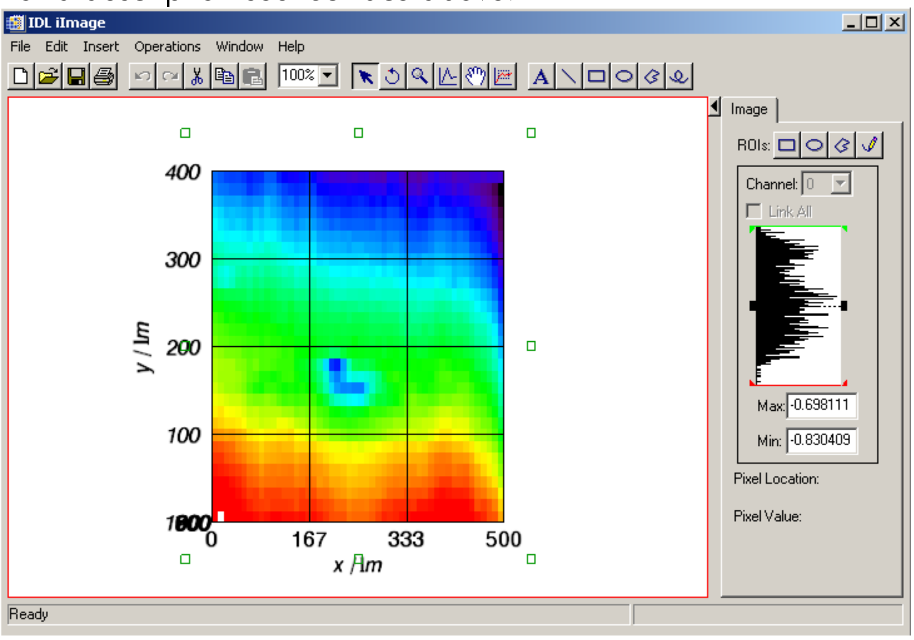


Fig. 24: Screenshot of iImage after startup.

3.2.8 iPlot

This plot is started with a data set only if a 2D data set is active in *Single Plot* or *Multiplt*. The operation is generally the same as described for iSurface.

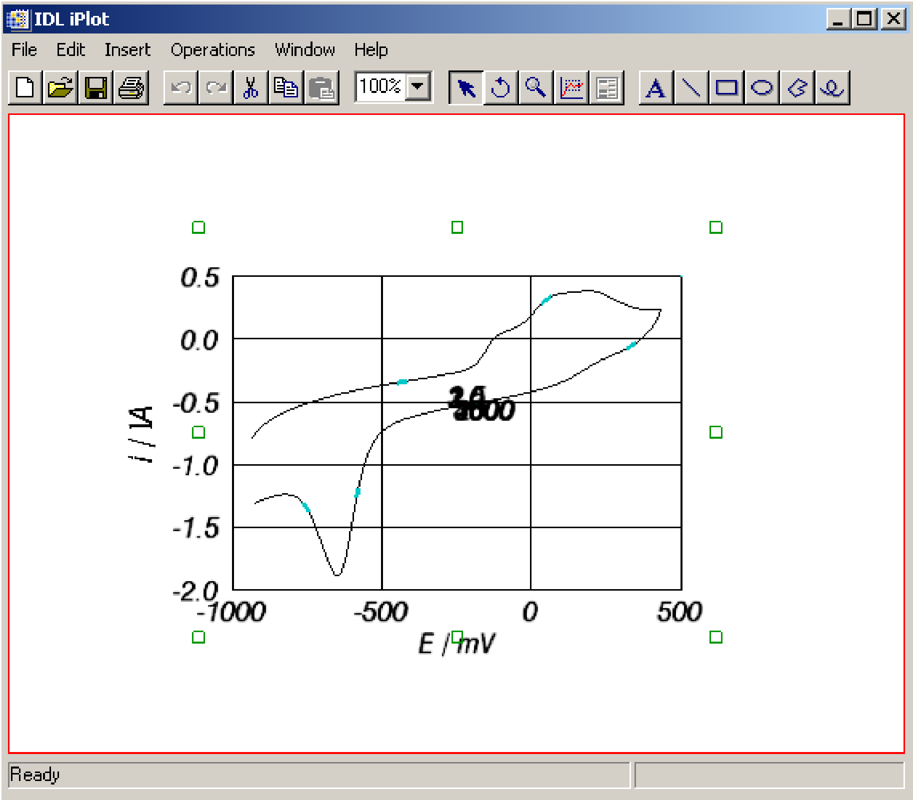


Fig. 25: Screenshot of iPlot after startup.

3.3 Data

3.3.1 Subsets

Select the range between the given borders for X- and Y-Axis. Acknowledge by pressing ***<Update>*** either under the text field or the graph windows depending on whether you would like the graphic or the text input to become the new value. You can go back to the start-up values or close the window.

For example:
The complete data set is shown in the upper right form. You can select a subset for closer inspection (Fig. 26). You can either give the index in the text field and press ***<Update>*** below. Alternatively you can simply draw a rectangle in the window on the top right side of the form. Press the left mouse bottom, hold and draw to the opposite corner, release (no border mark is drawn). The selected section will appear in the lower window. You can repeat this process many times. If you press update on the right side, the current subset will be updated in the text windows and on the main program. For changing the axis or legend format use options of *Axis Format*.

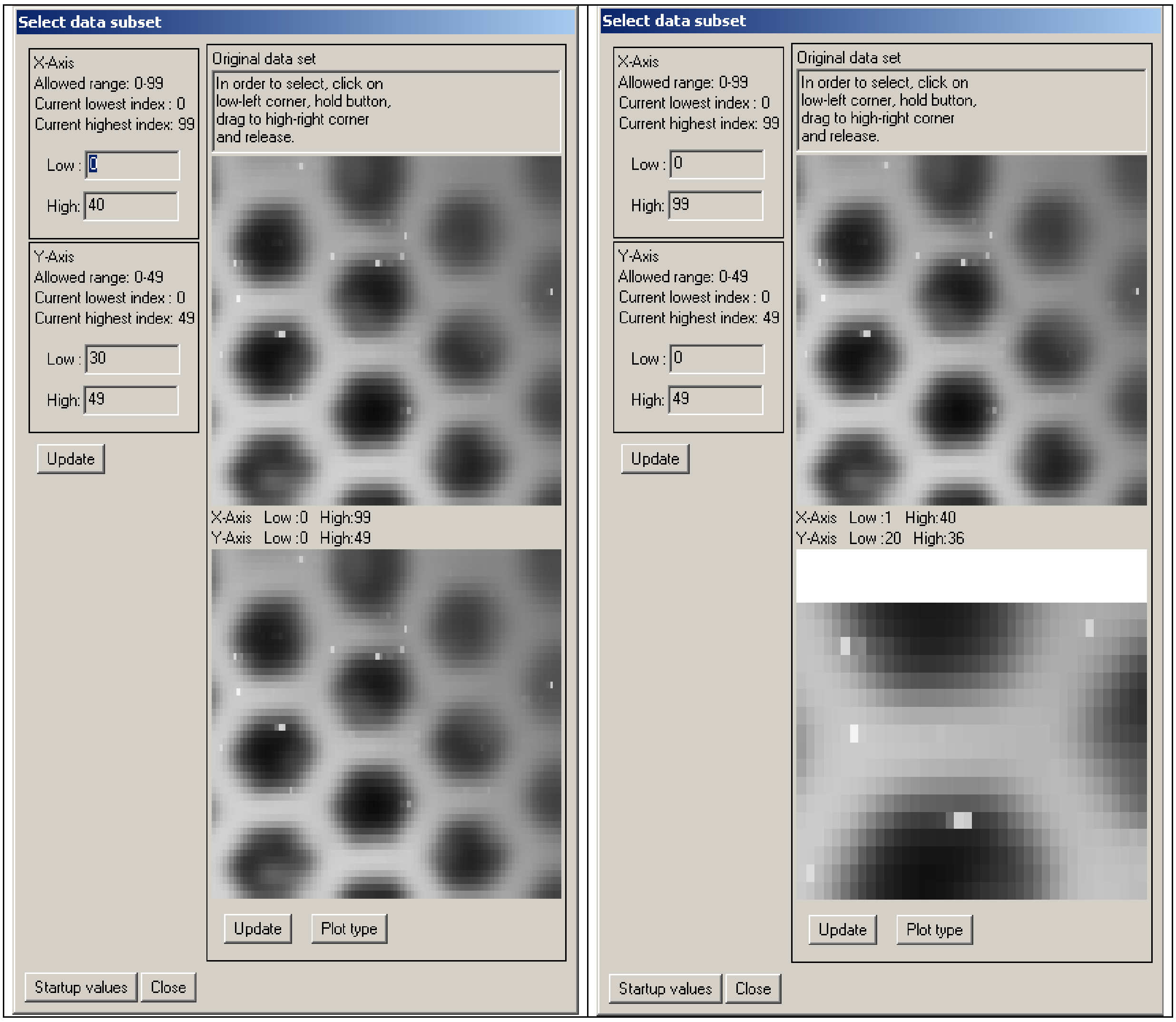


Fig. 26: Subsets: Plot before enlarging a part of it

3.3.2 Resize array

Change the array dimensions. Enter the favored factor to increase the pixel number in each direction. The new number of points is calculated by new pixel number = old pixel number * FX or pixel number = old pixel number * FY.

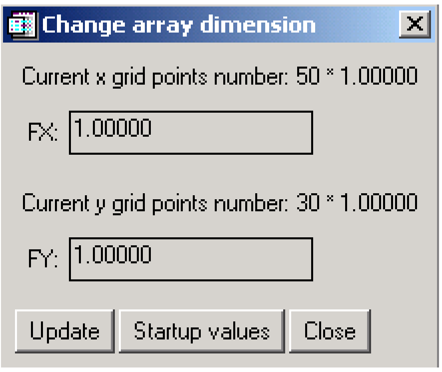


Fig. 27: Resize Array

3.3.3 Arithmetic

This function gives the chance to perform arithmetic transformation of the x, y or z data sets.

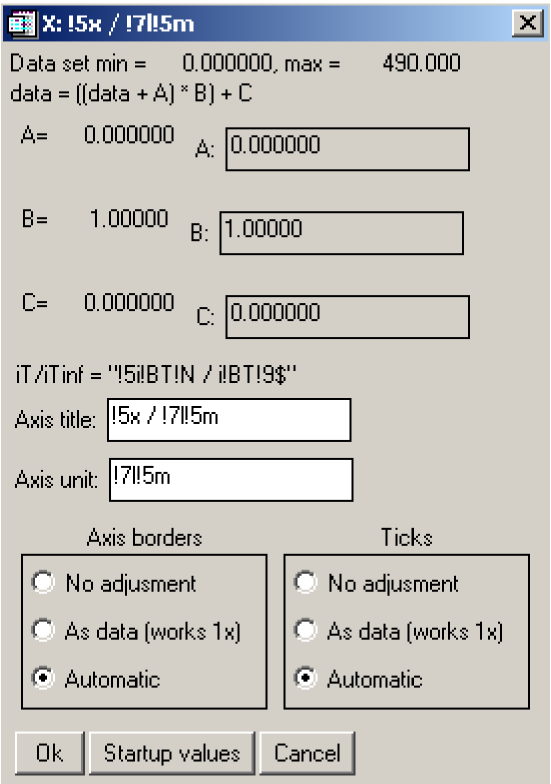


Fig. 28: Arithmetic, main screen

To normalize your data it is possible to multiply with constant value. You can also add a constant. Axis borders can be adjusted with the data set.**Data cutoff**

According to the smallest and the highest value for z you can cut off a part of your data range by changing the high or low border.

Figure 29 shows an area of a plot in which there are many spikes.

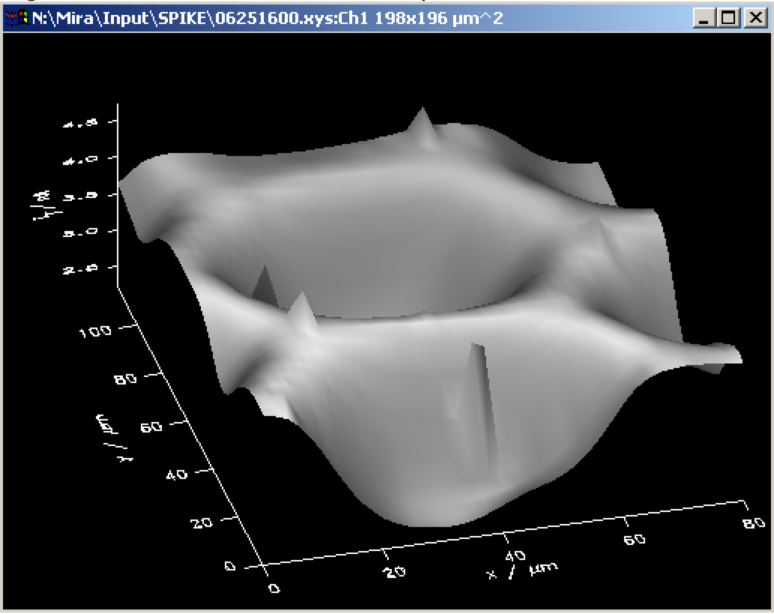


Fig. 29: Data cutoff: Spike area before flattening

To give an idea about the amplitude of the spikes another plot seems more practical:

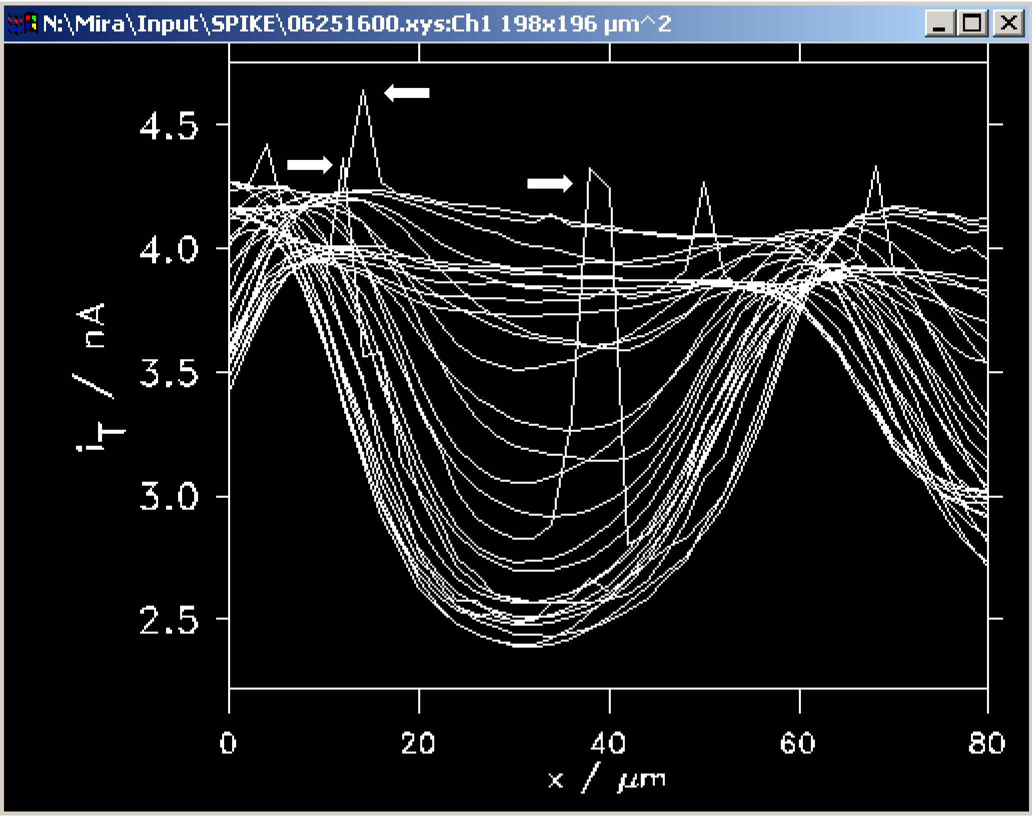


Fig. 31: Data cutoff: Spike area, shown in a two-dimensional plot

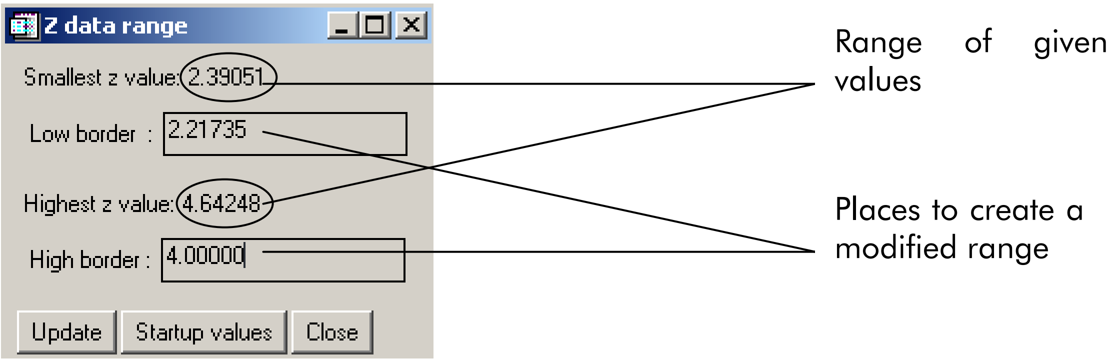


Fig. 32: Data cutoff, main screen.

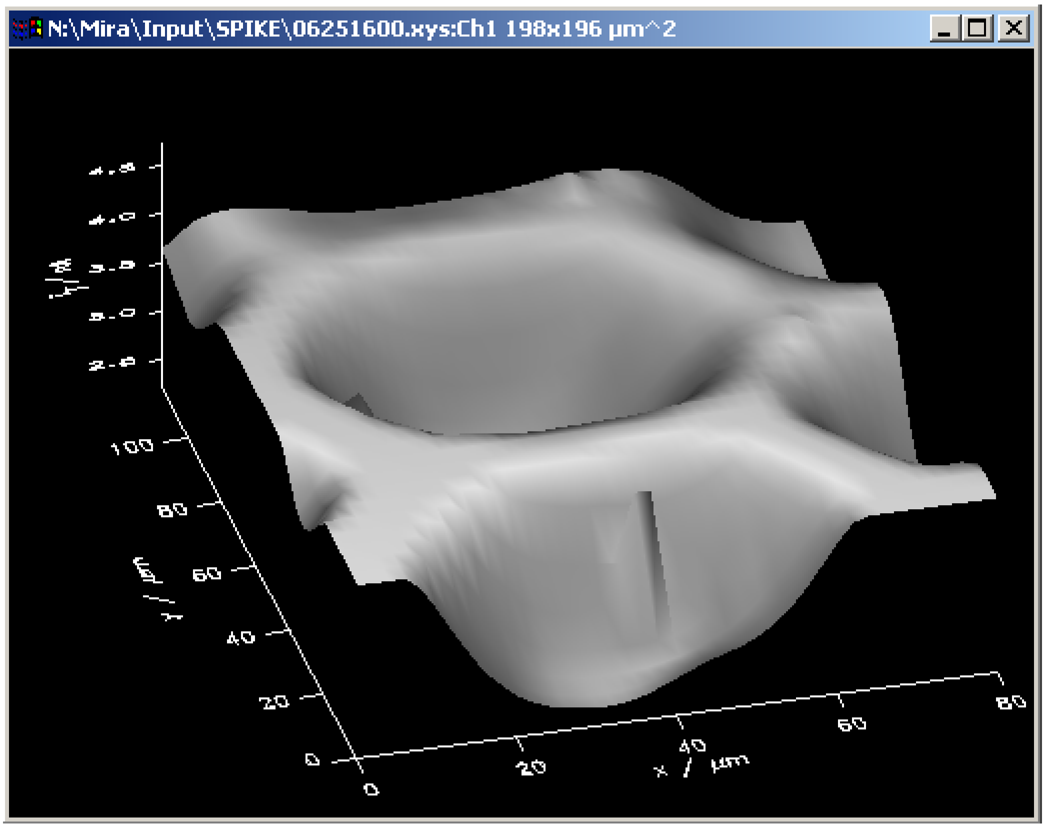


Fig. 33: Data cutoff: Plot after cutting the z data range.

The 2D plot will show the effect much more obvious:

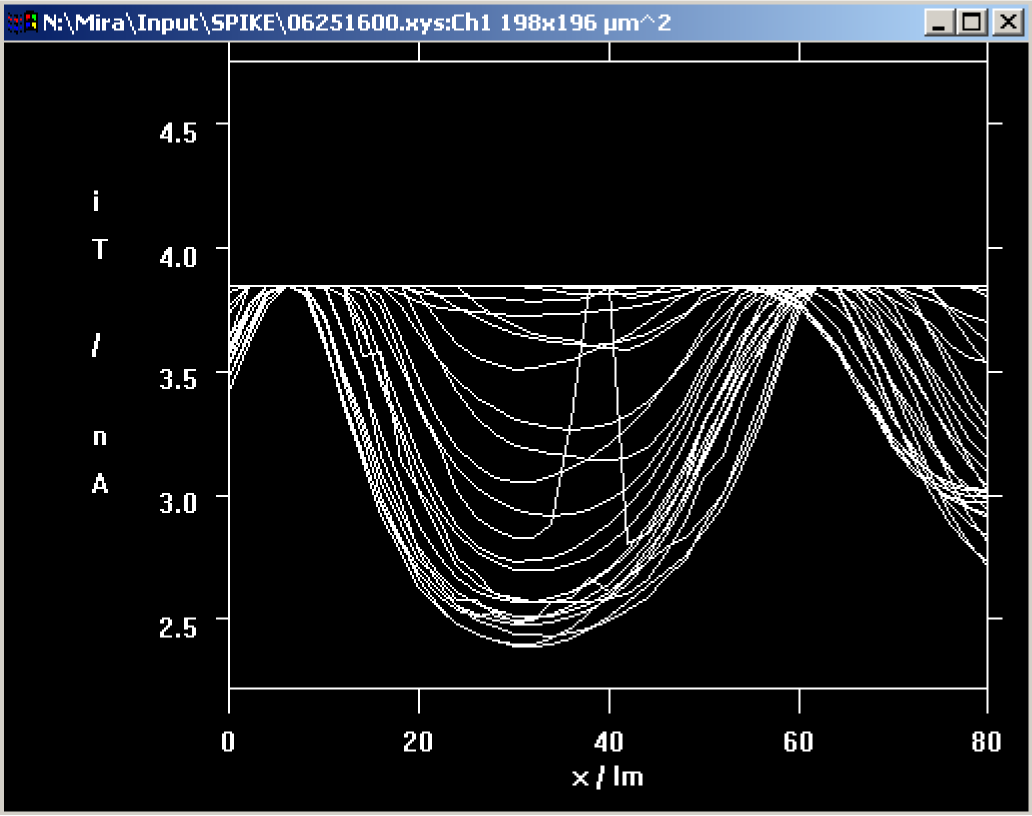


Fig. 34: Data cutoff: This setting of data cutoff value clips a considerable portion of the data points to the maximum value.

3.3.5 Rotate array

If you want to rotate your data set within the fixed coordinate system mark the choice of transformation. The program is able to rotate and transpose on 90°, 180°, 270°.

3.4 Plot format

3.4.1 Handle volume data

Volume data are data in which the probe performs the same mechanical movement as in imaging. However, at each grid point a complete 2D experiment (e.g. cyclic voltammetry or chronoamperometry) is performed. This experiment is called dependent experiment. These data can only be on a 2D paper by a projection. The Handle Volume data window provides access to automatise these functions. It shows an image (upper part) of the projected data and a time trace of the selected grid point in the image. In the example the lowest left point is selected an marked by a white rectangle around the point. If the projection method is ***Slice number***, the slice to display can be selected by the cursor in the time trace (vide infra).

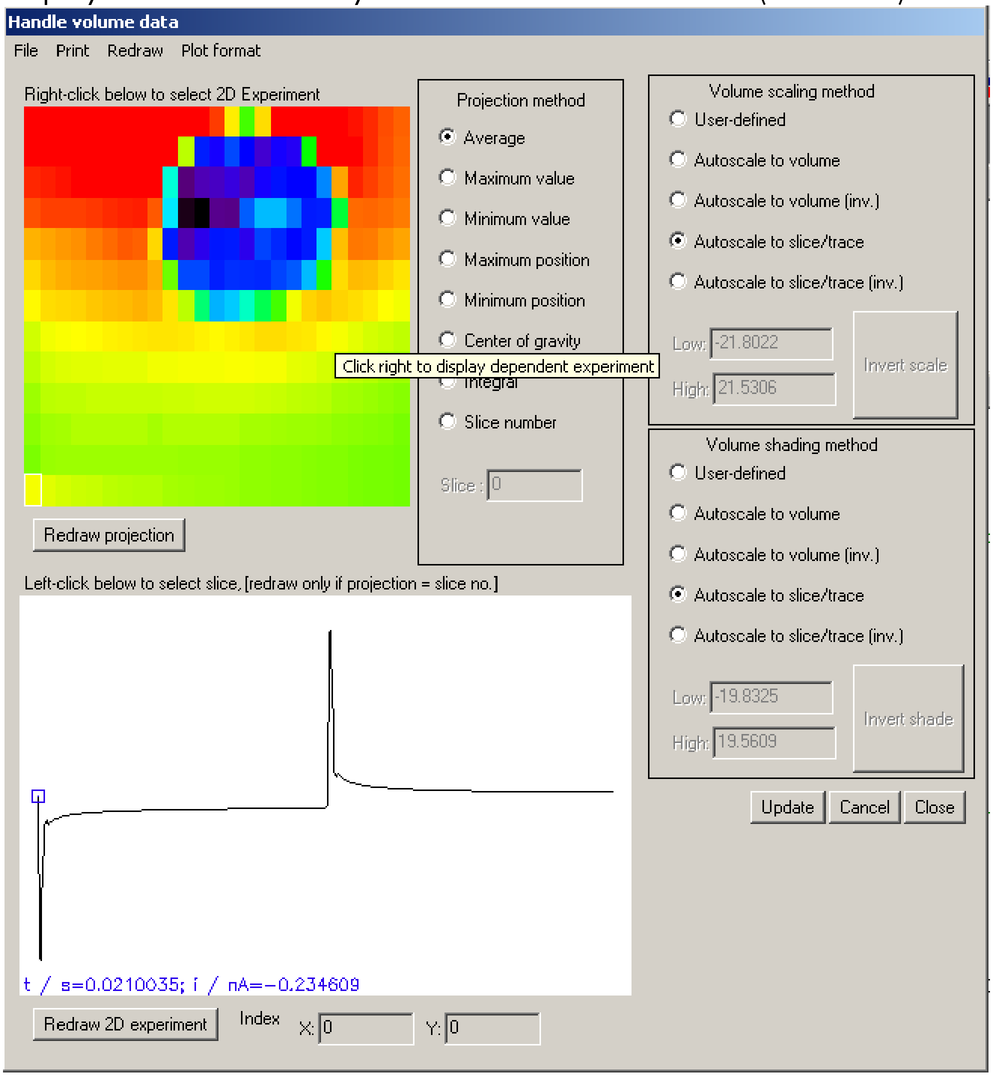


Fig. 35. Handling of volume data.

In order to obtain an image, the data at each grid point must be compressed to one data value. The method is selection by the radio buttons right of the image.

Average	The image is composed of the average *y* values of each of the dependent 2D experiments.
Maximum value	The image is composed of the maximum *y* values of each of the

	dependent 2D experiments.
Minimum value	The image is composed of the minimum y values of each of the dependent 2D experiments.
Maximum position	The image is composed of the x value of each of the dependent 2D experiments at which the maximum signal was recorded.
Minimum position	The image is composed of the x value of each of the dependent 2D experiments at which the minimum signal was recorded.
Center of gravity	The image is composed of center of gravity r of the dependent 2D experiments at which the maximum signal was recorded. $r = \frac{1}{n}\sum_{i=0}^{n-1} x_i y_i$ (x and y are the data pairs of the dependent experiment)
Integral	The image is composed of the integral of each 2D experiment.
Slice number	The image is composed of the y value of slice n of each 2D experiments.

The button ***Redraw*** projection causes the current projection to be redrawn in a separate graph window using the plot type selected in the main SPM window.

The ***Redraw 2D experiment*** causes a the currently selected time trace to be redrawn in a separate window as x,y-plot. Note there is a difference between time trace and *x,y*-plot, especially for cyclic voltammograms. The time trace in Fig. 35 shows the data a $y = f(t)$. The plot $y = f(x)$ can also give a loop if x is a triangle voltage ramp.

The radio button ***Volume shading method*** and ***Volume scaling method*** works in connection with the menu option ***Print/Print all slices***. This option exports a n images, one from each slice. The z axis is scaled according to the selection of the scaling method and the shading is made with the selection specified with Volume shading option. The n images can be combined to a movie that reflects the change of the signal in space and time.

The menu options are similar to other menus.

File/Return trace (2D) + Close	Returns the current trace as new 2D data set. The information on the 4D volume data is lost in SPM window, closes the window
File/Return projection (3D) Close	Returns the current projection as new 3D data set. The information on the 4D volume data is lost in SPM window, closes the window
Close	Closes the window
Cancel	Closes the window
Print/Selection of graphic format	Selects the graphic format for later output
Print/System printer	Selects the printer for later printing
Print/Print current projection	Prints the current projection to file or printer
Print/Print all slices (img)	Prints a series of all slices to file (for making a movie)
Print/Print current trace (2D)	Prints the current x,y experiment to file
Print/Print all traces (2D)	Prints all x,y experiments to file
Redraw/Redraw current	Redraws the current projection to a graph window

projection	
Redraw/Redraw all slices (img)	Redraws a series of all slices to a graph window (for inspecting a movie)
Redraw/Redraw current trace (2D)	Redraws the current x,y experiment to a graph window
Redraw/Redraw all traces (2D)	Prints all x,y experiments to a graph window
Plot format/Axis format	Allows to explicitly set axis format of x,y,z, time and x variable of the dependent experiment
Plot format/Scale user shade	Allows to set all the options for the user scale to plot the projections

3.4.2 Create view

Change the values for the graphic axis.

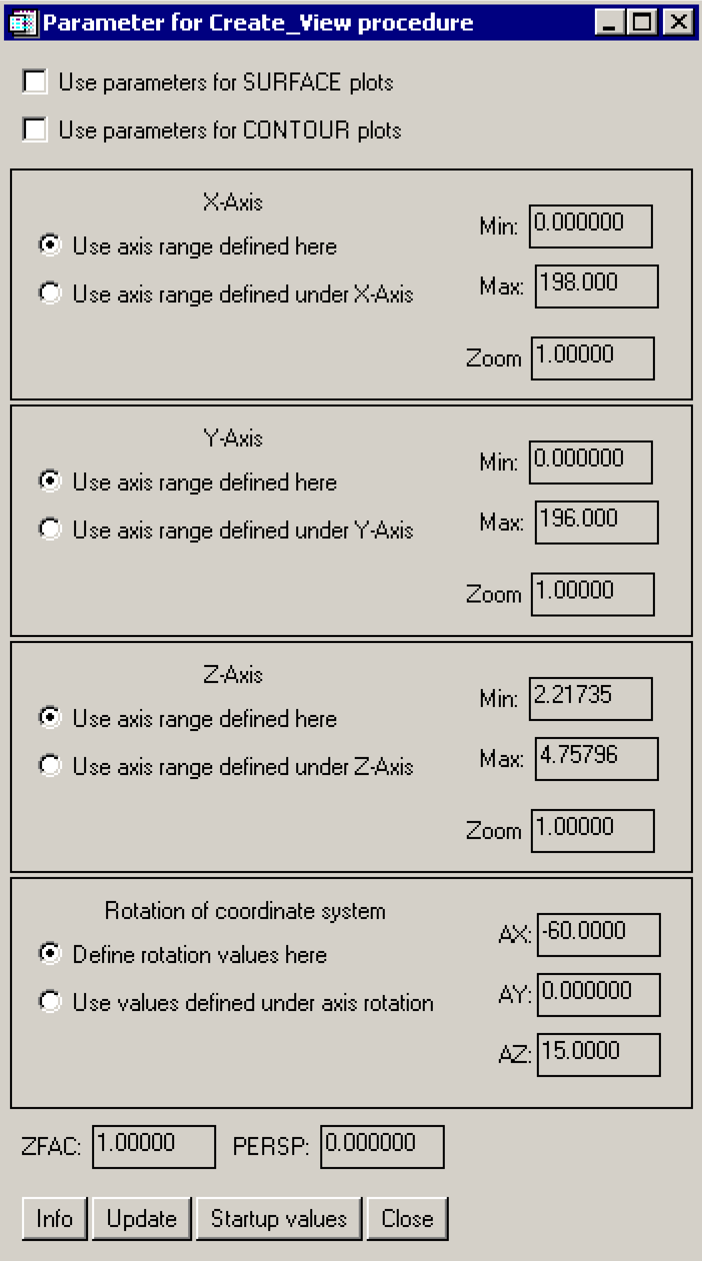


Fig. 36: Create view.

If you want to create a plot with a 3D coordinate system whose length is proportional to the real length in each direction you can define the viewing options here. This is good if the imaged areas deviates much from a square.

3.4.3 Plot-dep. margin

By choosing this function you will be able to change the plot-depending margin parameters. Startup values are given to which you can go back.

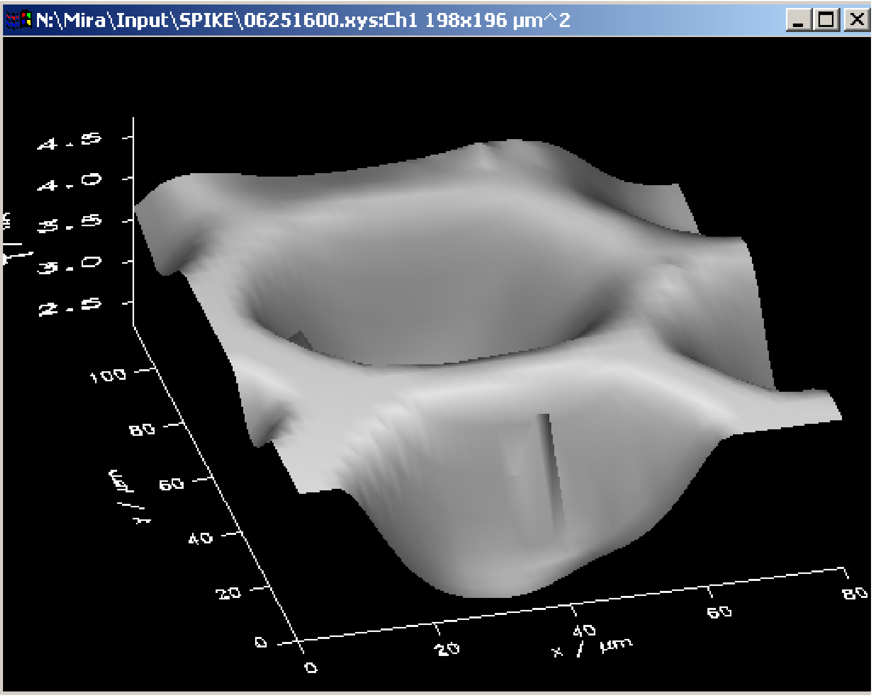


Fig. 37: Plot-dep, margin: Before changing margin.

As you can see in this plot (Fig. 37) the left margin should be set higher to make the axis label of the z axis readable. Choosing *Plot-dep, margin* the following window will appear:

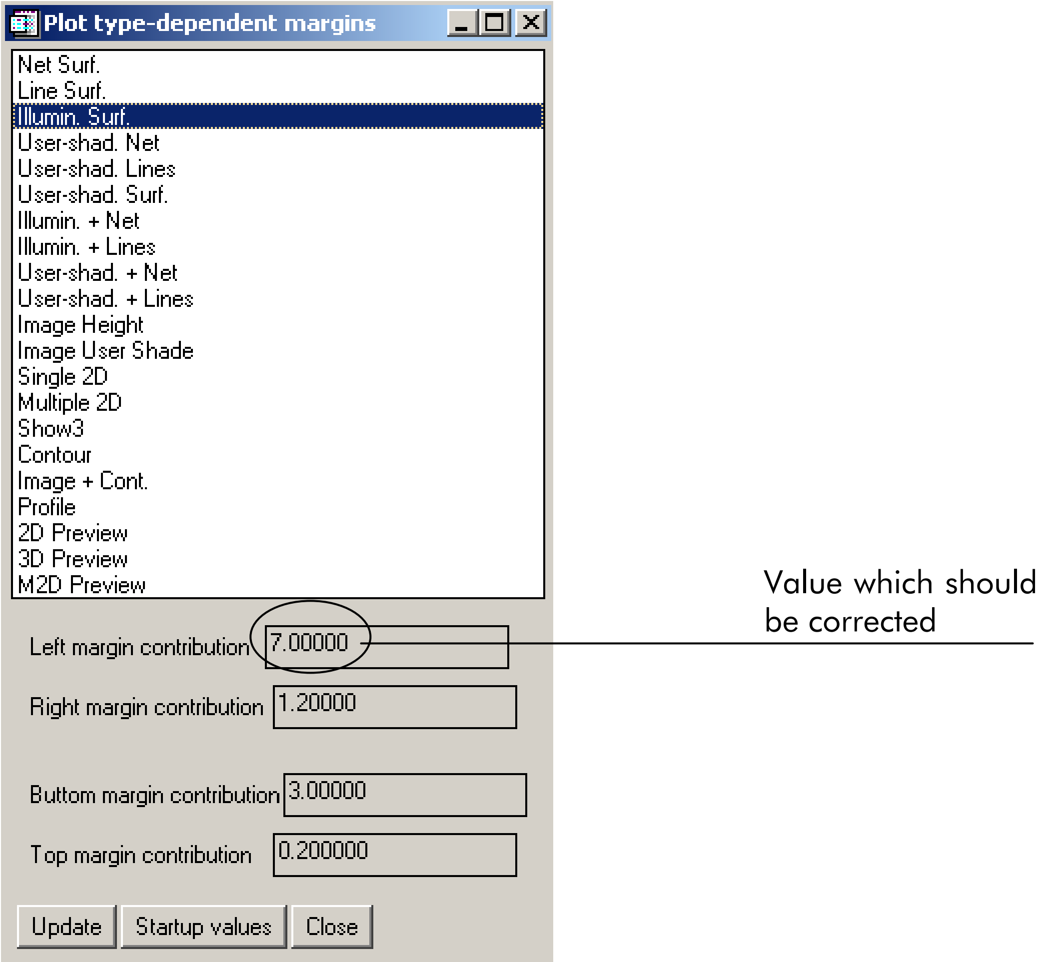


Fig. 38: Plot-dep. margin, main screen.

Standard values are given for every margin.
Changing the marked value into 10.00000 the result look like this:

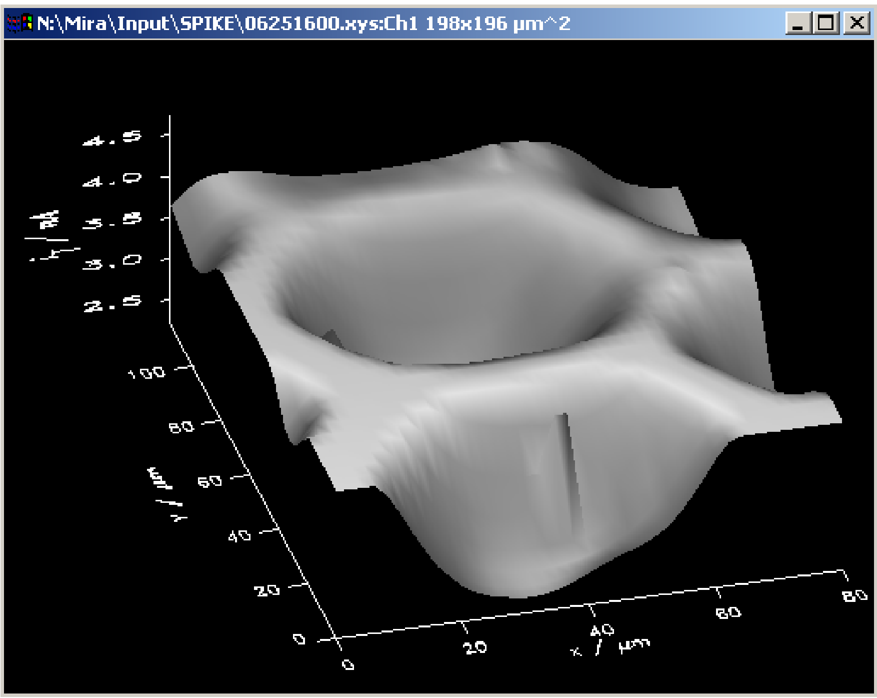


Fig. 39: Plot-dep. margin: Plot after correcting the margin contributions.

As you can see in Figure 39 the axis title fits into the plot window.

3.4.4 Plot region

Sets the limits of the plot region. This can be set here but will only affect Combined Plots. The position of the Single Plot is controlled only with the Plot-depending and hardware depending margins.

→ *Combined Plot: Example 2 - Create a Stacked Surface plot*

3.4.5 Skirt

Insert a skirt to your plot.
This option is only possible if you took a line- or net-structured plot. Every dot at the margin of the image is connected to the basis by a line.

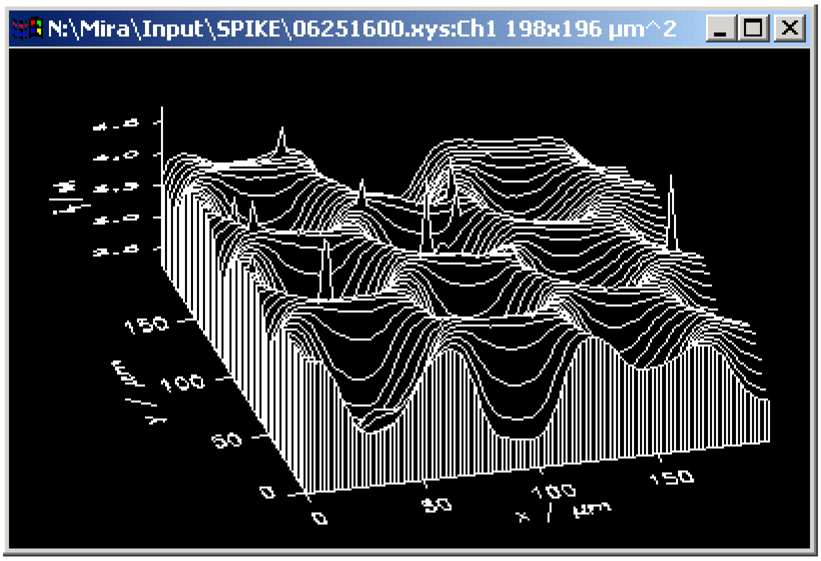


Fig. 40: Skirt: Plot including a skirt.

3.4.6 Axis rotation

Changing the rotation of the coordination system to get another view of the plot. Vertical and horizontal rotation is possible.

3.4.7 Axis format

Create the axis of the plot (X, Y, Z) by formatting everything depending on the ticks.

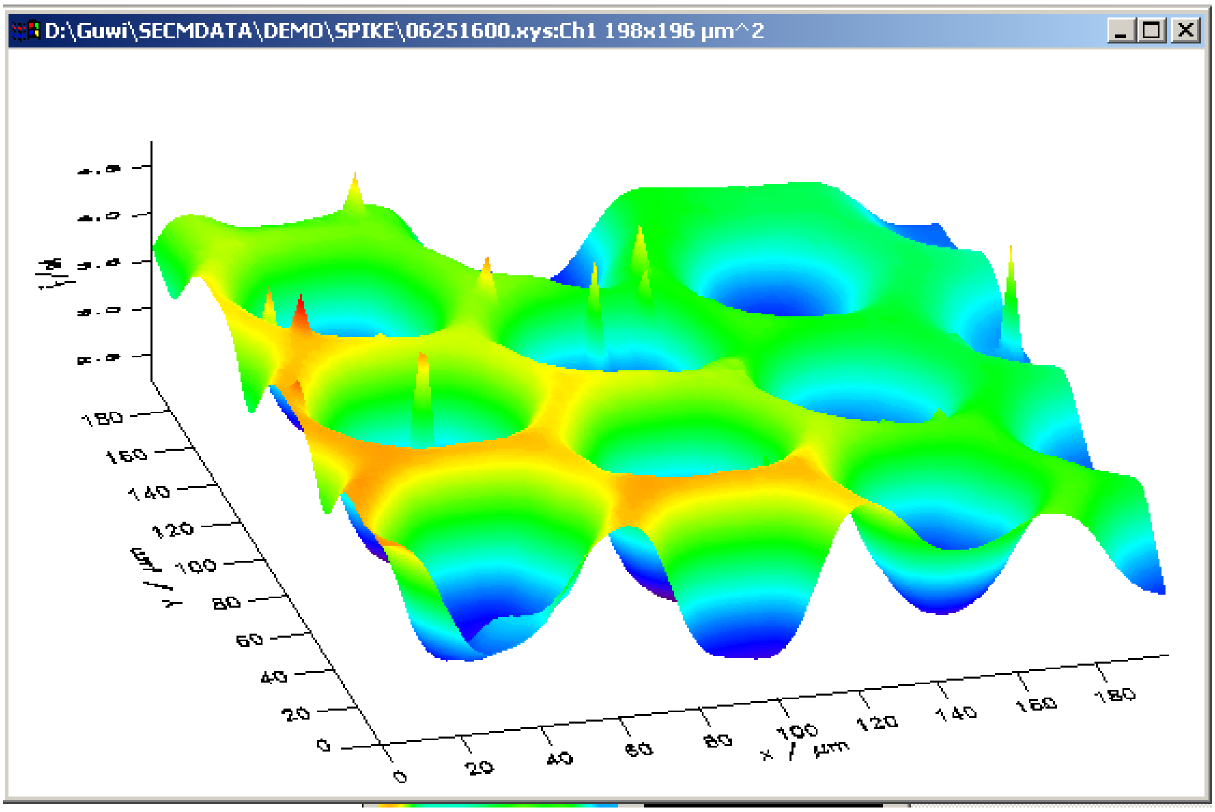


Fig. 41: Axis format: Plot before enlarging the values of z-axis.

As you can see in figure 41 the legend of the vertical axis is too small and not readable.

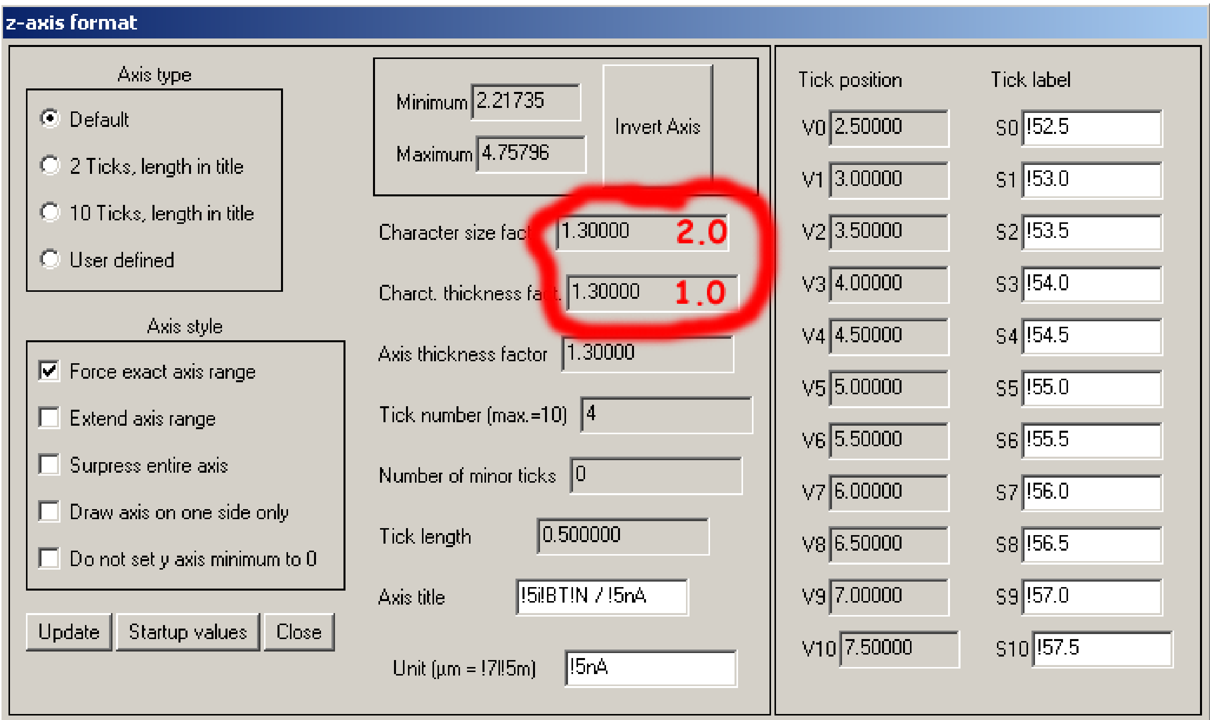


Fig. 42: Axis format - correction of character size and thickness of an individual axis.

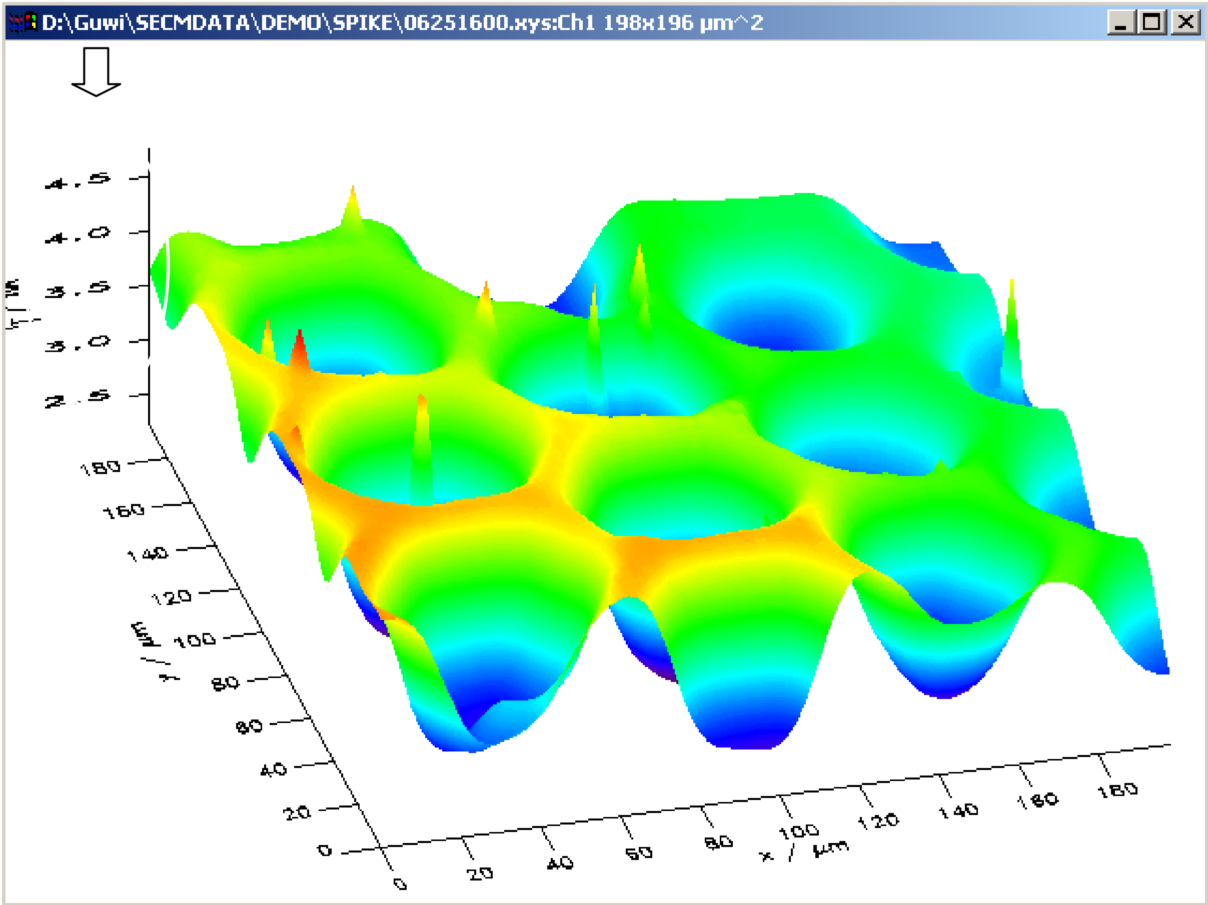


Fig. 43: Axis format: After enlarging the values beside the axis.

To change the margin contribution to complete the view of the axis information → *Plot-dep. Margin*.

3.4.8 Scale user shade

The form user scale can be used for two main purposes. The first one is to highlight small features on a rising background. Consider the following image. A small increase in the reduction current is present in the center of the image. In a standard 3D plot there are two problems (Fig. 44, right) i) the peak in reduction current points "downwards" ii) the shade does not highlight the feature because the slopy background cover a wider data range than the peak. This situation is quite common in SECM imaging with signals of small magnitude (e.g. from enzymatically active surfaces). One can enhance the image without altering the data itself, by inverting the content of the *Minimum* and *Maximum* text fields in the *Axis format* window. For this purpose, call *Plot format/Axis/Z* and invert minimum and maximum of the axis. Click *user defined* for *axis type* (Fig. 44, left).

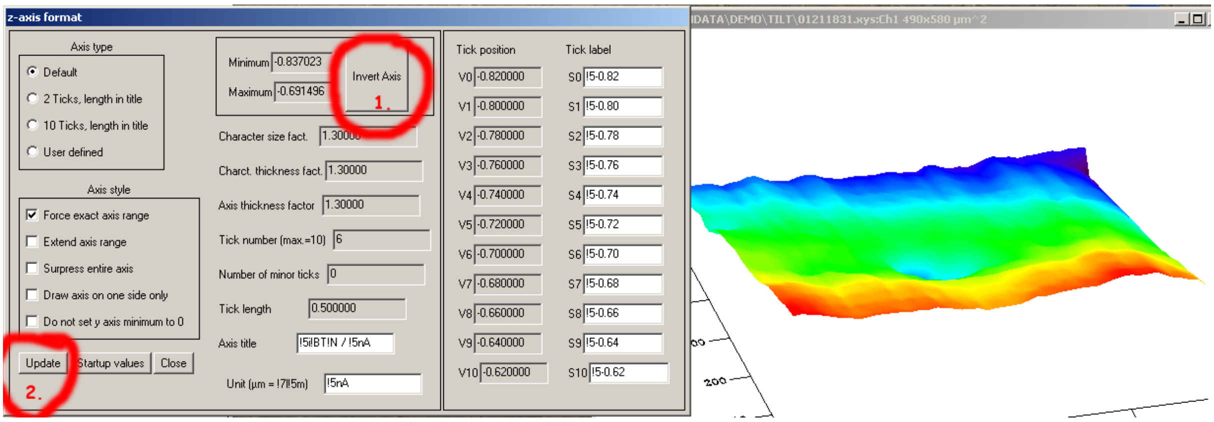


Fig. 44: Scale user shade: Only a part of the shade palette is used. The peak points "downwards".

Press ***<Update>*** in the *Plot format/Axis/Z* window and ***<Redraw>*** on the Single plot window. You should obtain the following graph.

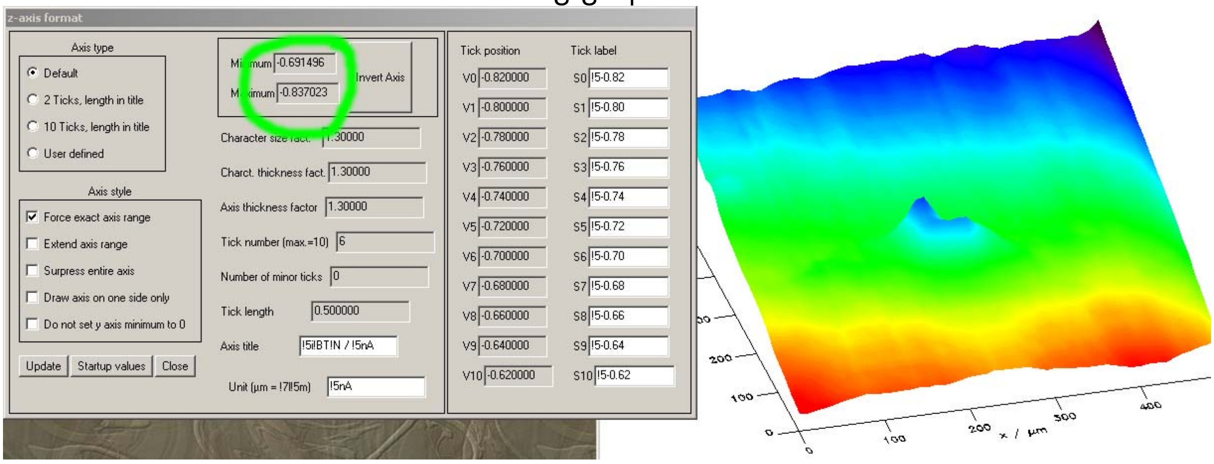


Fig. 45: Scale user shade: The peak points "upwards" now. The color shading is still not highlighting the feature in the center.

In order to use the scale of shades more effective than in Fig. 45, there are some options in the form *Plot format/Scale user shade*: The have in common, that a background is subtracted before converting the current values to a color scale. After subtracting the background, the resulting z array was scaled to the 0...254 (indicated in the left side of the image. This scales was used to color the surface plot. Gouraud interpolation was automatically used for the shading.
Furthermore, the color scale was inverted (option box in the lower left part of Fig. 46) and scaled to minimum and maximum values to make best use of the entire color scale. You can make any setting by selecting user-controlled shading. The inverted color scale emphasize that the feature is a maximum (in reduction currents) although arithmetically it is a minimum (reduction currents have a negative sign by IUPAC convention).
Please note, that in all cases the actual position of the z values is still the original. If you want to correct the z values itself and not just the shading (for tilt correction in a topographical AFM picture, use *Modify/Polynom flatten*, *Modify/Line by line flatten* and *Modify/Rolling sphere flatten*.

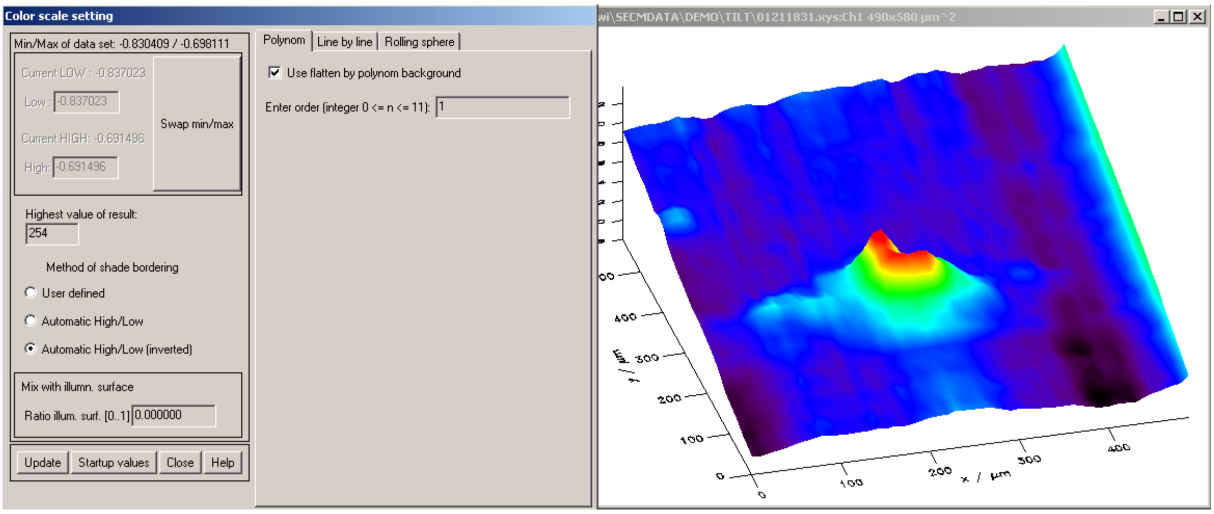


Fig. 46: Scale user shade with polynom background subtraction (order = 1, i.e. a plane) and the resulting plot.

Option a), see Fig. 46:
A polynom was fitted to the data set. this polynom was subtracted. The remaining variation in current was converted to a color scale. The order of the polynom can be between (0 = subtraction of a constant, 1 = subtraction of a tilted plane, ... 11). Experience shows that high polynom orders usually do not give good results. Try first 1 than 2 and so on. You also have to indicate in the Check Box "Use ..." that the polynom should be used.

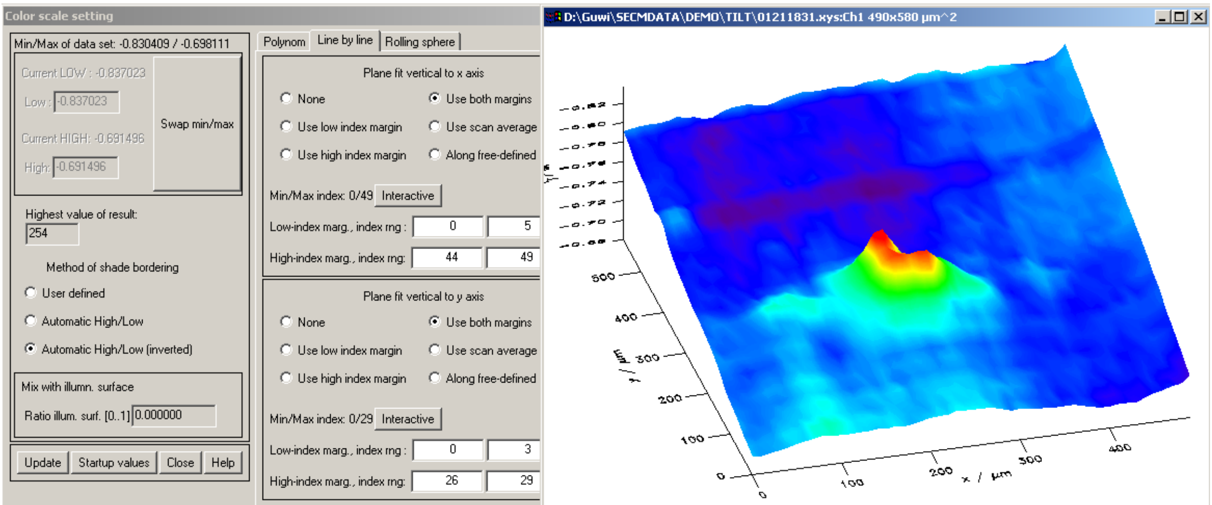


Fig. 47: Scale user shade with Line-by-Line background adjustment and the resulting plot.

Option b), see Fig. 47:
From z data at both margins of each line scan in x-direction and y-direction an average value of the currents for each scan was calculated. A temporary array for the z data was created. The mean values of each scan were subtracted from the measured z values. After subtracting the means of each line in x and y the resulting z array was scaled to the 0...254. The width of the margins used to calculate the mean of each line scan can be set by the white text boxes. For calculations of the mean you can use only one of the two margins, both margins or the entire line.

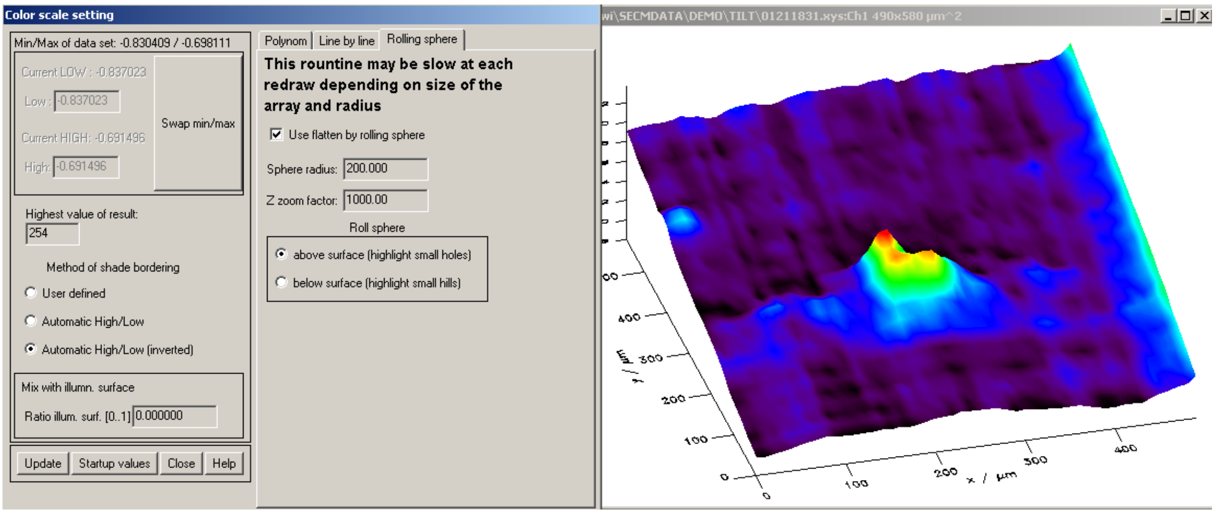


Fig. 48: Scale user shade with background adjustment by a rolling sphere above the data, followed by an inversion of the axis and the color scale and the resulting plot.

Option c), see Fig. 48:
The background calculation is done by calculating the path a sphere would roll above or below the data. If it rolls above, it highlights small depression, if it rolls below it highlights small elevation. Features of larger dimensions are removed. Important parameters are the size of the sphere and the z-zoom-factor that controls a stretching of the features during calculation.

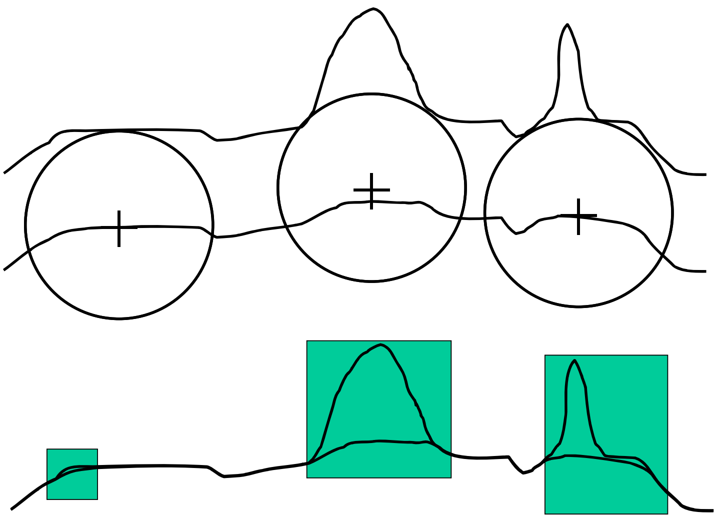


Fig. 49: Principle of the background removal by a rolling sphere. The path of the midpoint of the virtual sphere is taken as the background.

The second use of the *Plot format/Scale user shade* window is the creation of the hight proportional shading mixed with an illumination. Pure height-shaded images tend to hide small differences in data (the texture). An image that resembles how our eye receives texture is computed as an image *d*(*i*, *j*) that would arise from diffuse reflection of light. The incident light is described by a vector **L** (set by *Plot format/Light source*) and the surface normal **N**. **N** is computed for each image point *z*(*i*, *j*) from its four neighbors *z*(*i*-1, *j*-1), *z*(*i*-1, *j*+1), *z*(*i*+1, *j*-1), *z*(*i*+1, *j*+1). The gray or false color value is then computed from the scalar product of **L** and **N** (|**L**| |**N**| cos(<(**L**,**N**)). This algorithm together with Gouraud interpolation and consideration of ambient light and depth cueing is implemented in MIRA as well as in other image processing packages.

The image computed for diffuse reflection and height scale can be mixed by a linear combination in different ratios. Set the contribution [0...1] of the illuminated surface in the text field right above the ***<Update>***-button.

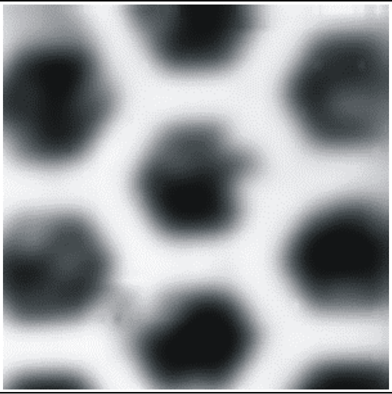
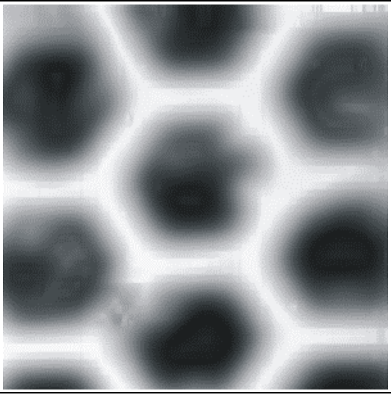
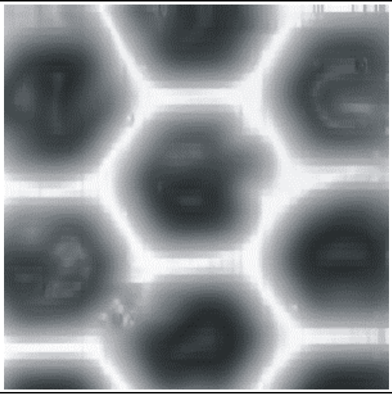
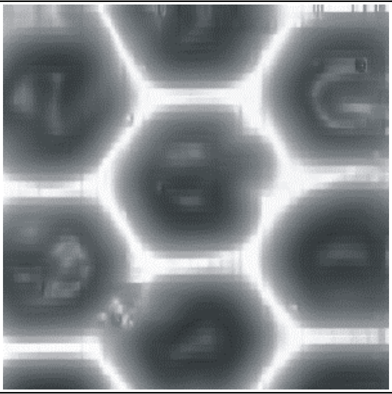
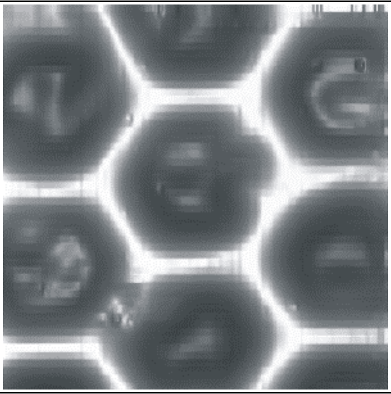
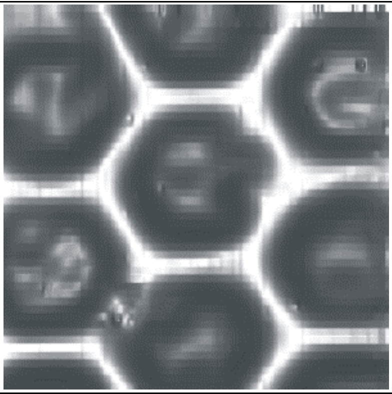
		
a:b = 100:0	a:b = 80:20	a:b = 60:40
		
a:b = 40:60	a:b = 20:80	a:b = 0:100

Fig. 50: Results of mixing height scale and diffuse reflection in different ratios a:b. a is the heigth-porportional shading, b in the image computed for diffuse reflection. Incident light comes from z direction.

3.4.9 Light source

Choose the direction of the light. Direction is given in (x, y, z) coordinates of the binary system. The example in the window indicates the light coming from the z direction (default). Incident light from the side tends to produce shades that highlight small features.

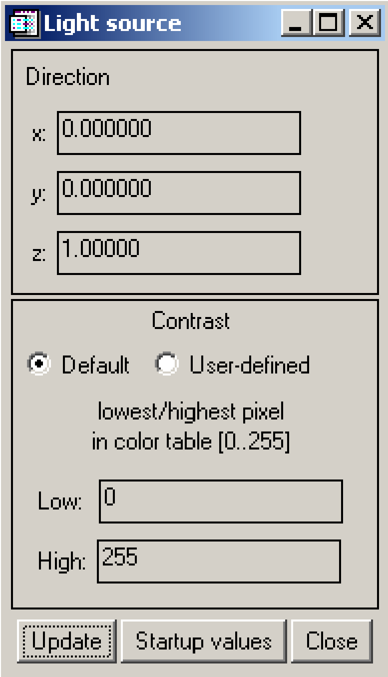


Fig. 51: Light source.

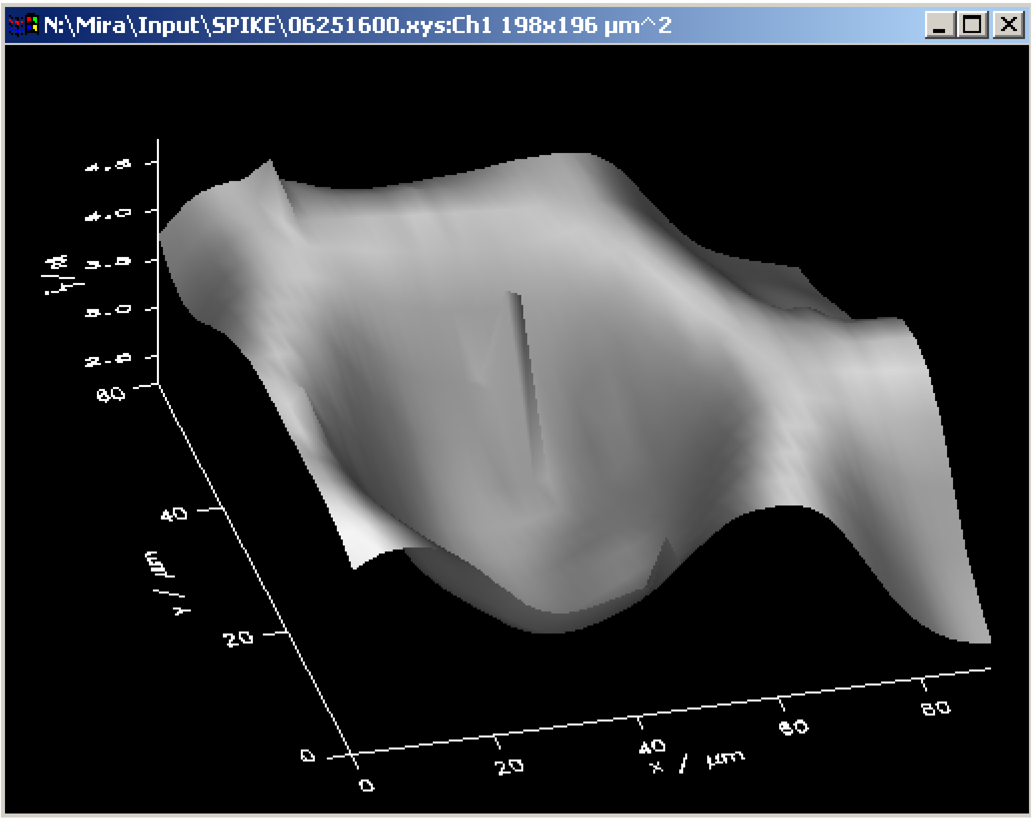


Fig. 52: Light source: Before changing the direction.

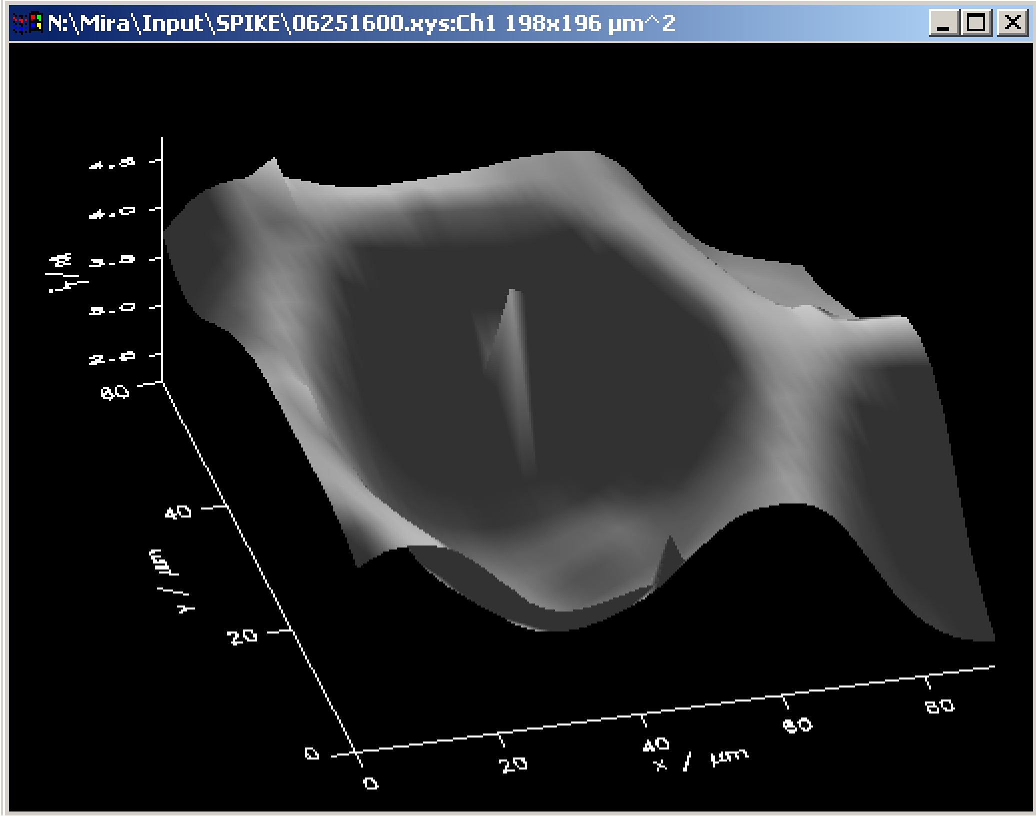


Fig. 53: Light source: After changing the direction off the vertical direction.

Figure 52 and figure 53 show the same plot. The only difference is the direction the light comes from. To point out a detail this functions allows to enlarge the contrast of an ambit without changing plot-internal parameters.

3.4.10 Symbol

If 2D plots are generated you can control the appearance of the individual data points in the window *Plot format/Symbol*. The current setting would draw a thin line only (default). In order to draw symbols select *Line and symbols* or *Symbols only* on the left side. The symbol itself is selected on the right side.

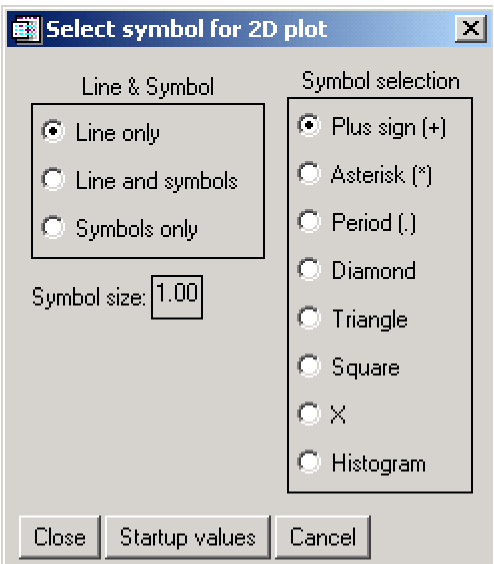


Fig. 54: Symbol.

3.4.11 2D Line Color

Sets the color for lines and symbols in 2D Plots. Than can be used to distinguish data sets in Combined Plots. A graphical selection tool opens with the color palette of the currently selected palette (Fig. 55). Working with line colors requires a fundamental understanding of the color system. MIRA works with the color tables provided by IDL. Each color tables consists of 256 color. The may be viewed with the tool XLOADCT (→*Single Plot: Tools/XLoadct)* In one plotting comand only colors from one color table ca be used. The color selection tool selects a color index within this table. The actual color may be different depending on the selected color table. (Using the same index with different color tables will usually produce different colors!) In addition white and black are inverted on some output devices or graphic file types. In order to avoid the difficulties with that., MIRA has predefined standard foreground and backgroudn colors that typically produce black liens on white background. If you intend to use colors by index from a specific color table, you have to indicate that by checking the option below the color display! Otherwise the selected color will be stored but not used.

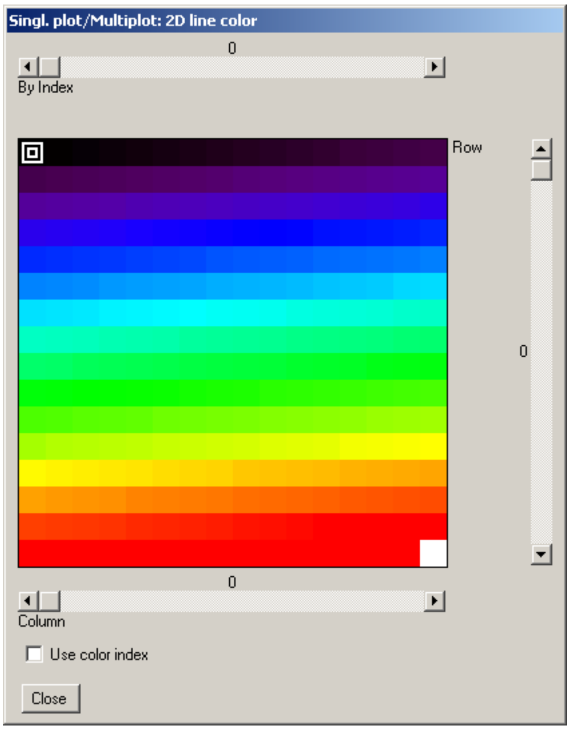


Fig. 55: Selection tool for line color.

3.4.12 Font System

Overview font system

There are three font system: i) vector fonts (the default), ii) hardware fonts (not recommended), and iii) TrueType fonts. Vector fonts give excellent quality when printed to PostScript files. Displays on the screen and in TIF and BMP files may leave wishes open. In this case you may either wish to increase the font size or change to TrueType fonts. TrueType fonts shall appear approximately equal on different file types.

Hardware fonts are specific to certain output devices. It can not predicted how output will appear on different devices. In particular formatting codes will not work in hardware fonts as well rotation of text lines.

The font system will be switched using the window under *Plot format/Font system*.

Overview over font size
At several places of the program you may use to change the font size in the output. Although they all influence the final size of characters on the screen and on the printout, they should be used for a specific purpose.

Menu Plot format/Font system in Single Plot
Here you should set the overall size of the characters and the distance between text lines. This will apply to all subsequent outputs of all graphic formats.
From *Multiplot* this menu is accessed via *Single Plot/Plot format/Font system*.

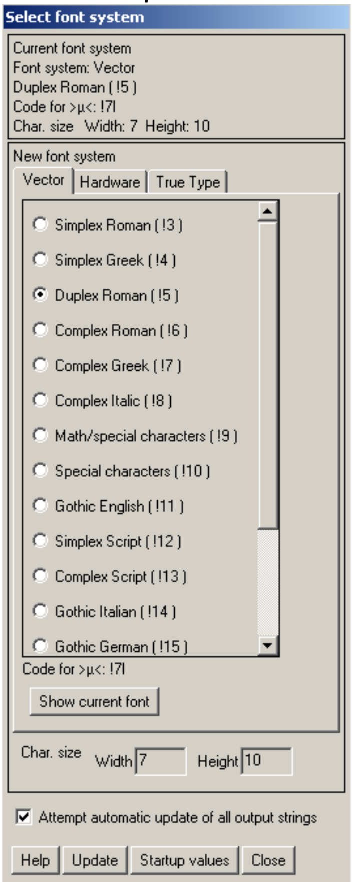


Fig. 56: Dialog for selection of the default font system.

You make all your selection on the right part of the form. The left part only gives information about the current status.

With the tab controls you select the font system (vector, hardware TrueType). By the radio button you select a specific font within the above group as the default font (for instance Helvetica). The command button allows you to view the font of the currently selected radio button of the vector and TrueType tab.

Tab. 1: Available fonts

Command string	Vector font	Post Script font, i.e. example for hardware fonts	TruteType fonts
!3	Simplex Roman (default)	Helvetica	Helvetica
!4	Simplex Greek	Helvetica Bold	Helvetica Bold
!5	Duplex Roman	Helvetica Narrow	Helvetica Italic
!6	Complex Roman	Helvetica Narrow Bold Oblique	Helvetica Bold Italic
!7	Complex Greek	Times Roman	Times
!8	Complex Italic	Times Bold Italic	Times Italic
!9	Math/special characters	Symbol	Symbol
!M	Math/special characters (change effective for one character only)	Symbol	Symbol
!10	Special characters	Zapf Dingbats	Symbol *
!11	Gothic English	Courier	Courier
!12	Simplex Script	Courier Oblique	Courier Italic
!13	Complex Script	Palatino	Courier Bold
!14	Gothic Italian	Palatino Italic	Courier Bold Italic
!15	Gothic German	Palatino Bold	Times Bold
!16	Cyrillic	Palatino Bold Italic	Times Bold Italic
!17	Triplex Roman	Avant Garde Book	
!18	Triplex Italic	New Century Schoolbook	
!19		New Century Schoolbook Bold	
!20	Miscellaneous	Undefined User Font	
!X	Revert to the entry font	Revert to the entry font	Revert to the entry font

Know problems: No meaningful dispaly is generated for the vector fonts Simplex Roman, Simplex Greek, Duplex Roman.

The following fonts are currently available.

You can select the default font size and the line distance.

All your selection become only active if you press the command button *Update*. If the check box *Attempt automatic update of all output strings* is selected, MIRA will replace the the font selection switches (e.g. !5) in all output strings. The program will also search for all string segments that code for the substring "μ" in outputs. In the future more special characters can be replaced on demand. Meanwhile all other special character may require manually coding them with command strings. If the check box is not selected, only the font system will be changed but all switching codes will be untouched. You have to change them manually.

Menu File/Selection of graphic format and the setup button of the corresponding graphic format
The field *Character size factors* determines a factor with which the character size set under *Plot format/Font system* will be multiplied. This factor will be applied to all printout to a specific file format but not to other file formats. The default values are intended to provide an approximately corresponding size/figure relation in all graphic formats. This setting should be used to equalize the appearance of screen and file output.

From *Multiplot* this menu is accessed via *File/Selection of graphic format* and then setup button.

Menu Plot format/ Axis format/ X (or Y, Z)
The field *Character size fact.* determines a factor with which the character size set under *Plot format/Font system* and *File/Selection of graphic format* will be multiplied. This factor applies to all printout formats for the specified axis. The factor is intended to make characters of a specific axis different from the other axes. This can be useful for instance for the z-axis if it is displayed under a small angle.

From *Multiplot* this menu is accessed via *Single Plot/Axis/X* or */Y* or */Z*.

Using the dialog Select font system

3.4.13 Window size

Choose the size of the screen by changing the number of bits of x- and y-dimension of the screen window. The number of pixels of your screen is given to let you which portion of the screen would be covered by the window. If you are not satisfied with your selection you can go back to the startup values.

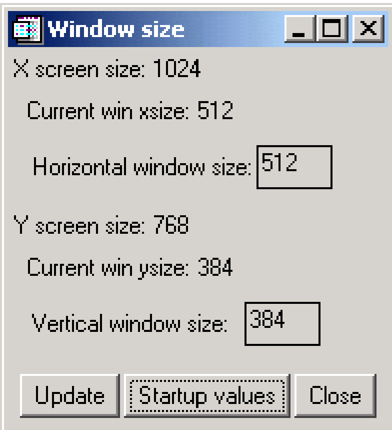


Fig. 57: Window size

3.4.14 Window title

To change the title of the graph window which appears after clicking the ***<Redraw>*** button. This function is useful if there is no high quality printer available and you want to make a copy of the screen to the clipboard to generate a BMP image.

For example:

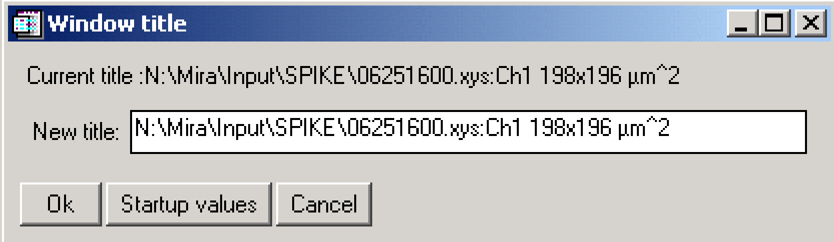


Fig. 58: Window title.

The standard title is the full file name of the data set and the dimensions.

3.5 Options +?

3.5.1 Extended widget, Minimal Widget, Extended widget + infobox, Minimal widget + infobox

The general meaning of this term is explained in the introduction of *Single plot*. You can change the appearance of an existing Single plot widget with the menu options. The

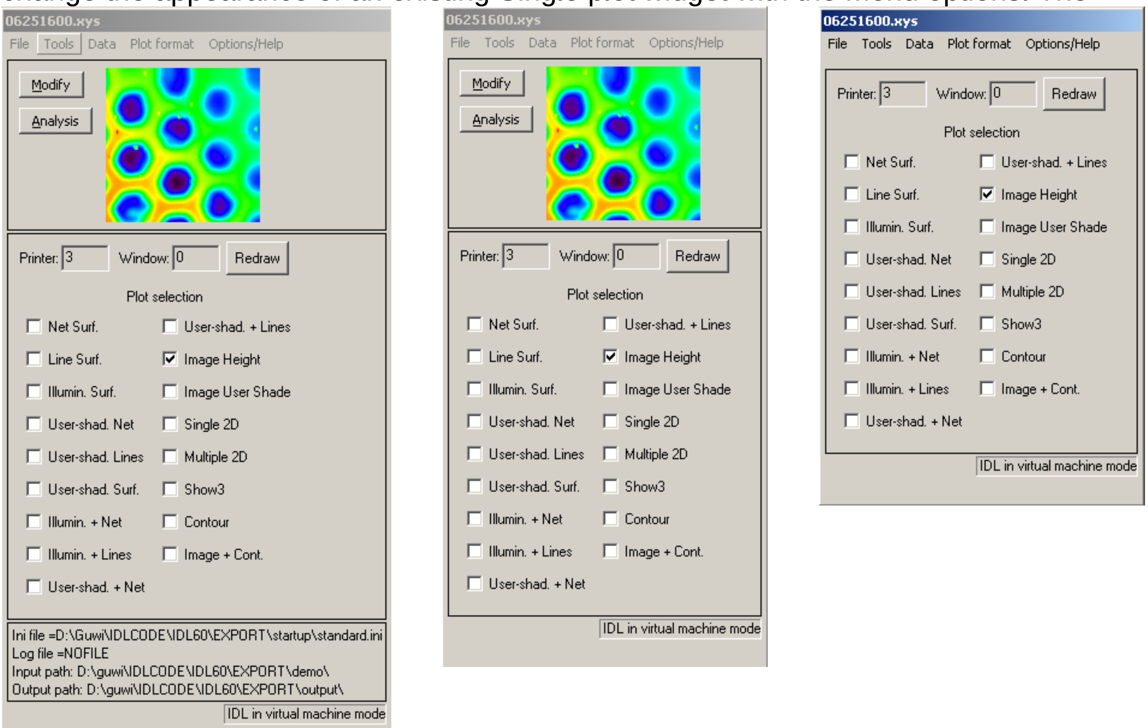


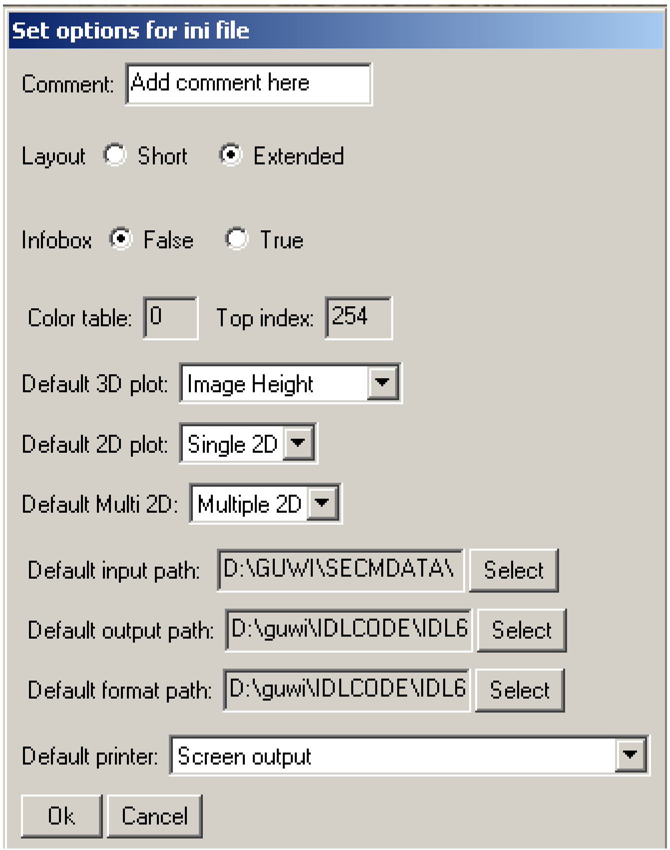
Fig. 59: Different layout of the Single plot widget from left to right: Extended + info box, Extended, Minimal (Minimal + info box is not shown).

3.5.2 Load INI file

Usually you will select the desired initialization file in the main screen of the program (Fig. 9). If you want change the initialization file later, this option gives you the chance to do so. This may be useful if you have predefined settings for a certain filetype (such as color tables or different input path).

3.5.3 Save INI file

A number of defaults can be set during the saving of an initialization file:



Label

Information about layout

Presence of the info box

Index of color table, highest values to be used out of [0..255]
Default plot types

Default path for data input, graphic output and formating input/output

Default printer or graphic output format

Fig. 60: Default options

3.5.4 Information about MIRA

This displays information about MIRA

3.5.5 What's new in MIRA VM xx

This displays recent changes to the MIRA software to direct experienced users to the things that might be different from the behavior of MIRA in the past,

3.5.6 Manual about MIRA

Displays this manual in Acrobat Reader.

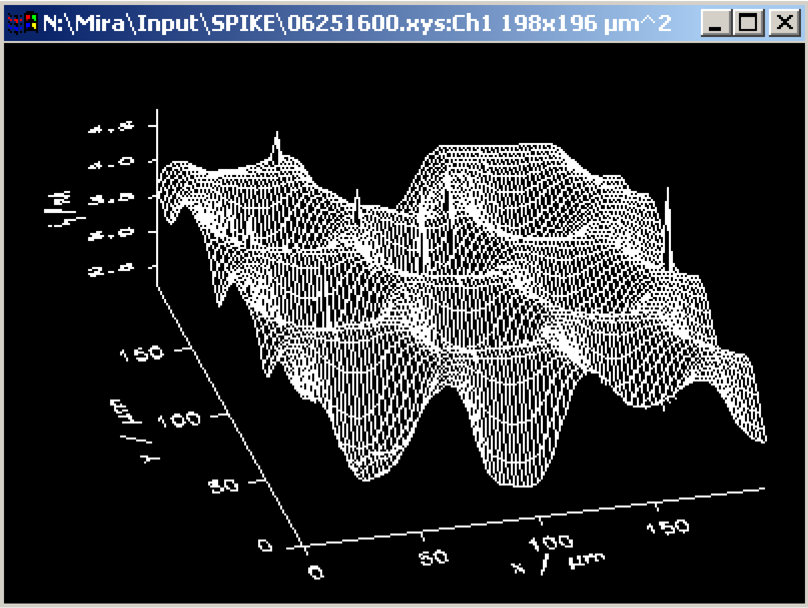
3.5.7 RSI manual about iTools

This displays a manual about the iTools. This manual comes from RSI and Gunther Wittstock is not the author nor was the content checked for agreement with the program. Usually I found the RSI manuals quite helpful.

3.6 Plot selection

Select a plot out of the choices given in the main window of *Single Plot*. The following plot types are there by default. Most plots require a 3D data set. The color of line and background can be changed. Current default for all devices is black lines on white background.

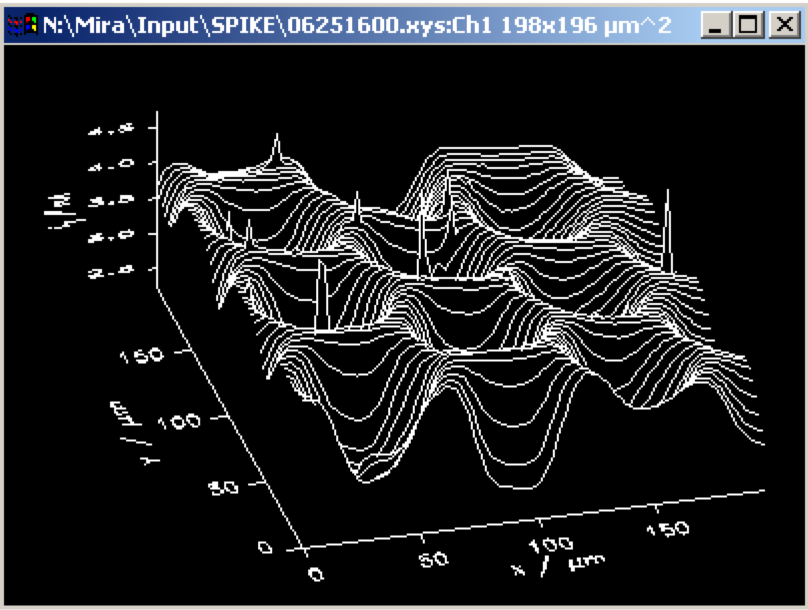
3.6.1 Net Surf.



Net constructed surface

Fig. 61: Net surface

3.6.2 Line Surf.



Line constructed surface

Fig. 62: Line surface

3.6.3 Illumin. Surf.

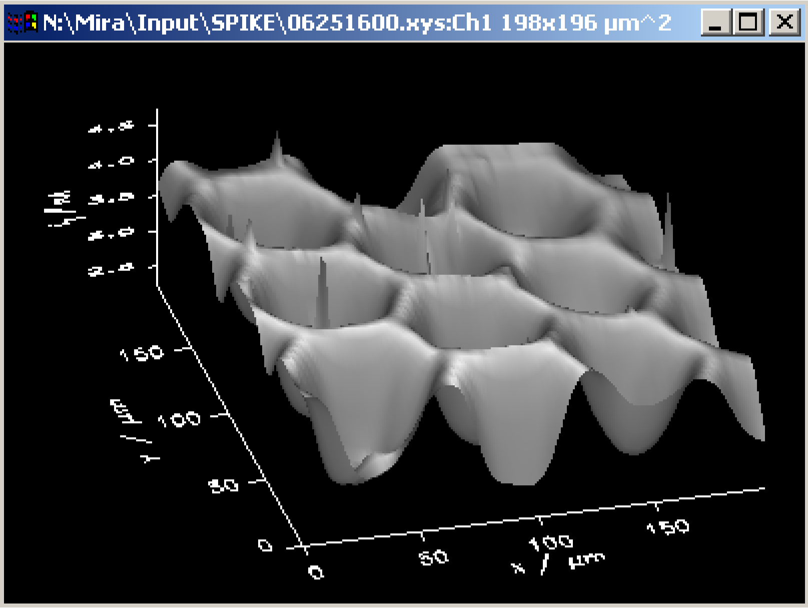


Fig. 63: Illuminated surface

This plot gets a pseudo 3D outlook because of being illuminated by one light source. The light direction can be set using *Plot format/Light source*

3.6.4 User-shad. Net

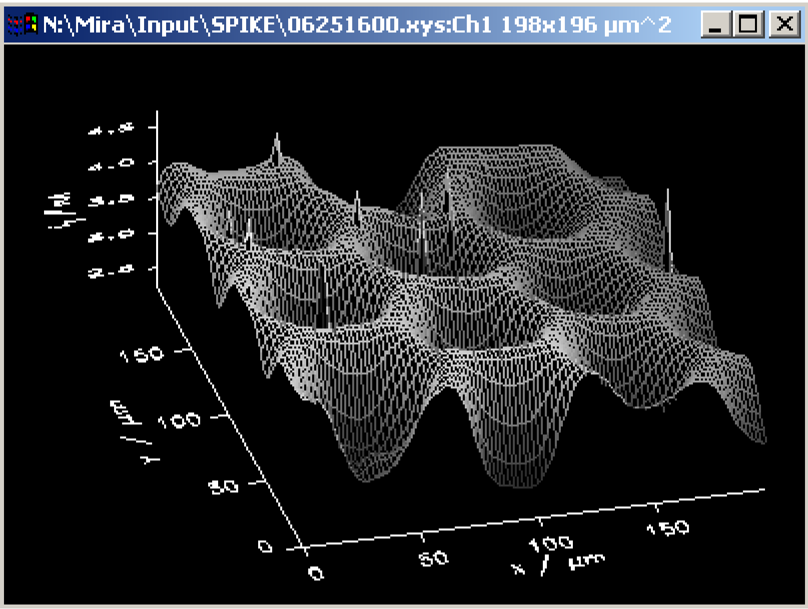


Fig. 64:User-shaded net

Net constructed surface, color of the net is given by the value of z-axis. It can be modified in the window *Plot Format/Scale user scale.*
Colors are mapped in the user-selected color scale.

3.6.5 User-shad. Lines

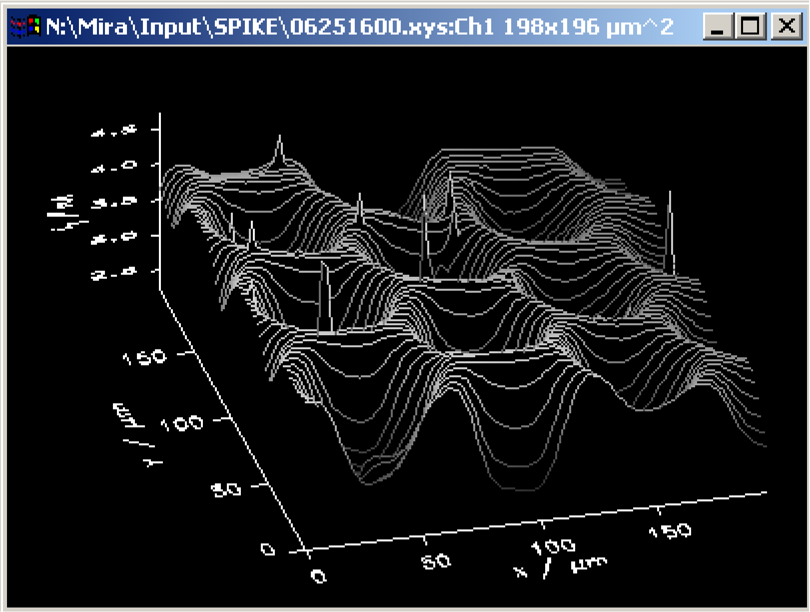


Fig. 65: User-shaded lines

Line constructed surface, color of the line is given by the value of z-axis. It can be modified in the window *Plot Format/Scale user scale.* Colors are mapped in the user-selected color scale.

3.6.6 User-shad. Surf.

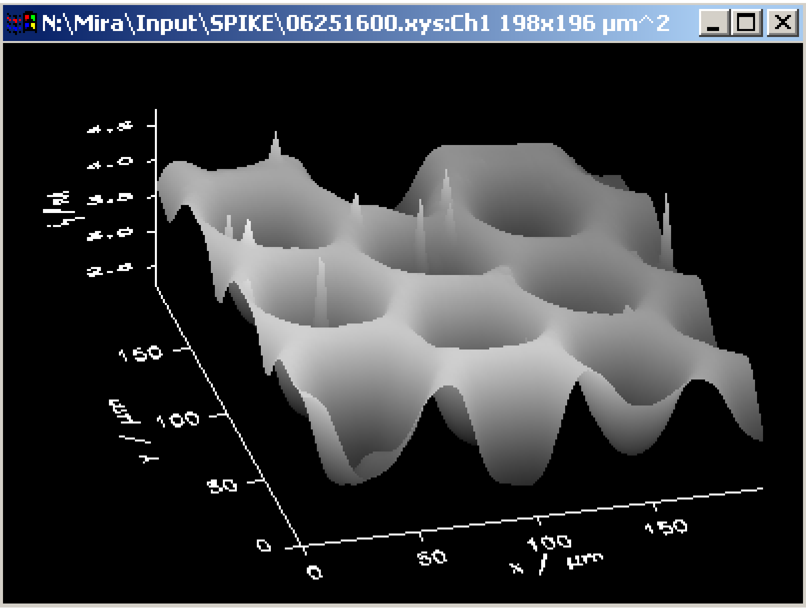


Fig. 66: User-shaded surface

Color of every pixel is given by the value of z-axis. It can be modified in the window *Plot Format/Scale user scale.* Colors are mapped in the user-selected color scale.

3.6.7 Illumin. + Net

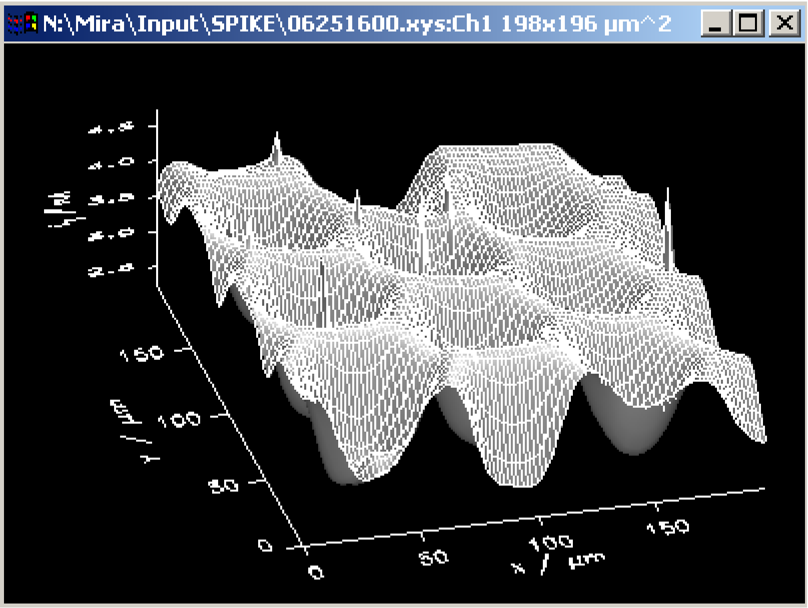


Fig. 67: Illuminated and net

Overlay of monochrome net on an illuminated surface.

3.6.8 Illumin. + Lines

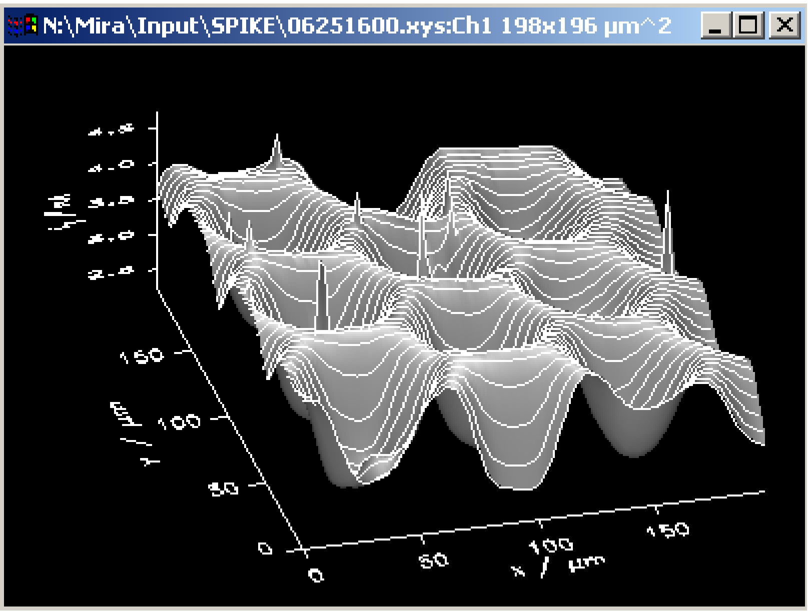


Fig. 68: Illuminated and lines

Overlay of monochrome net on illuminated surface.

3.6.9 User-shad. + Net

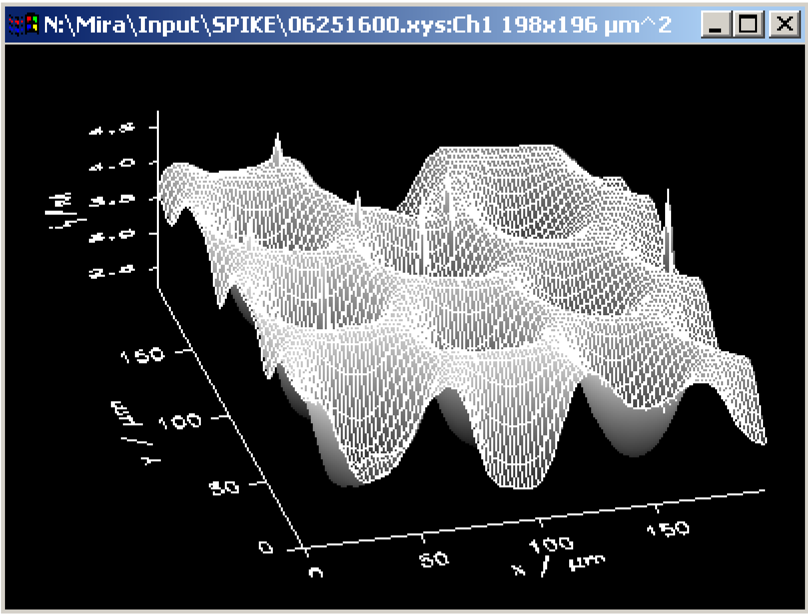


Fig. 69: User-shaded and net

Overlay of a net construction (monochrome) on a surface for which every pixel is given by the value of z-axis. The shading can be modified in the window *Plot Format /Scale user scale.*

3.6.10 User-shad. + Lines

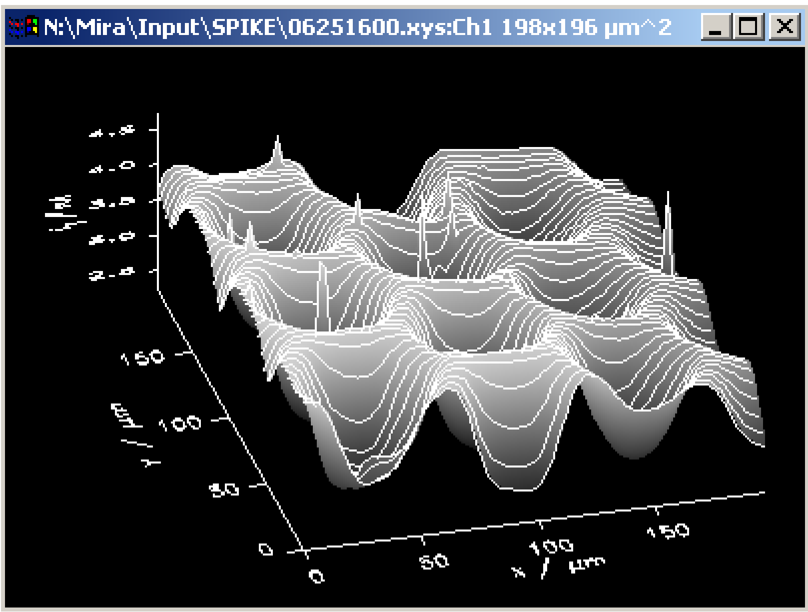


Fig. 70: User-shaded and lines

Overlay of a line construction (monochrome) on a surface for which every pixel is given by the value of z-axis. It can be modified in the window *Plot Format/Scale user scale.*

3.6.11 Image Height

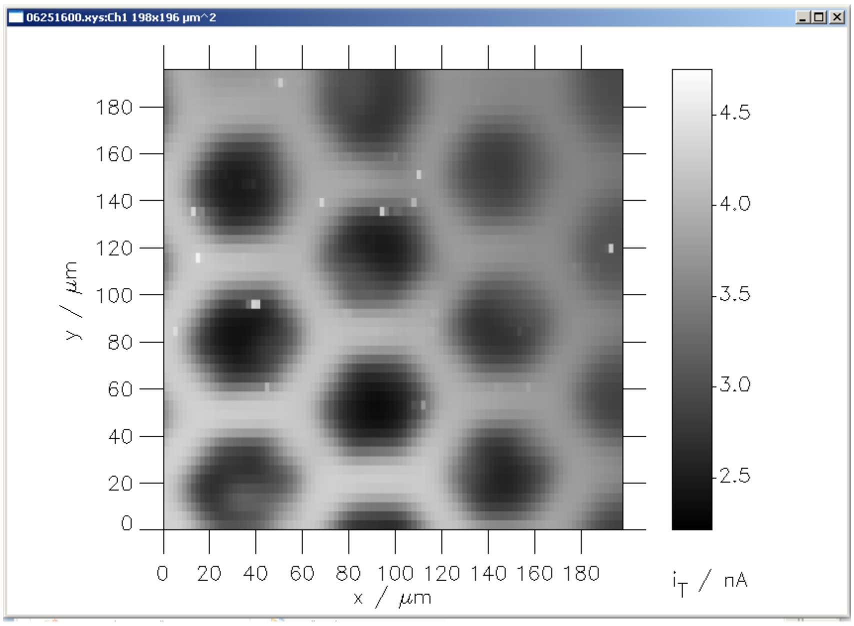


Fig. 71 Image Height (not interpolated)

2D graphic, current differences are pointed out by using different shades out of the color table.
On the right there is a false color scale to indicate the value for which the shade stands for.

The current values look pixeled because they are not interpolated-

3.6.12 Interpolated Image Height

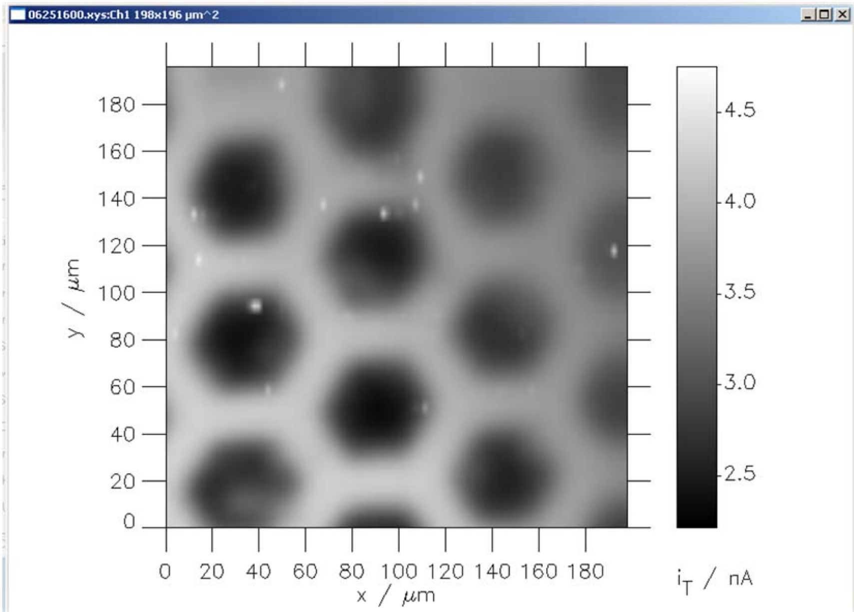
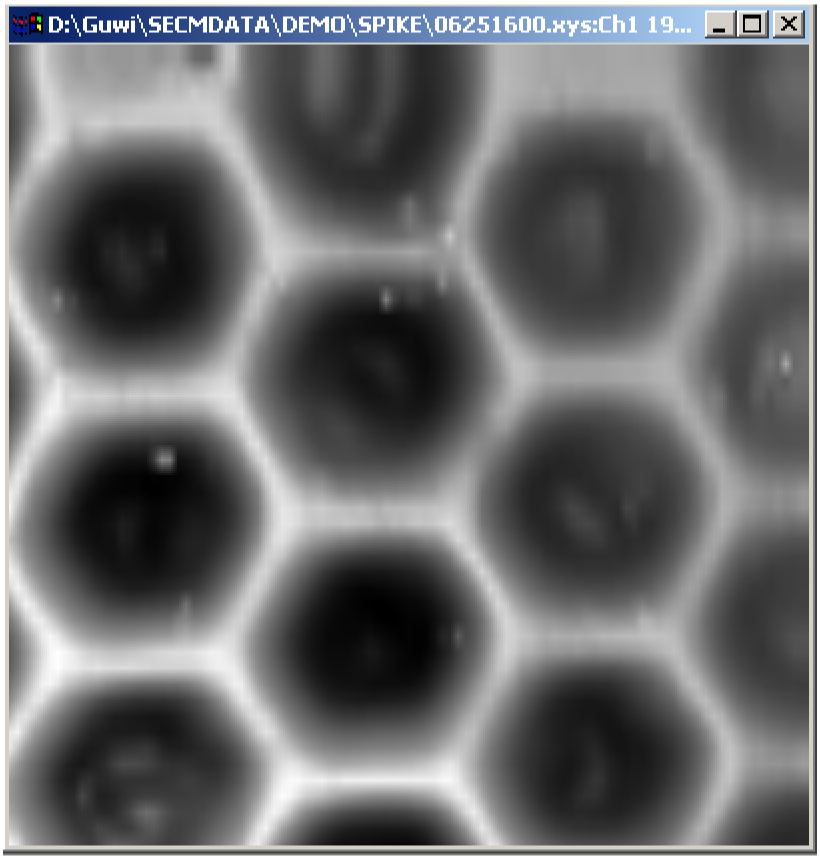


Fig.: 72 Interpolated Image height

2D graphic, current differences are pointed out by using different shades out of the color table.
On the right there is a false color scale to indicate the value for which the shade stands for.

The dataset looks smooth because the gray scale values are interpolated.

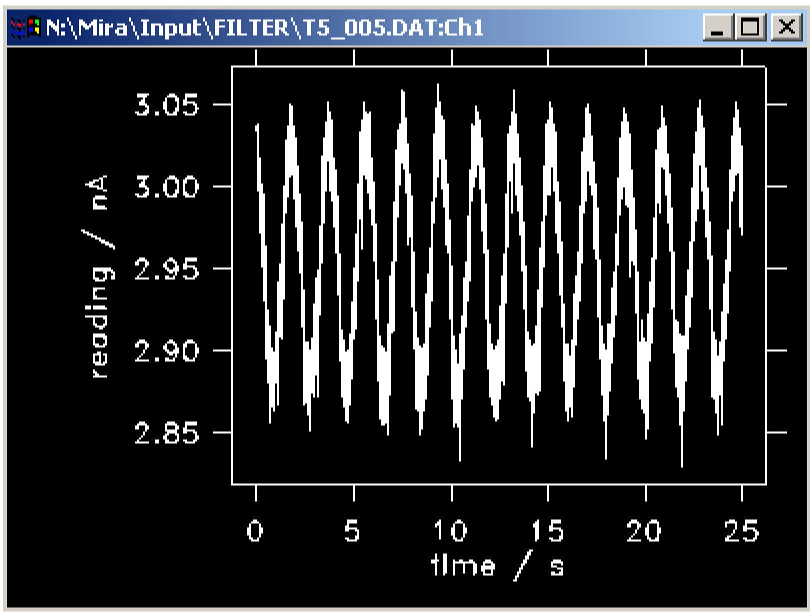
3.6.13 Image User Shade



2D graphic, altitude differences are pointed out by using different shades out of the color table. In contrast to *Image Height*, it can be modified in the window *Plot Format/Scale user scale.*

Fig. 73: Image user shade

3.6.14 Single 2D



2D axis plot is possible only for (x,y) data sets like time series, cyclic voltammograms etc.

Fig. 74: Single 2D

3.6.15 Multiple 3D

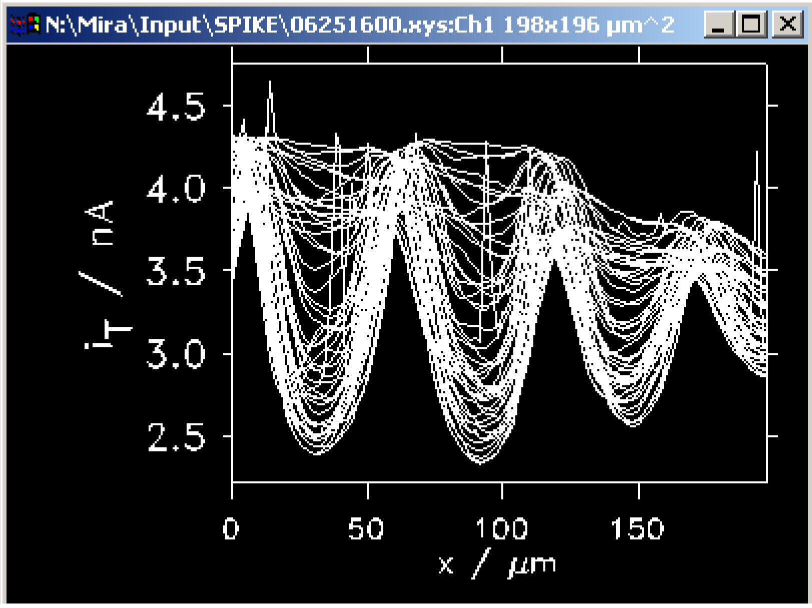


Fig. 75: Multiple 3D

This plot is usable for data sets containing two or three variables.
If there is a third variable the plot will be a stacked and overlaid plot of (x,z) data sets. For each value of y there will be one 2D plot. As a result you get as many curves as there are different y values.

3.6.16 Show3

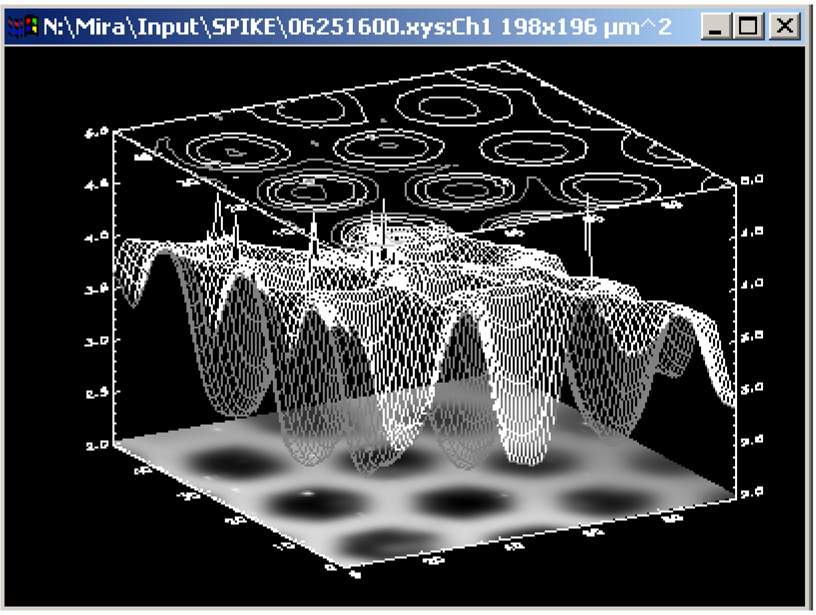


Fig. 76: Show3

Plot which is composed of three different data representation in one axis system.
On the bottom there is a 2D graphic in which a false color height-proportional image.
Additionally a 3D monochrome net is given and on the top there is a contour plot.

3.6.17 Contour

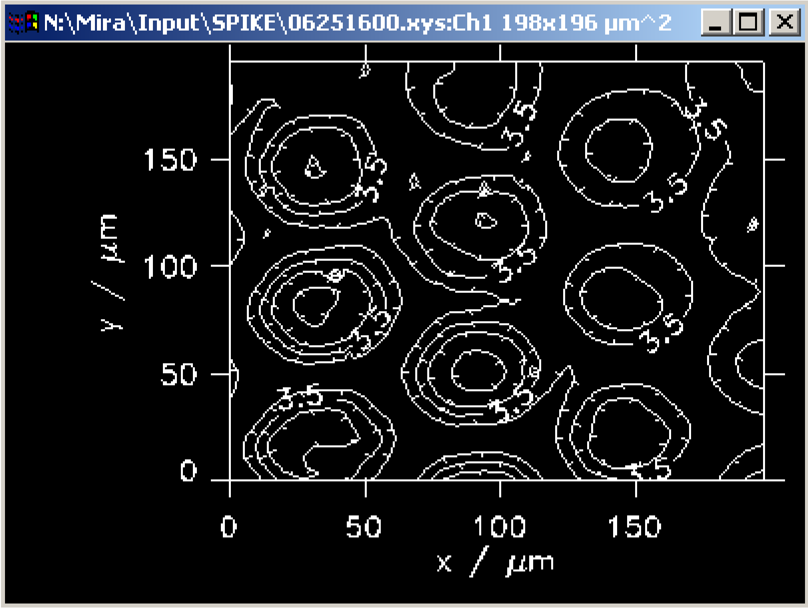


Fig. 77: Contour

2D plot in which data values are indicated by contour lines of the plot connecting image points with the same height. Ticks show direction of increasing altitude.

3.6.18 Image + Cont.

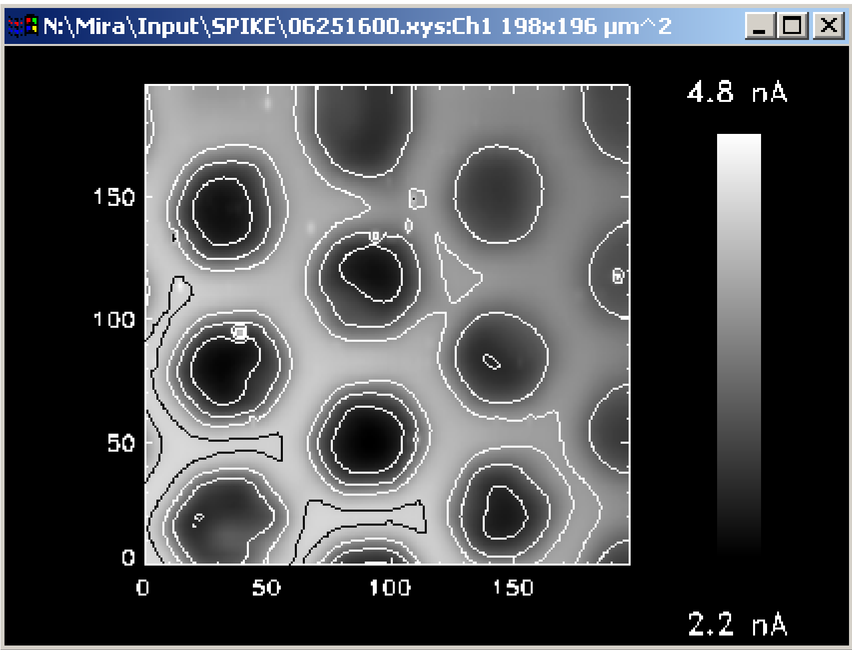


Fig. 78: Image and contour

Overlay of a height scale image and a contour plot.

Redraw

Each selected type of diagram will be presented in a separate graph window. If several graphs are selected, they will be placed in separate graph windows. If you want to compare different data sets plot the first data set in window 0. Change the entry into the window field to 1. Load the next data set and press redraw. Both data sets are now in different graph windows. However, the plot for the first data set cannot be changed. Alternatively you can load both data sets to *Multiplot* and switch between manipulating both data sets (recommended).

The following options are only available if you choose extended layout.

3.7 Modify

All these routines will make changes to the data itself rather than to format the corresponding graphs. Therefore a warning will appear before going to the actual windows. There is no undo function. In order to undo, you have to re-load the data set.

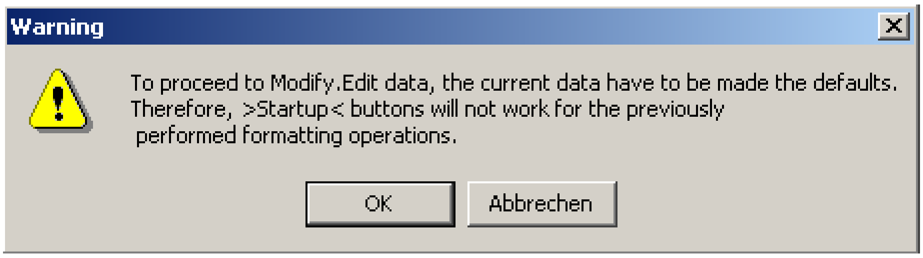


Fig. 79: Warning of flattening.

3.7.1 Linear flatten

If your plot plane has a tilt, you can subtract it from the data set itself. See the difference to

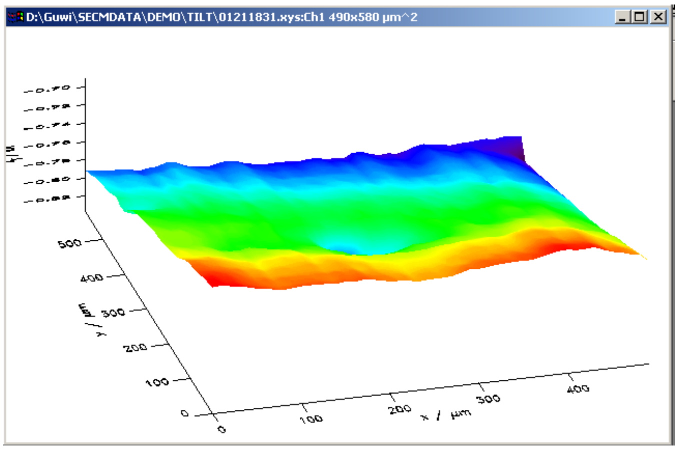


Fig. 80: Plot with tilted background.

As you can see in this graphic, the complete area looks inclined. In order to focus the view on the feature in the middle, you can subtract from each image line a value to align the image in one plane but to preserve height variations. In contrast to *Plot format/Scale user shade*, the changes is done on the data set itself. This is a common practice in AFM height measurements.

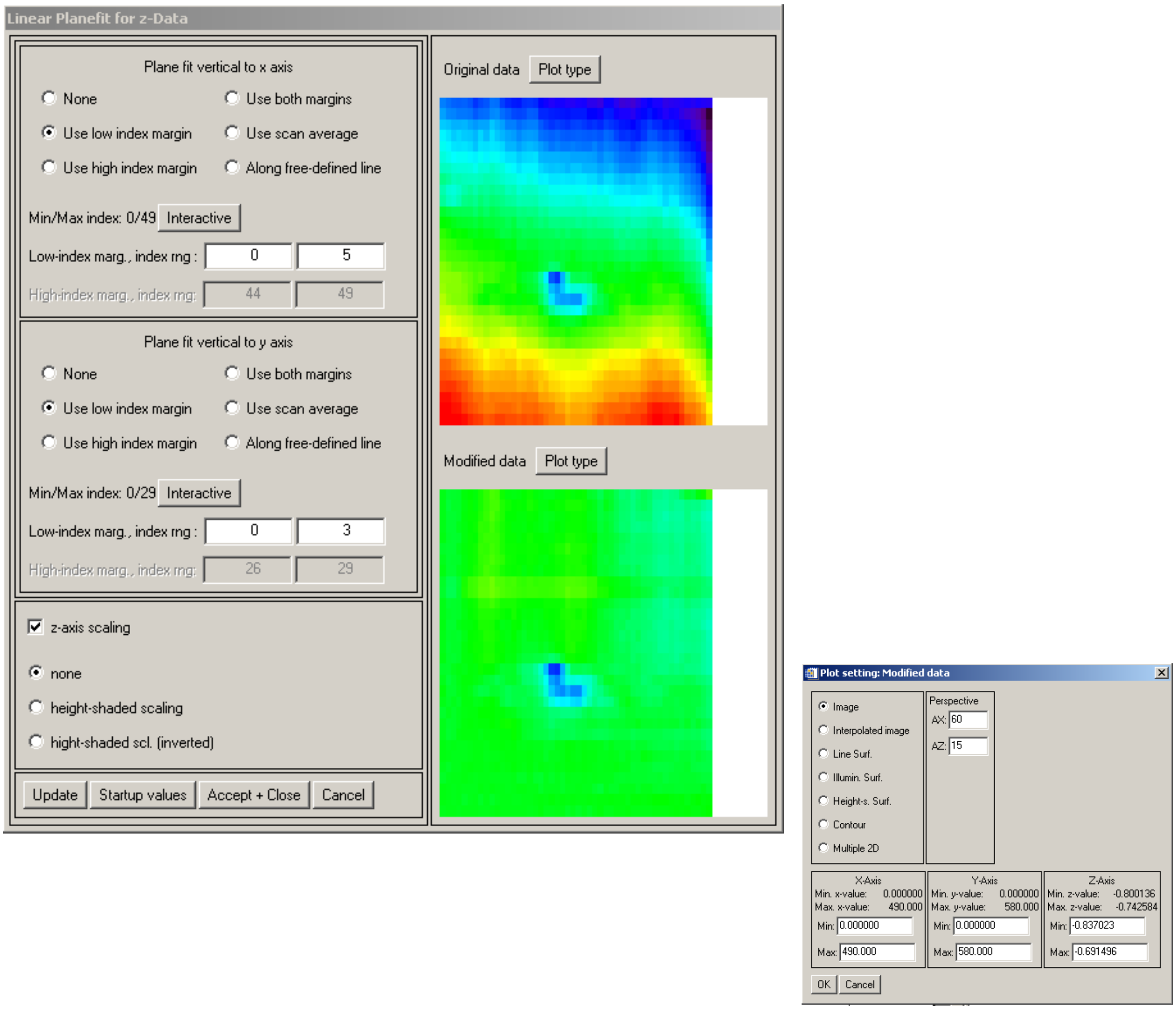


Fig. 81: Linear flatten, main screen. The display of original and modified data can be selected in the right window.

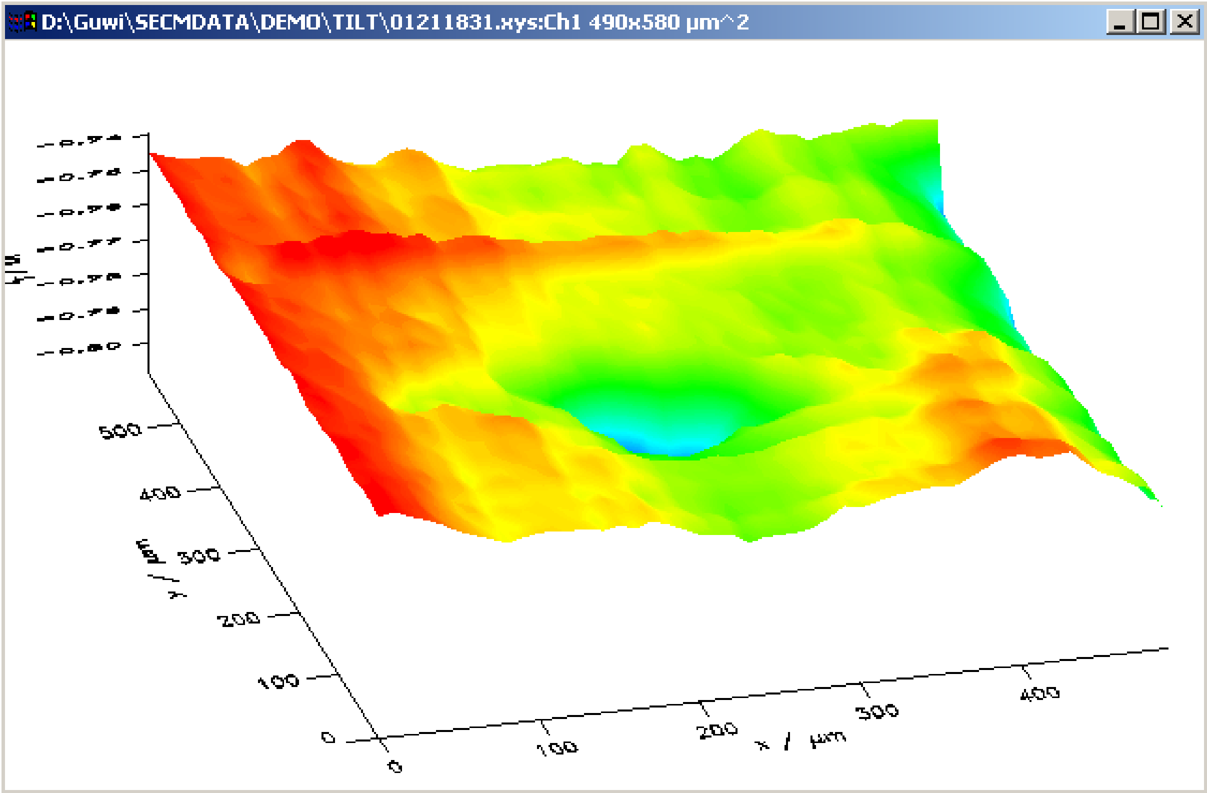


Fig. 82:Plot after leveling.

Figure 82 shows the plot after setting the line average as described in the Window of Fig. 81 to a unified value. The height differences within a scan are still o.k. The absolute current values have changed substantially.

3.7.2 Polynom flatten

Another algorithm to flatten your data than the one described in 3.7.1 is to subtract a polynom that was calculated as the best fit to your data. You can select the order of the polynom [0...11]. Zero order will subtract a constant, 1 will be a tilted plane and so forth. High polynom orders only seldom make sense. The form shows you the original data, the calculated background and the resulting data. You can select different plot representations under the *Plot* menu. To accept the changes to the data it self, select *Data/Accept changes* and then *File/Close*. To exit without changes select *File/Cancel*. The option button "Retain mean value" will ensure that not just the difference between background and data value will be returned but that the mean of the returned array is equal to the mean value of the input data.

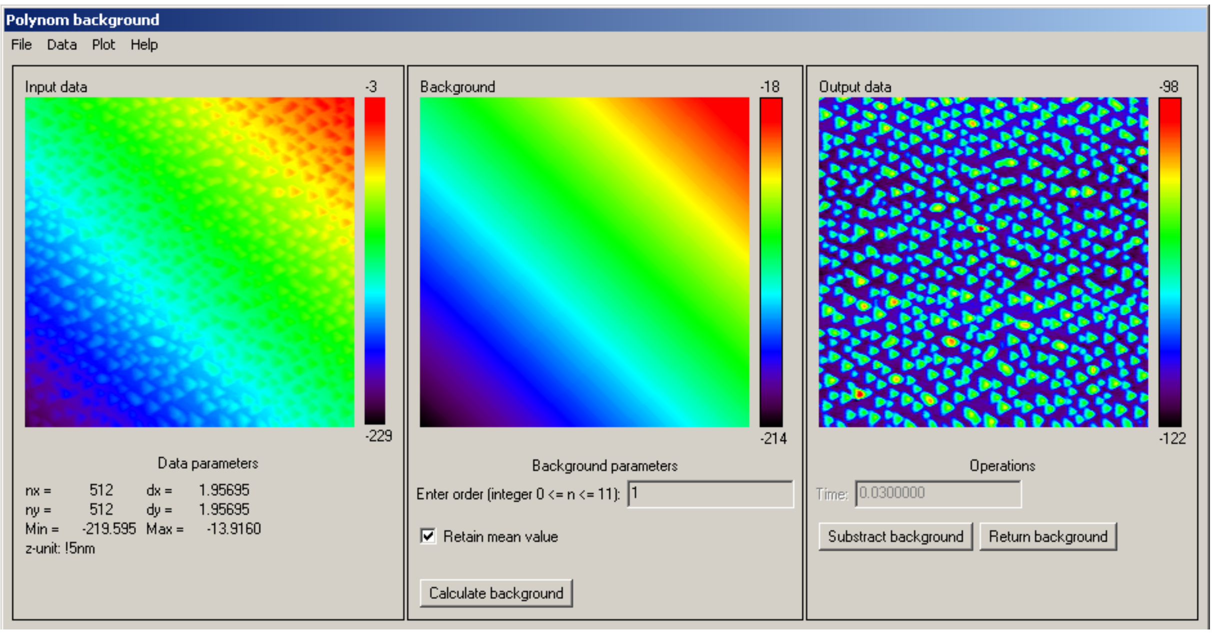


Fig 83: Window for polynom flatten. The operation is applied to the data itself.

3.7.3 Rolling sphere flatten

If the background cannot be described by a polynom or if line-by-line flatten does not yield the desired result (artifacts) the background can be calculated by the path a sphere of a defined radius would roll below or above the surface. Thei si illustrated in Fig. 84.

The window to start this option is similar to the other modify windows (Fig. 85). The filter radius determines from which change in z values is considered to be background. Only signals with considerable smaller radius than the calculated sphere will not be removed. The z-zoom-factor will be multiplied with the data. After the background subtraction the resulting array will be divided by the z-zoom factor. The option above/below determine whether small depressions or small elevations will be high lighted. If you want to highlight small depression you must role the sphere above the data. If you what to emphasize small elevation you should roll the sphere below the data (as shown in Fig. 84). You can select different plot representations under the *Plot* menu. To accept the changes to the data it self, select *Data/Accept changes* and then *File/Close*. To exit without changes select *File/Cancel*. The option button "Retain mean value" will ensure that not just the difference between background and data value will be returned but that the mean of the returned array is equal to the mean value of the input data.

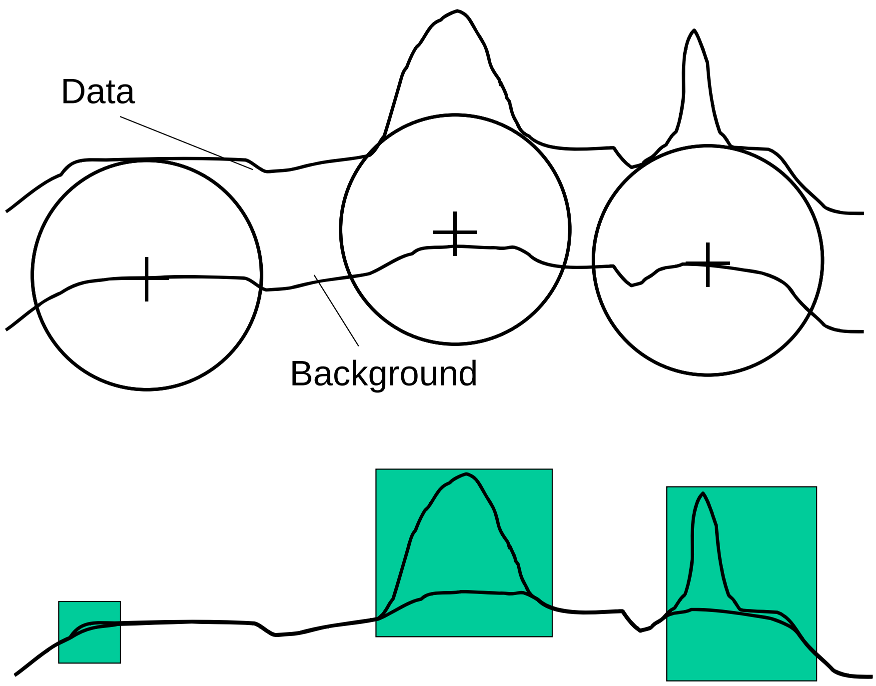


Fig. 84: Principle of the background calculation by the path of a rolling sphere.

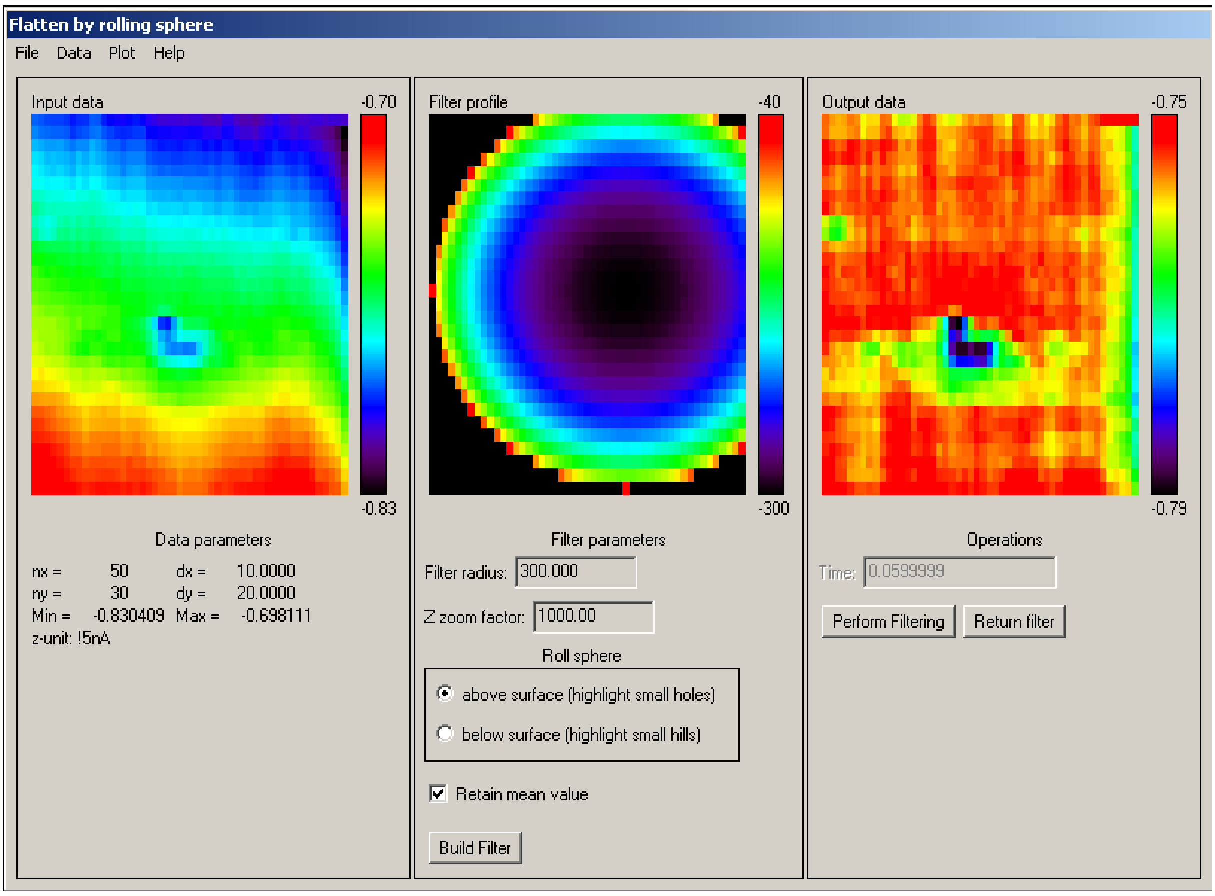


Fig. 85: Principle of the background calculation by the path of a rolling sphere.

3.7.4 Spike removal

Spike in SECM images may occur do to electromagnetic interferences or temporal mechanical collision of the probe and the sample. These signals usually are smaller than a signal can be hen imaged with a probe of finite size. This can be used to identify points that might be influenced by such phenomena.

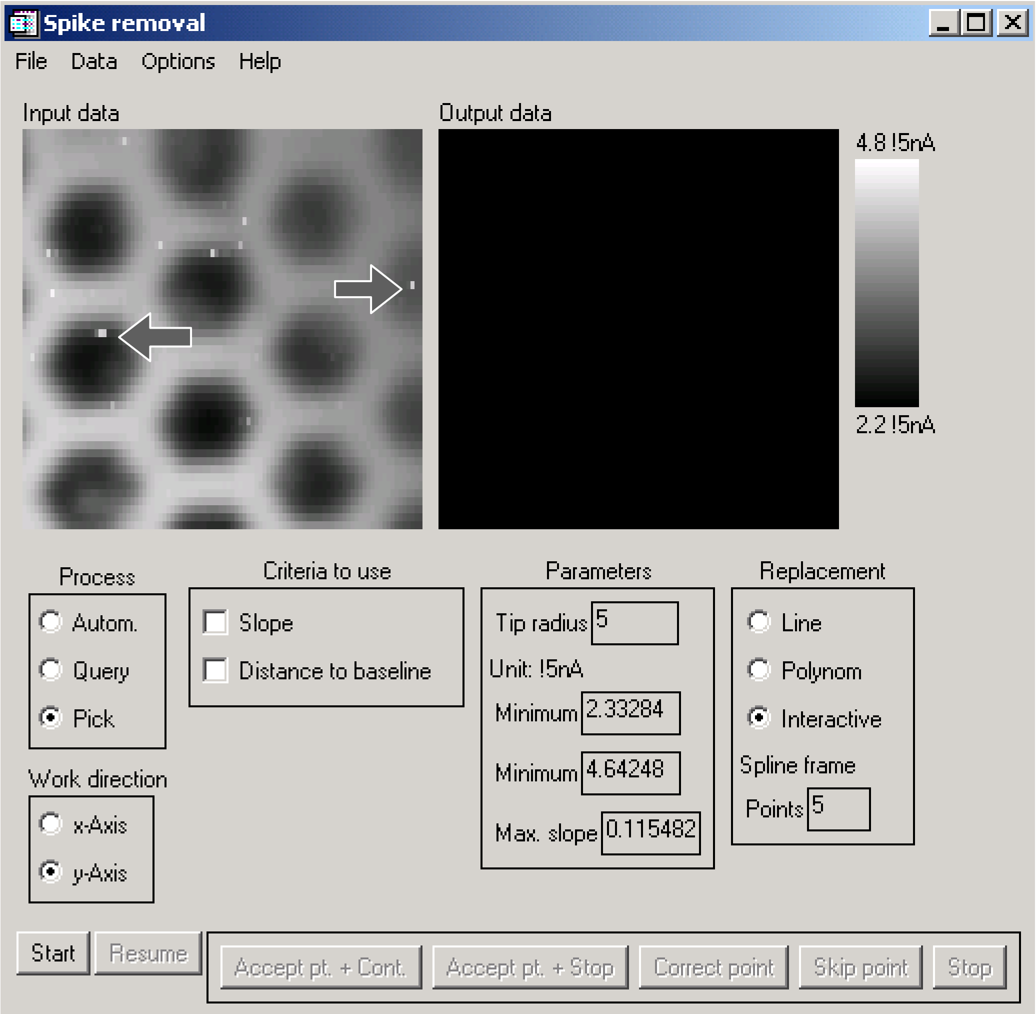


Fig. 86:Data set input.

As you can see in the Input data window (Fig. 86) there are some spikes (white). With help of the value for the tip radius as an input parameter, this function will identify data that might be a spike. You can also manually select them.
After choosing the wanted configuration press ***<start>***.

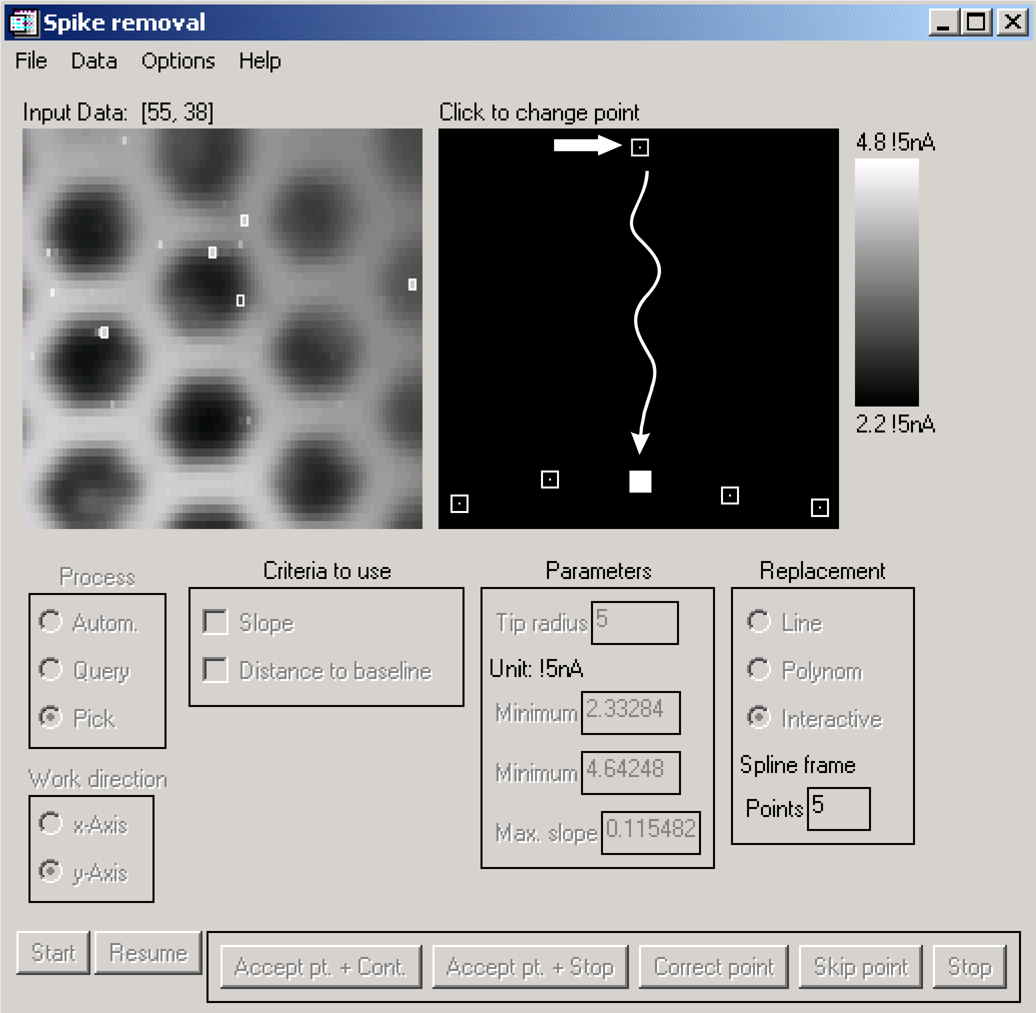


Fig. 87: Data set after marking.

Afterwards possible spikes are identified either manually or automatically. The point together with the neighboring data points are shown in the right. Select a position for the modified position of the suspected spike either by clicking on it or by linear or polynomial interpolation. For optimum performance use work directions (x, y) after another. After completing one work direction confirm changes *Data/Accept changes*.

This routine can be automatized in several steps. Instead of you selecting suspected points this can be made by the program (Options *Autom.* and *Query* under *Process*, left). The replacement can than be done either by hand or by fitting a line or a polynom through the neighboring data points.

The right image displays the modified data set. If you are satisfied, modify the working data set under *Data/Accept changes*. You may then consider to further working on the data set (e.g. along the y-Axis). After finishing with one setting you should used *Data/Accept changes*. To return to the *Single Plot* option use *Data/Accept changes* and *File/Exit* and confirm once again the changes.

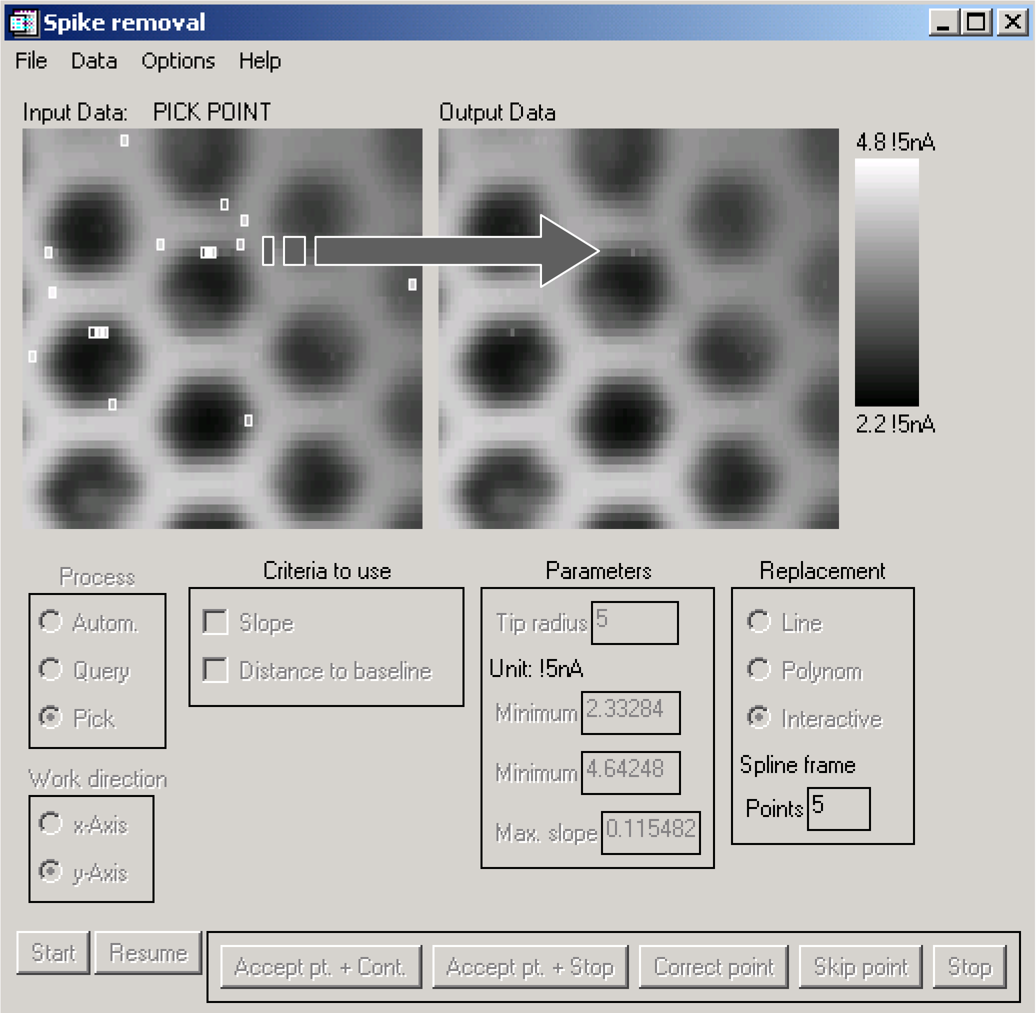


Fig. 88: Output data in comparison with Input data.

Figure 88 shows both data sets: The input set and the output set.

3.7.5 SECM debluring/edge enhancement

This filter restores the image by subtracting the diffusional blurring from the measured image. It is useful for SECM data. The filter is described in C. Lee, D.O. Wipf, A.J. Bard, K. Bartels, A.C. Bovik; *Anal. Chem.* **1991**, *63*, 2442-2447. It has some serious disadvantages: i) the edge has to be discarded, depending on the size of the filter. ii) reasonable results are obtained only if the density of points in x and y direction is equal. While the parameter sigma of the filter is correlated to the radius, *tau* can be set arbitrarily. We found that this routine extremely seldom gives acceptable results and a modification of the shading by mixing a height-shaded image and one calculated based on diffuse reflection as described under Plot Format/Scale user shade give often better results without the disadvantages of this procedure. Details are described in G. Wittstock, T. Asmus, T. Wilhelm; Investigation of Ion-Bombarded Conducting Polymer Films by Scanning Electrochemical Microscopy (SECM). *Fresenius J. Anal. Chem.* **2000**, *367*, 346-351.

In order to operate the window, set the parameters for the filter based on the information shown under the input data on the left, press <***Build Filter***> and then <***Deblur***>. The filter is displayed in the middle and the result in the right window. The plot type for showing input data, filter and output data can be modified under *Plot/Input*, *Plot/Filter* and *Plot/Output* as described in Fig. 81, right.

Instead of the modified data set, the filter can be returned to single plot when using <***Return Filter***> and *File/Close*.

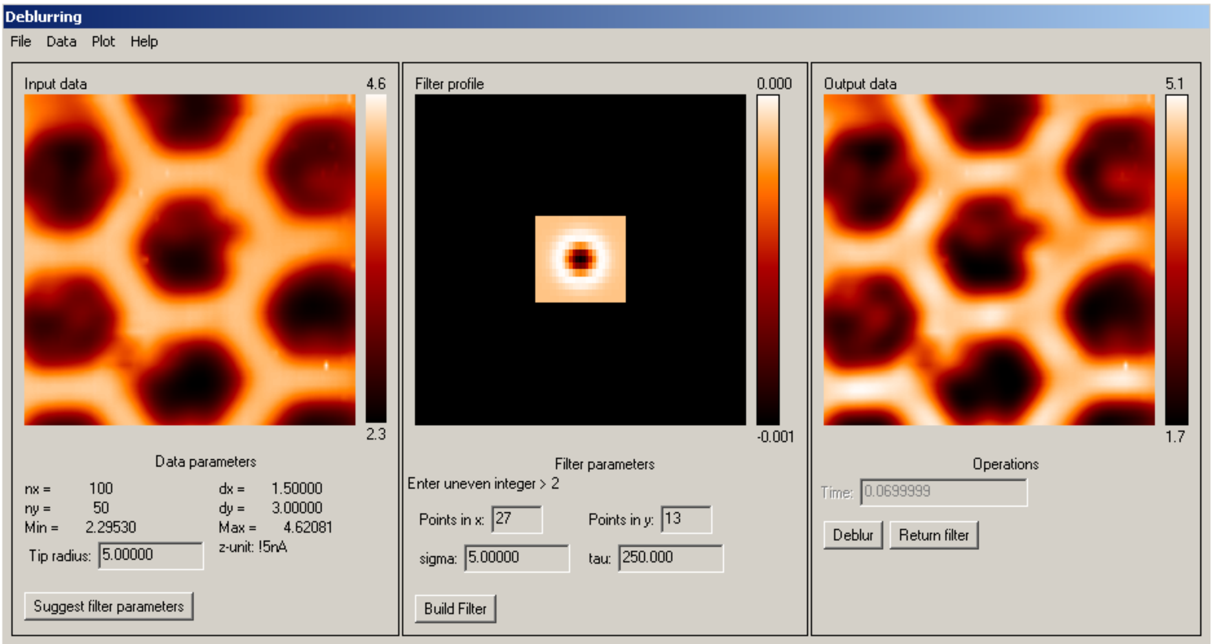


Fig. 89: Window for performing the deblur operation.

3.7.6 Adjust bundle setting

"Bundle" is the term used for electrodes (sensors) that are measured simultaneously by a multipotentiostat, typically in a multi-tip scanning probe microscope. The tips may not be of the same sensitivity (for instance due to slight variations in their size). They may also have a positional offset on the sample. MIRA reconstructs the image from the measured data and correction values. The following corrections are used

***x* position offset *xoffset*.** *xoffset*[*i*] = 0 means the *i*-th electrode has the same *x* coordinate as positioning system

***y* position offset *yoffset*.** *yoffset*[*i*] = 0 means that electrode *i* has the same *y* coordinate as the positionong system.

z value offset zoffset. *zoffset*[*i*] = 0 means that no offset correction is applied to the values coming from sensor *i*.

correction factor of the sensitivity *scale factor*. *scalefactor*[*i*] = 1.0 means no correction is applied for electrode *i*.

The *Adjust bundle setting* form allows editing the correction values and the measured values itself.

The corrected values are obtained as

$$x_{i,corr} = x_i + xoffset[i] \tag{1}$$

$$y_{i,corr} = y_i + yoffset[i] \tag{2}$$

$$z_{i,corr} = (z_i - zoffset[i]) * scalefactor[i] \tag{3}$$

The data are placed in three tables on a tab form. The tab *Conversion values* contains the *xoffset*, *yoffset, zoffset* and *scale factor* for each electrode (sensor) of the bundle.

In order to allow more precise correction all data from a certain sensor or all data from a sensor and a spcfied scan can be displayed in a different color (all scans from sensor #5 in Fig. 90)
The tab *Tab data* contains the tabulated data for *x*, *y*, and z data.
The tab *Use values* allows to exclude and include/exclude data from an individual sensor or a particular line scan from all sensors.

In order to edit the data, click on the cell, type the new value and press *[Enter]*. Without *[Enter]* the new value will not be copied into the table. Changing the value in the table, does not lead to an immediate change of the data itself. You have to press *<Update>* to make the change effective in the *Adjust bundle setting* form. The edited data will be displayed on the right side as multi 2D-plot showing the lines recorded for each sensor in an overlayed plot. If the data can be processed to an image, the image is displayed in the upper graph. The crosses which can be displayed under *Display/ Show point location* mark the positions of the provided data (tabulated x and y data with corrections) from which the interpolation of all other points was performed. The color of the crosses is white if the false color on the scale 0...255 is below 205 and black if it equal or larger than 205. The current scales give the min-max values of the data set after applying the correction values.

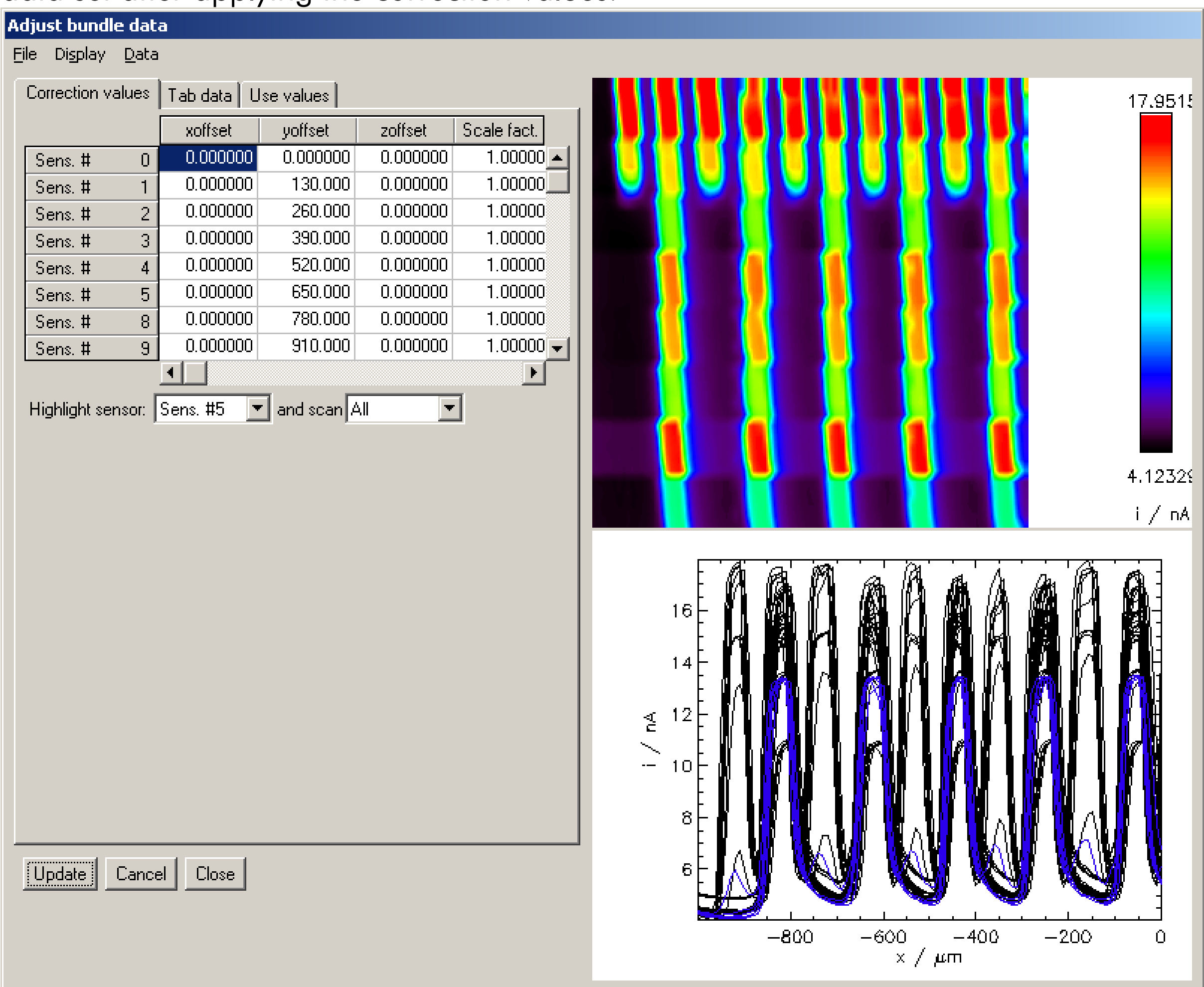


Fig. 90: Window for adjusting bundle data.

The tab *Use values* also allows using extrapolation for making an image by checking "Extrapolate to rectangle". The extrapolation is connected with a particular way of interpolating data from the neighbouring points. The effect becomes visible if different *xoffsets* for the sensors are entered. If extrapolation is not used, the edges of the image looks rugged because each sensor covers a different range of *x* coordinates in one scan. Extrapolation estimates the values from the neighbouring ones. This gives excellent results if there is not too much slope towards the edge of the image. However, situations can occur in which there is a slope and then the extrapolated points tends to be the largest/smallest of the image. Then extrapolation must be switched off. The situation can also occur if a certain region was imaged two times. This means that the last scan of one sensor scanned the same area as the first scan of the next sensor. In this case, very high slopes may occur within an image because different values are measured at (almost) identical horizontal coordinates and the slope approaches infinity. Then the computed images usually contain a few very large and very small data and all the rest looks flat because the color scale is spoiled by the very large and very small values. Also in this situation extrapolation should be switched off.

If the box "Extrapolate to rectangle" is checked, the interpolation is made by IDL's routine using Akima's quintic polynomials from "A Method of Bivariate Interpolation and Smooth Surface Fitting for Irregularly Distributed Data Points" in *ACM Transactions on Mathematical Software*, 4, 148-159. If the extrapolation is not checked, linear interpolation will be used.

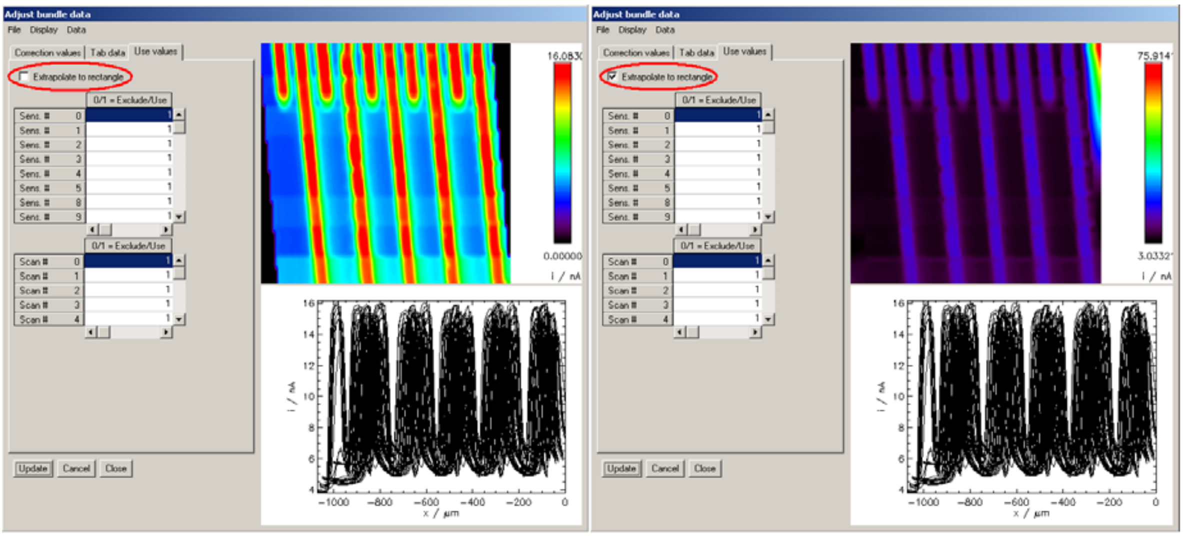


Fig. 91: *xoffsets*; without (left) and with (right) Extrapolation.

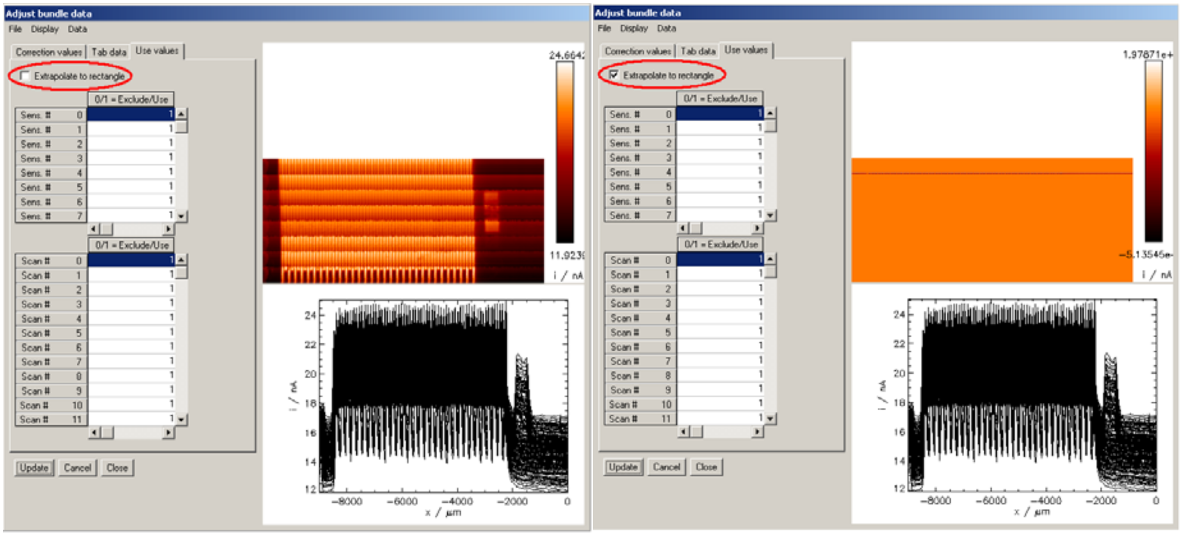


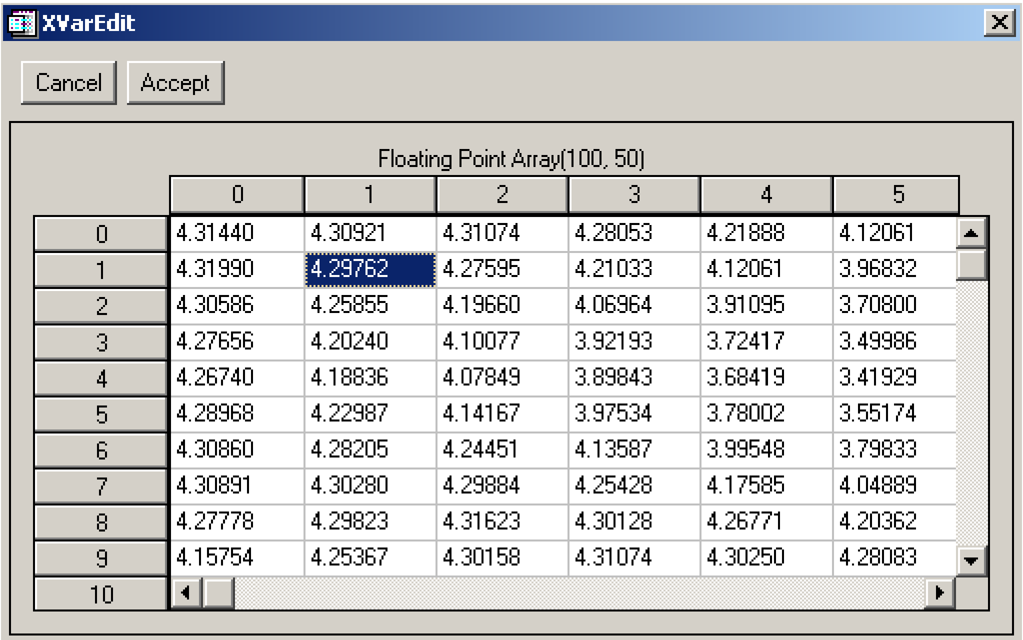
Fig. 92: Double scanned areas; without (left) and with (right) Extrapolation.

<*Cancel*> closes the window without transferring any changes to the original data set. <*Close*> transfers the edited data to the data handling routines.

It is recommended to use *Adjust bundle data* first, and then perform further fine tuning of the image (subsets, rotations etc.)

3.7.7 Edit data

With this options individual values can be edited in a manner known from speadsheats (spikes in 2D data sets). For a (x,y,z) data set, a table of all z values in matrix format will appear. For a 2D data set only a column or row of the dependent values (y) will appear.



	0	1	2	3	4	5
0	4.31440	4.30921	4.31074	4.28053	4.21888	4.12061
1	4.31990	4.29762	4.27595	4.21033	4.12061	3.96832
2	4.30586	4.25855	4.19660	4.06964	3.91095	3.70800
3	4.27656	4.20240	4.10077	3.92193	3.72417	3.49986
4	4.26740	4.18836	4.07849	3.89843	3.68419	3.41929
5	4.28968	4.22987	4.14167	3.97534	3.78002	3.55174
6	4.30860	4.28205	4.24451	4.13587	3.99548	3.79833
7	4.30891	4.30280	4.29884	4.25428	4.17585	4.04889
8	4.27778	4.29823	4.31623	4.30128	4.26771	4.20362
9	4.15754	4.25367	4.30158	4.31074	4.30250	4.28083
10						

Fig. 93: Unchanged data sets.

In order to change a value, click on the cell and press <***Enter***>. The value becomes editable. After changing the value, press again <***Enter***>.

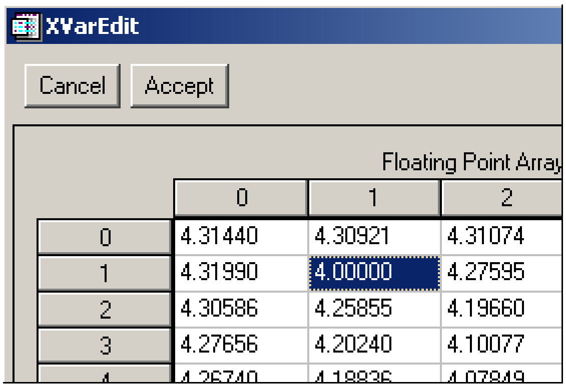


Fig. 94: After editing.

After pressing <***Accept***>, a window appears showing the input data and the result after editing individual values. You may change the plot type under Plot/.. (Fig. 81, right).

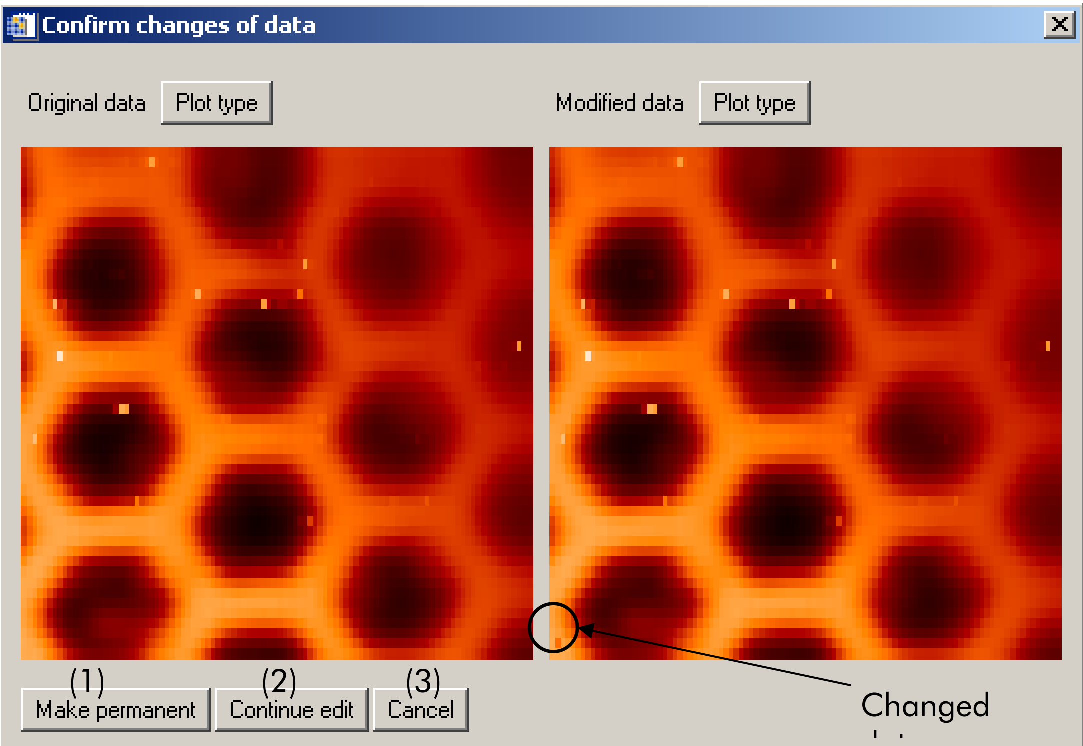


Fig. 95: Changed data in comparison with the unchanged version.

Three options are available now:
You get the last chance to cancel your changes (3).
You can make your changes permanent (1).
You can return to the table for editing (2).

3.8 Analysis

3.8.1 Profile

This option gives you the chance to analyze a profile along a freely defined line. In Fig. 96 the window is shown in which you can select the line for the profile. **NEW:**

Place the cross-hair on the begin of the line. Click and hold the left mouse button. Move to the end of the line and release the mouse button. The profile is presented below the plot. Inputs for the printer/graphic format number and the thickness of the profile line in the upper plot are included, too. Results may be exported as table or graphs with options under *File/..*. The menu options are analogous to the File menu options in *Single Plot*.

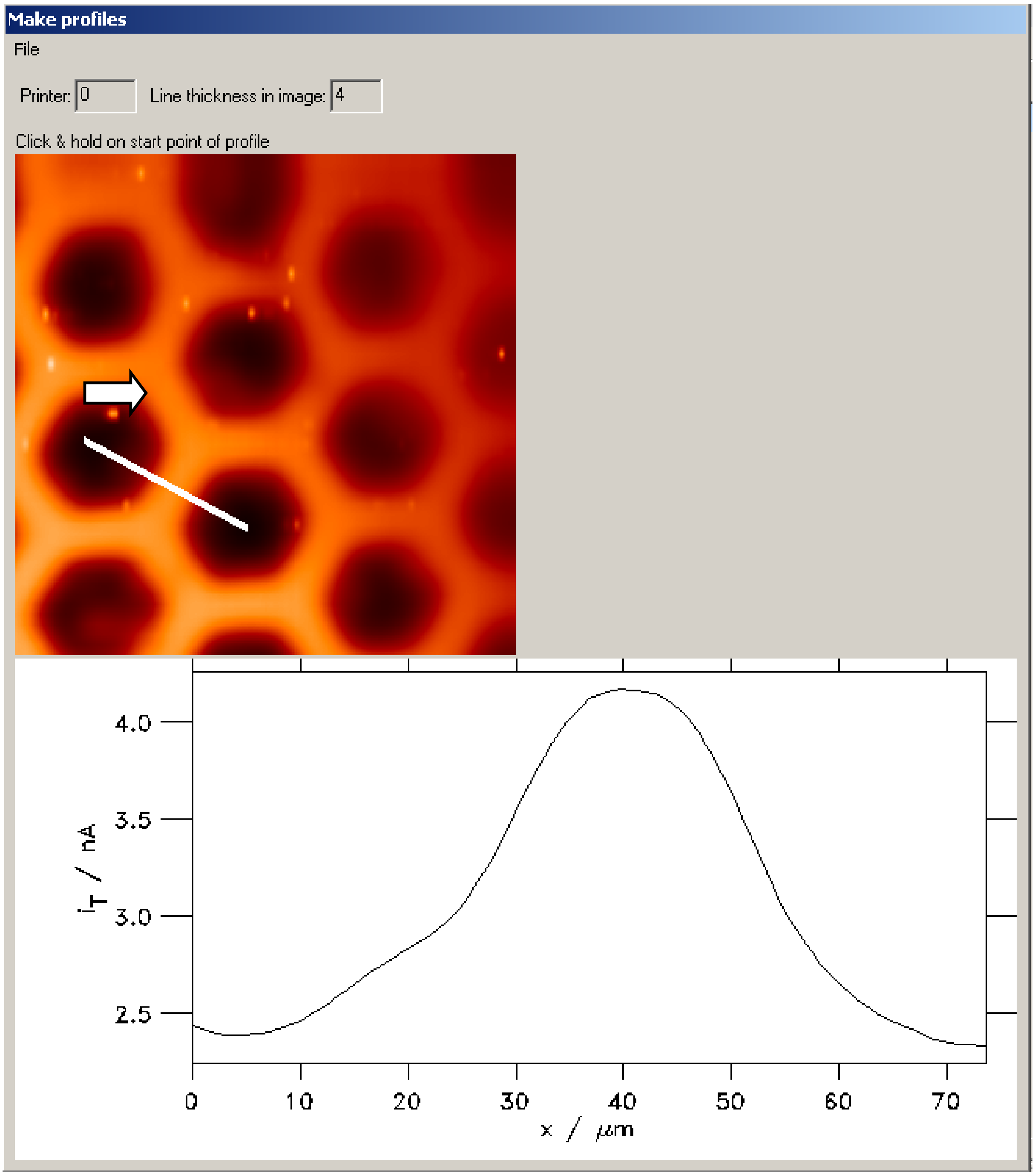


Fig. 96: Profile along the white line in the upper image.

3.8.2 Histogram

Histograms show the occurrence of values within a given interval. Such plots can be used to optimize color shadings to show the important details. If for instance, a few values are much larger or much smaller than the bulk of the data, it might be worth setting the upper and lower limit of the color scale such that it is spread only about the bulk of data points. Histograms are characterized by a minimum and maximum value considered and the interval (*binsize*) over which the occurrence is counted. The initial settings are min/max of the data set and 2 % of the data interval for *binsize*. They can be changed and new histogram plots are calculated after pressing <***Excecute***>. The result can be exported in all graph formats or as an ASCII data set. The menu functions in the histogram window are equivalent to the ones in *Single Plot*.

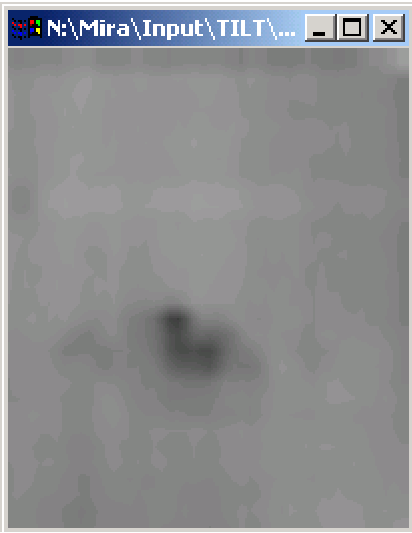


Fig. 97: Example plot.

The histogram of Fig. 97 will look like this:

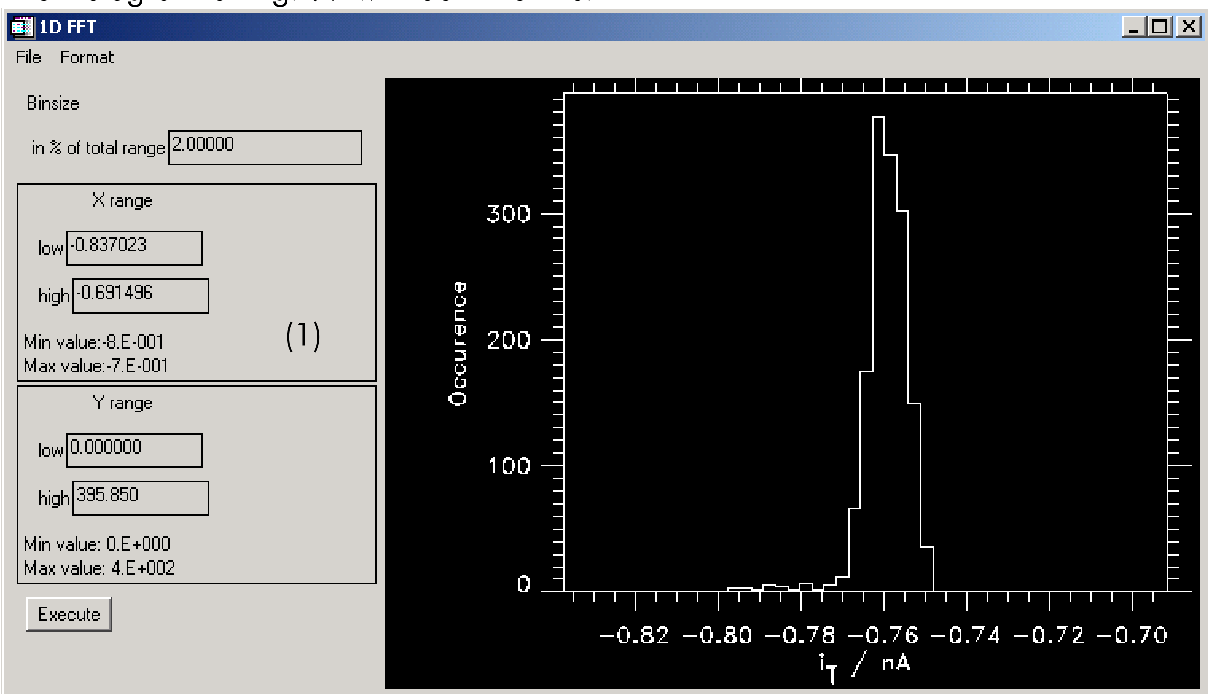


Fig. 98: Histogram Fig. 97.

3.8.3 1D FFT (Fast Fourier Transformation)

1D data sets (time series) are using the Fast Fourier transformation. You may have to change min/max of the plot to see the results in an optimized way.

3.8.4 Optimize AD Filter

This is a special function helping in optimize custom made instruments using Analog-Digital (AD) Converters. Often certain frequencies show up in the recorded signals (line frequency). Because of analogue-digital-commutations interferences get inducted to the plot. Using simple, but specifically optimized digital filters can eliminate these discrete frequencies almost totally. In our laboratory we accumulate and average the AD values with the maximum frequency of the AD card over one period (1/50 s, 1/60 s in the USA). The average value contains as many points on the negative half cycle of the noise component as on the positive half cycle. Both contributions are cancled, if the accumulation time is exactly the period (or multiple) of the line frequency. The maximum AD conversion rate given in the product description is only realized approximately. Therefore it turned out to be important to optimize this number for each system. This functions helps to do it. It loads a time series recorded with the maximum AD conversion frequency and searches for the size of the best box-car filter.

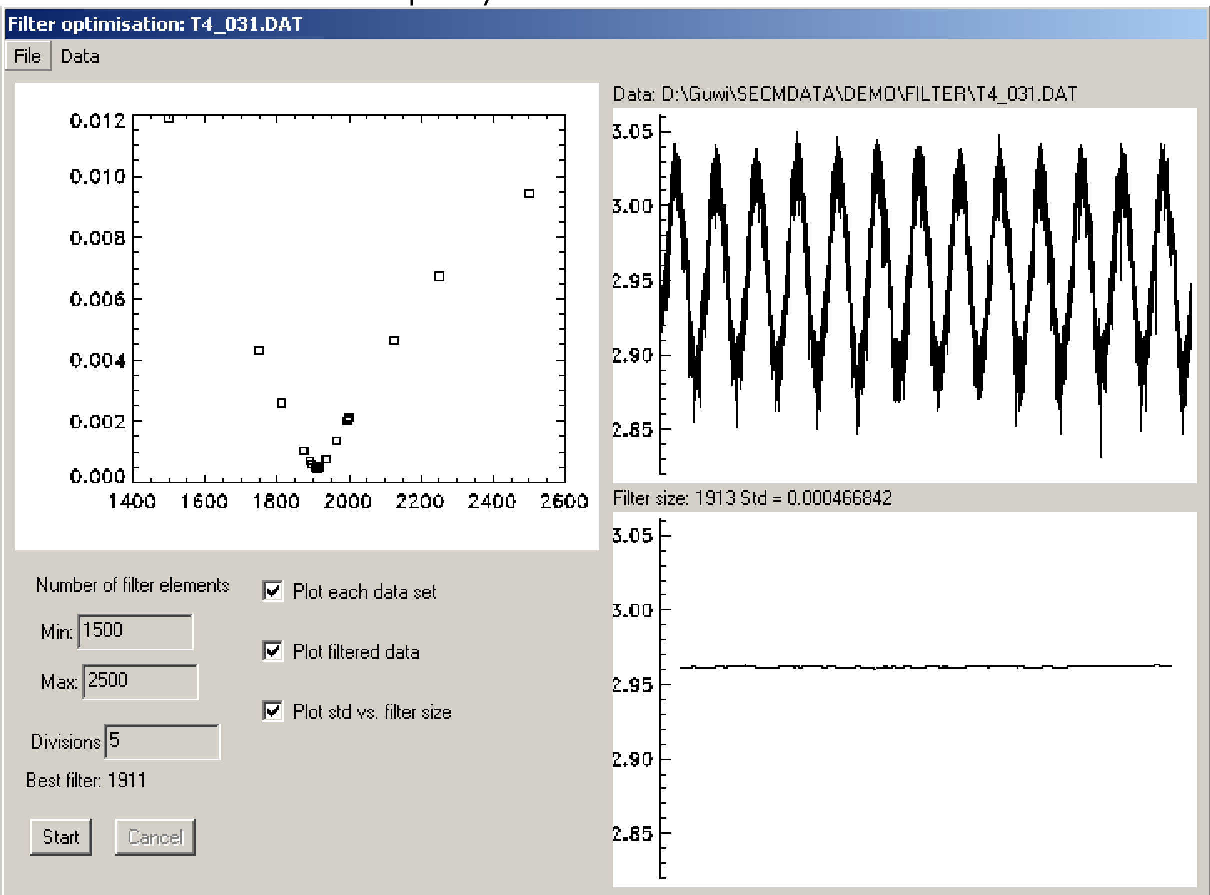


Fig. 99: Window for optimizing AD filters.

Select *Min/Max* and press <***Start***>. *Min/Max* should be selected such that the theoretical best count number ($n = k * (1/\text{line frequency}) * \text{frequency of AD card}$) is in the middle of the interval. The settings in Fig. 99 are appropriate for a line frequency of 50 Hz and AD card of 100 kHz and k=1. The check marks on the right control the graphic output during operation. Unchecking these options accelerates the processing. This can be significant when treating many data sets. This procedure can also be performed with several time series in order to get a statistically sounder analysis. In order to do so, load several data sets into *Multiplot* (see description on *File Open* or *Batch Processor* in the *Multiplot* chapter of this manual). Display the first AD time series in one of the graph windows in *Multiplot*. Start the *Optimize AD Filter* from the *Multiplot* window. Now all loaded AD time series are analyzed one after the others and the optimized filters are given (Fig. 100). For larger data sets the processing may take several minutes. The plots during processing (if checked) are the same as in Fig. 99. They are updated as the processing proceeds from filter size to filter size and from data set to data set. The final output contains a histogram of the best filter size (top left), the best filter for the data sets in sequence of the file list in *Multiplot* (top right) and the standard deviation of the filtered data after application of the best filter for each data set (buttom right).

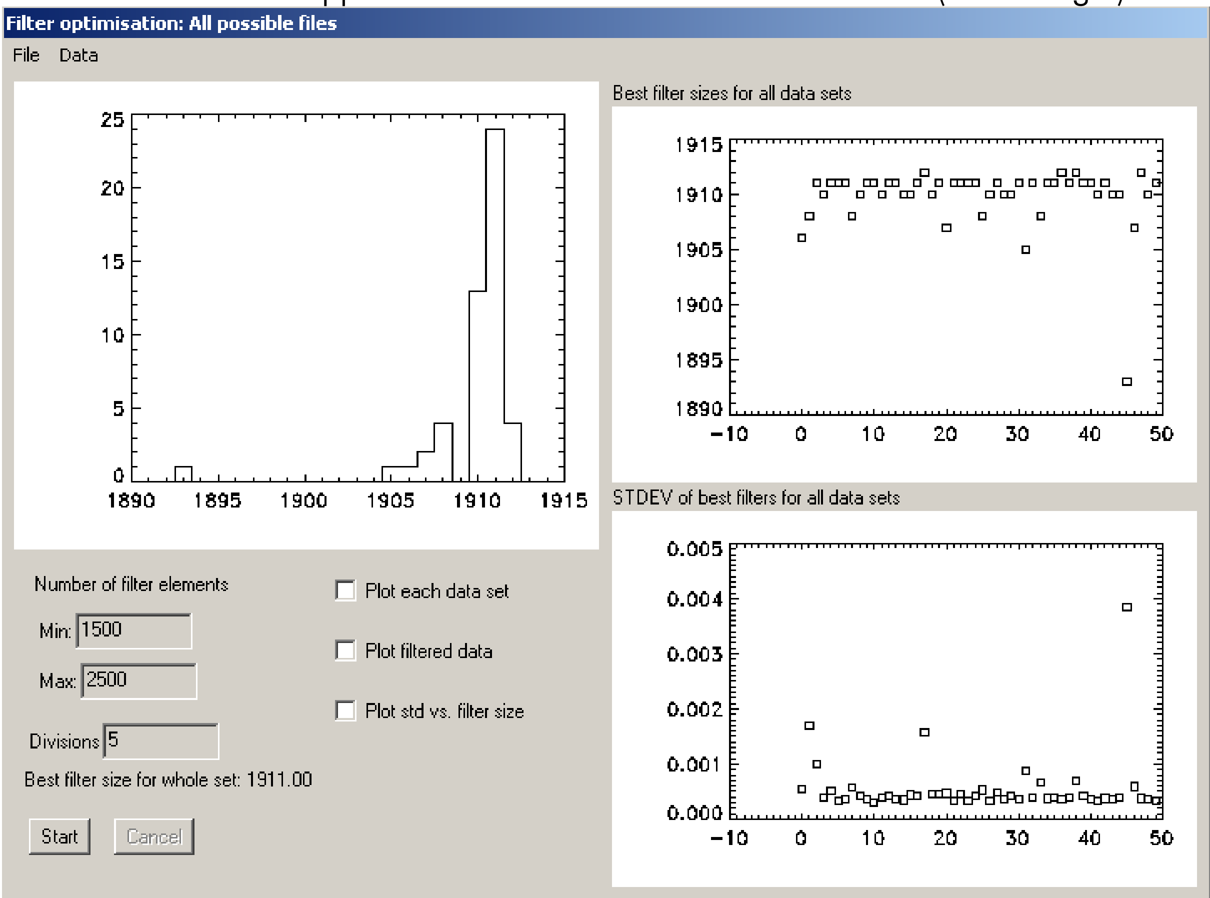


Fig. 100: Output for processing 50 time series in *Optimize AD filter*.

3.8.5 Curve fit

Curve fit is a module that fits SECM approach curves to the theory for infinite fast electron transfer at the sample and for very slow electron transfer at the sample.
Further models that might be of interest are included: generation collection (GC) horizontal line scan across the center of a pore from which particle are diffusing into the SECM cell. GC approach curve above a pore center. Michelis-Menten kinetics. All models are fitted by non-linear least-square fitting.

Theoretical models from the following papers are included.
Amphlett, Denuault; *J. Phys. Chem.* **1998**, *102*, 9946.
Shao, Mirkin; *J. Phys. Chem.* **1998**,*102*, 9915

Mirkin, Fan, Bard; J. *Electroanal. Chem.* **1992**, *328*, 47
Scott, Bath, Lee, White, Scott; *Anal. Chem.* **1998**, *70*, 1047.

The general aim of the curve fitting consists in extracting physico-chemical constants from the measured curve. The theoretical response is available as an analytical function. The analytical functions results either from a mathematical treatment of the problem or from an interpolation of digital simulations for discrete points.
WARNING: The proper use of fitting programs requires a detailed understanding of the underlying theory. Neither the program nor this manual can replace a thorough study of the original papers. Users must be aware of the limitations of each model and their experiments. This manual does not attempt to give a complete overview on the curve fitting. It intends only to explain the proper use of the program. If questions remain open, please contact Gunther Wittstock.

As an example, we consider the approach curve of a UME to a gold surface. Load the curve into *Single Plot*. If loaded into *Multiplot*, display it into one of the graphs to make it the present data set. Select the color table 39 (Rainbow + White) tin order to get the same colors as used here. Start *Analyse/Curve Fit*. The following window appears.

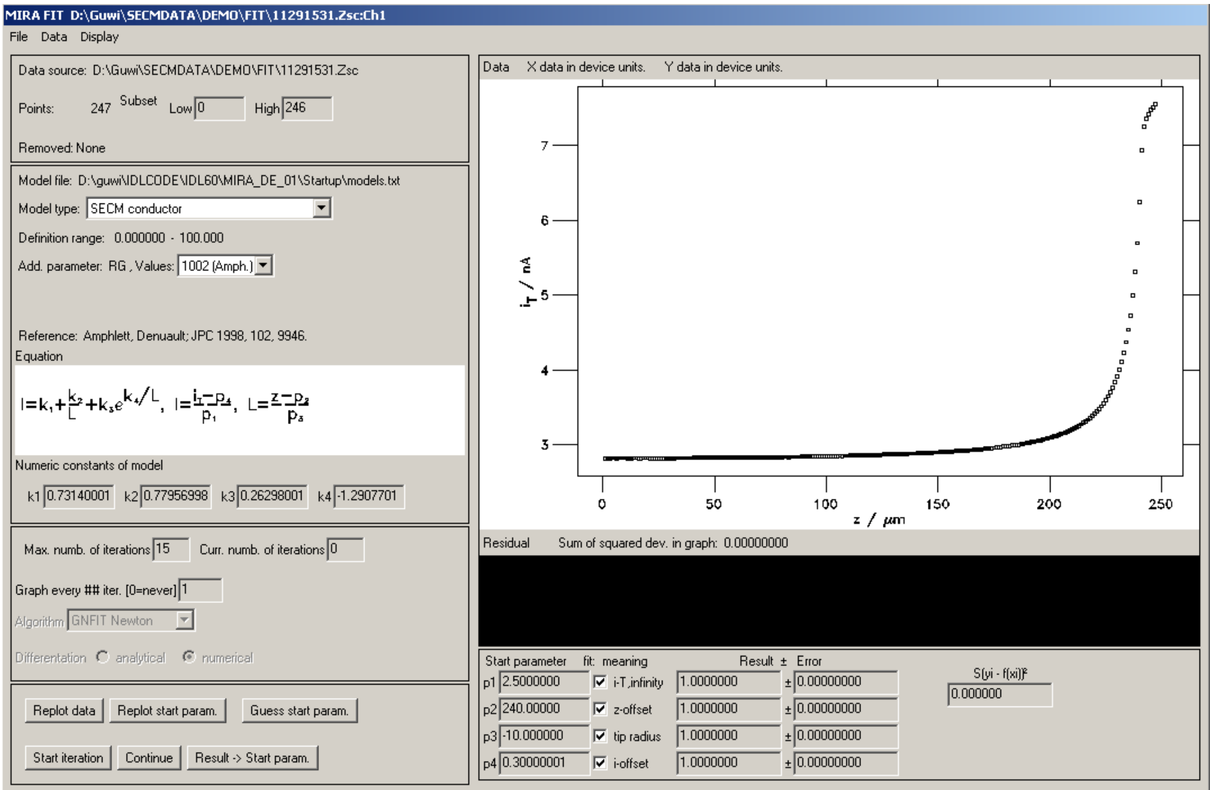


Fig. 101: Startup-screen for *Curve Fit*. Data set is a SECM approach curve to gold.

In order to prepare the processing proceed from top to down and left to right of the different controls.

The last 6 points of the data set at the right side of the display clearly do not follow the theory probably because the glass sheaths of the electrode touched the sample. Such data points should be excluded from the fitting procedure. To do so set the field High: on 246-6 = 240. You can press <Replot data> (left bottom) to see the new selection.

Individual data points (spikes etc.) can be excluded by a spreadsheet. This is accessible via the menu Data/Spreadsheet. The last column initially contains 1. By setting this value to zero, the data point will be excluded from fitting.

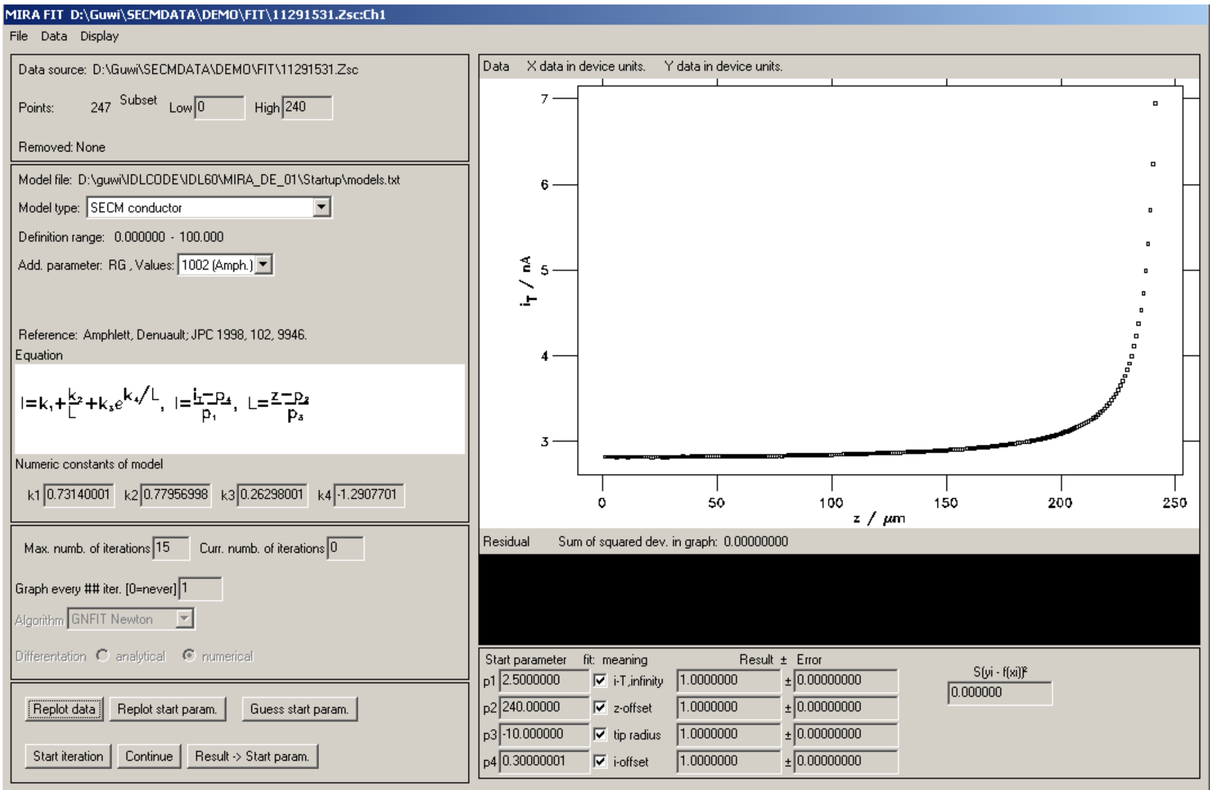


Fig. 102: Curve fit window after excluding the last six data points from fitting and pressing <***Replot data***>.

Now the appropriate model can be selected. For this data set we know that the experimental current offset of the potentiostat is zero. We can, therefore, select the model in the second frame on the left side with *SECM conductor without i_offset*. The window is rebuilt and has now only three adjustable parameters on the bottom right. The RG value of this electrode was 16.5. In order to fit the data, we can either use the closest value give in the filed *Add. parameter, RG, Values* = 10.2 or select a freely selected RG value (= *?)*. The freely selected RG value is interpolated from the neighbouring RG values, for which constants are known. Since the RG affects approach curves to a conductor only little, we want to stay with the predefined value RG = 10.2 from the paper of Amphlett and Denuault. (For fits with insulators model, more RG values are available since the curves are much more sensitive to this parameter.) The program will update the equation and the numerical constants as well as the literature reference from which the data are taken. (For some situations, more than one numerical solution is available as a model). The resulting appearance of the window is shown in Fig. 103.

Now details for the numerical fitting routine can be selected. For the SECM models the program usually converges after 7-8 iterations. The settings of *Max. number of iterations* should be set higher. Since processing is so fast it does not hurt to set them to 15. The *Curr. numb. of iteration* will display the progress of the program and cannot be edited. *Graph every ## iteration* controls how often the graph window will be updated. Only for older computers (Pentium 1 and lower) it makes sense to have a value other the 1. "1" means that a graph update will be initiated for each iteration cycle. This will usually be so fast, that you cannot see the individual iteration steps clearly.

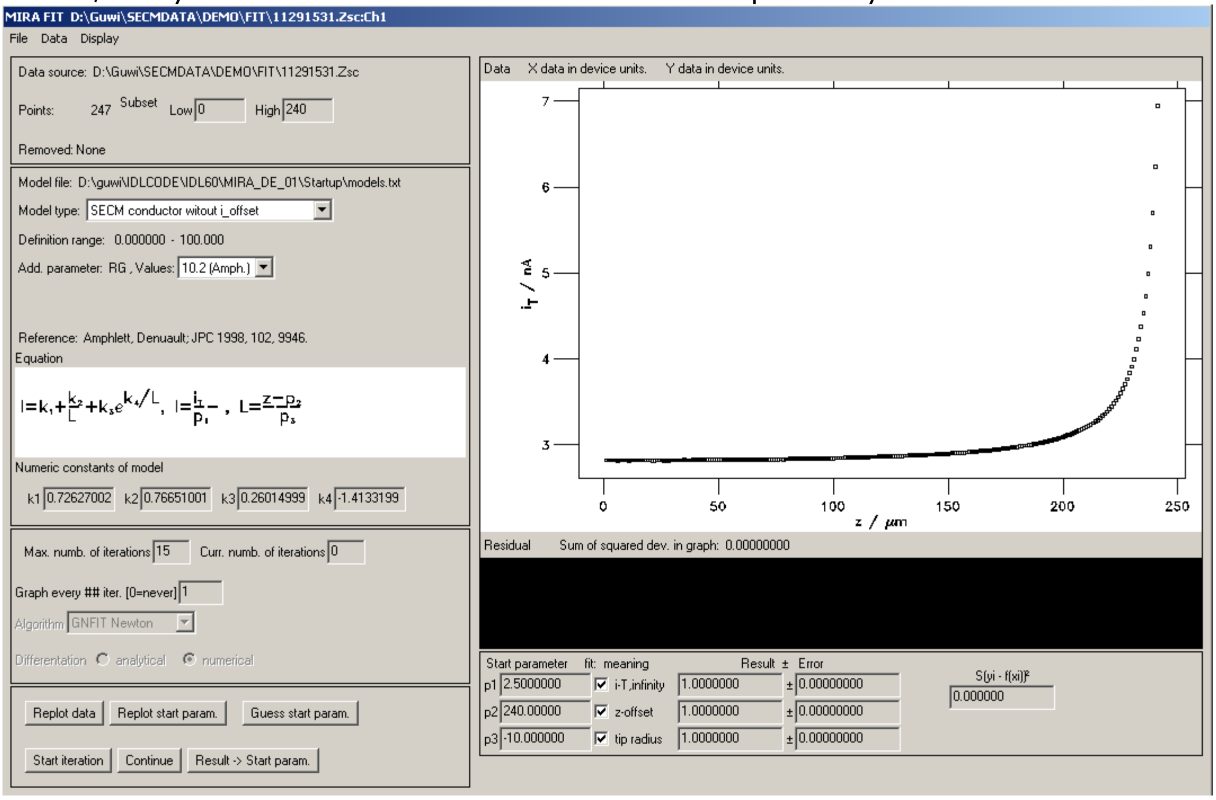


Fig. 103: Screenshot after selecting details of the model.

The field *Algorithm* and *Differentiation* cannot be edited. The program can work with several algorithms for non-linear curve fits and analytical and numerical differentiation. Previous testing showed that the results of the different algorithms are identical. However, the Gauß-Newton fit with numerical differentiation is the easiest to implement and works most reliable, while other algorithms showed problems with some data sets and are more prone to problems. Therefore, the further development of these algorithms is discontinued and will be dropped in the future if experience will not call for the opposite.

The quality of non-linear least square fitting depends on the starting parameters. It is a main advantage and accelerates the data processing enormously that MIRA can provide a good set of starting parameters for most models. For those models that do not have the <***Guess start param.***> function implemented, nothing will happen. After pressing <***Guess start param.***> the window will show the data points and the theoretical function with the start parameters. The experimental points which are within the definition range of the function are displayed in Blue (all for the example). The function with the start parameters is given in Red (Fig. 104).

On the bottom right, the fitting parameter are listed in a table. The enumeration p1 … pn corresponds to the labels p_1 .. p_n in the formular display on the left side. The window give the start value of the parameter. The values can be edited after clicking on them. The results can be explored by pressing <***Replot start param.***>. A plot similar to Fig. 104 will appear calculated with the new start parameters. Please be aware that for some models the parameters of the numerical model are not an individual physico-chemical parameter but a combination of them (e.g. $p_1 = k_{cat} * [E_0]$ in a Michalis-Menten curve). Please note the sign for the electrode radius. The sign should be negative if the z-values of the experimental approach curves are counted positive if the electrode approaches the sample. It should be positive if the z-values increase with increasing distance to the sample.

The check marks after each parameter indicates that this parameter can be varied during the iteration. For some models parameters are known from independent experiments and the curve could be fitted by more than one parameters sets. In order to avoid this situation, parameter known from independent measurements (e.g. electrode radius) can be set constant in the procedure by unchecking the box. Such a parameter will not be varied and now uncertainty is calculated for this parameter. The small graph below the data set shows the deviation between model and experiment for each data point. The field $S(y_i\text{-}f(x_i))^2$ gives the sum of the squared deviations between experimental points and the model.

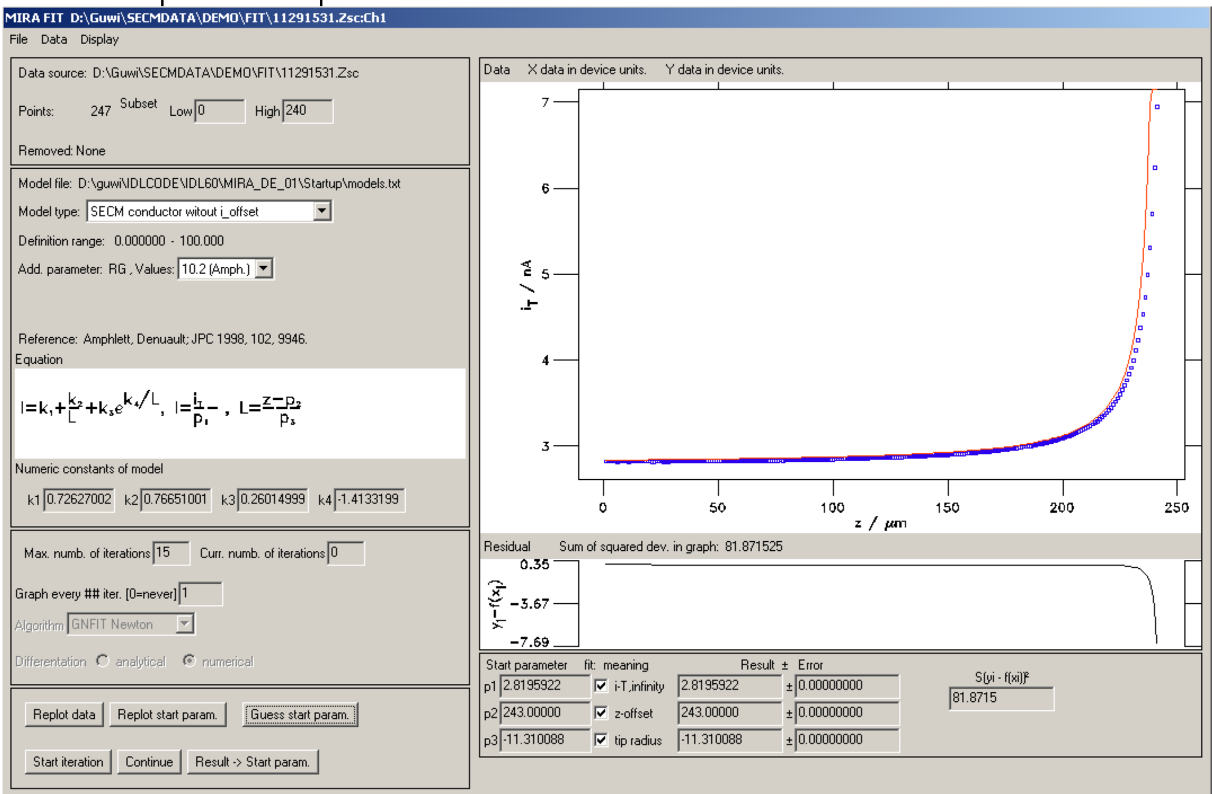


Fig. 104: Screenshot after <***Guess start param.***>.

If the start parameter are sufficiently close (what is "close" may depend on the model), the fit can be started by <***Start iteration***>. If the result is not sufficient, iterations can be continued by <***Continue***>. If the model shall be refined with a different model, or algorithm (currently disabled) the result can be made the new start parameter by <***Result->Start param.***>. For the example the result of the fitting looks like Fig. 105. The model with the optimized parameters is plotted in Green. The optimised parameters are plotted in the table together with an estimation of the uncertainty of each parameter. The estimates are given as ± one standard deviation.

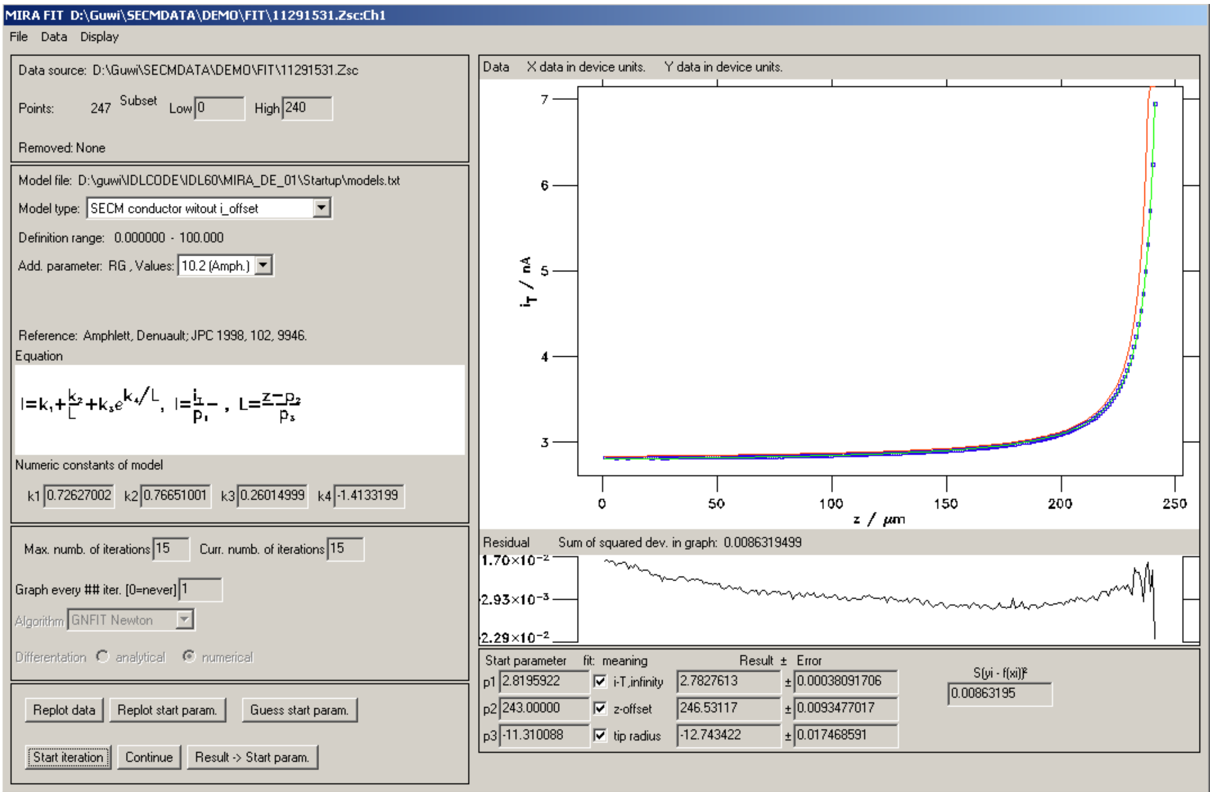


Fig. 105: Screenshot after <***Start iteration***>.

Working with the result:

Menu <u>*File*</u>

The menu works mostly like the menu in *Single Plot*. Here is a summary

Change Default Path: use it to select the output directory for graphic and text files

Save/Load IDL binary: This is for short term storage of fitting (for preparing discussion). It should not be used for long term archiving as each version of MIRA can only work with its own binary files.

Export fit to ASCII: Exports data, fitted data and deviations to text file in spreadsheet format

Export parameter to ASCII: Exports only the fitted parameter to a file (avoids writing numbers from screen displays.

Select graphic format: Selects the output format as in Single Plot.

System printer setup: Sets up the windows system printer, if you want to direct the output directly to a physical printer.

Print text results: Puts the result to graph window.

Sun Nov 07 20:07:40 2004
D:\Guwi\SECMDATA\DEMO\FIT\11291531.Zsc, Channel: 1
Number of used data points/data points in set: 241/247
Excluded (0–based index): 241–246

Model: SECM conductor witout i_offset

$$I=k_1+\frac{k_2}{L}+k_3e^{k_4/L},\quad I=\frac{i_T}{p_1},\quad L=\frac{z-p_2}{p_3}$$

Lit.: Amphlett, Denuault; JPC 1998, 102, 9946.
Add. constant: RG = 10.2 (Amph.)
Numeric constants: 0.72627002, 0.76651001, 0.26014999, –1.4133199

Numeric procedure: GNFIT Newton , Computation method for derivatives: numerical
Number of iterations: 15
p_1 from 2.8195922 (i–T,infinity), fitted
p_2 from 243.00000 (z–offset), fitted
p_3 from –11.310088 (tip radius), fitted

Fig. 106: Graph output from *File/Print text results*.

Print graph:

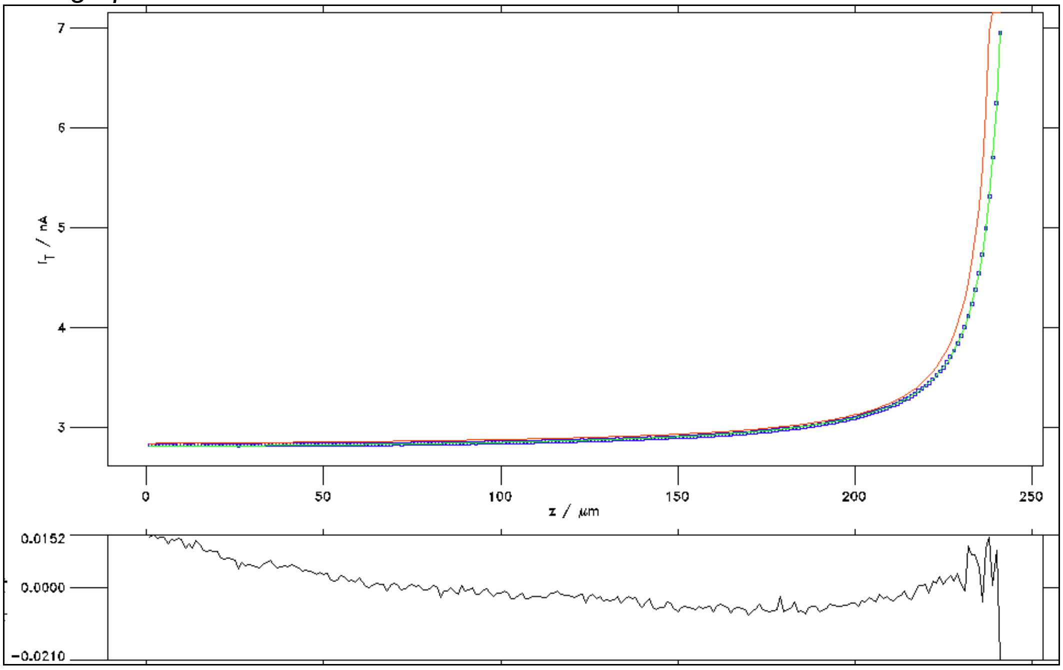
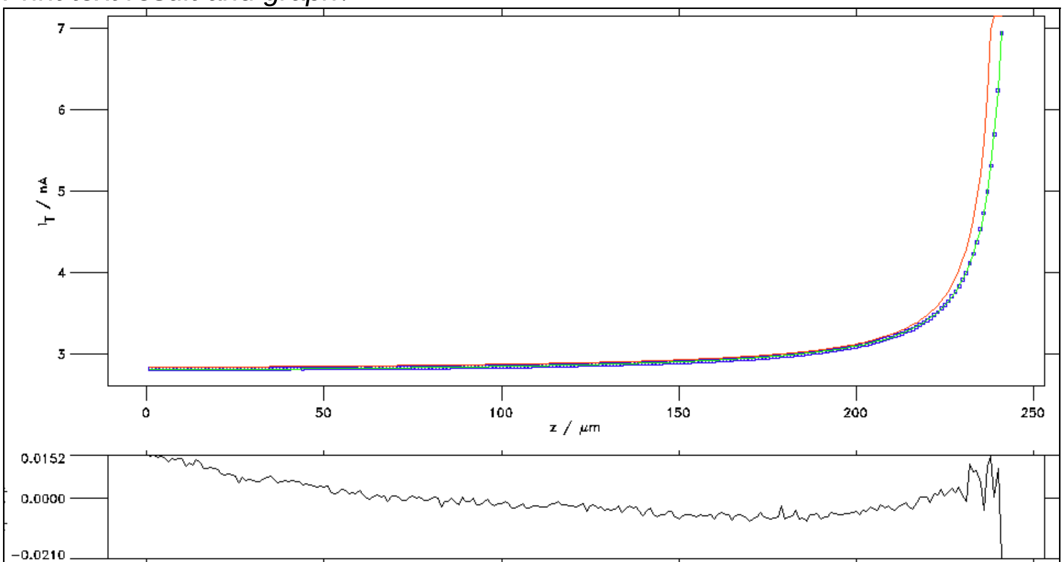


Fig. 107: Graph output from *File/Print graph*.

Print text result and graph:



Sun Nov 07 20:09:46 2004
D:\Guwi\SECMDATA\DEMO\FIT\11291531.Zsc, Channel: 1
Number of used data points/data points in set: 241/247
Excluded (0−based index): 241−246

Model: SECM conductor witout i_offset

$I=k_1+\frac{k_2}{L}+k_3 e^{k_4/L}$, $I=\frac{i_T}{p_1}$, $L=\frac{z-p_2}{p_3}$

Lit.: Amphlett, Denuault; JPC 1998, 102, 9946.
Add. constant: RG = 10.2 (Amph.)
Numeric constants: 0.72627002, 0.76651001, 0.26014999, −1.4133199

Numeric procedure: GNFIT Newton , Computation method for derivatives: numerical
Number of iterations: 15
p_1 from 2.8195922 −> 2.7827613 ± 0.00038091706 (i−T,infinity), fitted
p_2 from 243.00000 −> 246.53117 ± 0.0093477017 (z−offset), fitted
p_3 from −11.310088 −> −12.743422 ± 0.017468591 (tip radius), fitted
Sum of squared deviations: 0.0086319499 (in graph: 0.0086319499)

Interpretation of SECM approach curves
Distance of closest point to surface: (5.53117 ± 0.00934770) µm
Distance of closest point in normalized coord.: 0.434041 ± 0.00132851

Fig. 108: Graph output from *File/Print text result and graph*.

Print text start and graph:

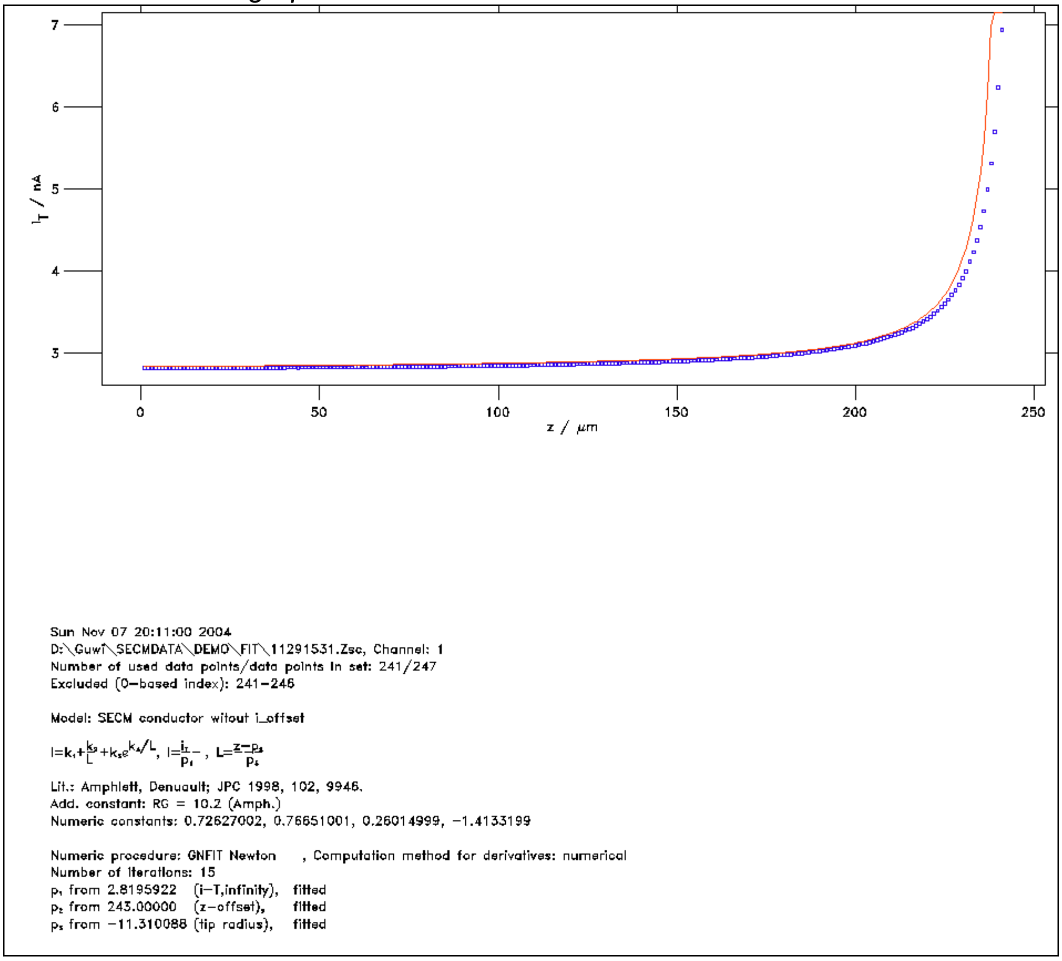


Fig. 109: Graph output from *File/Print text start and graph*.

Close/open log file: All operations within *Curvefit* can be recorded in a log file. Here it can e closed and a new one be opened.
Exit: Return to *Single Plot* or *Multiplot*

Menu <u>*Data*</u>
Spreadsheet: Individual data points can be edited or excluded from fitting.

Menu <u>*Display*</u>
Show matrix of 1st part. derivatives: Shows a vector of the first partial derivatives dS/dp_i for each parameter. S is the sum of squared derivatives. This gives an idea on how well determined a parameter is by the current data set.
Show matrix of the 2n part. derivatives: Shows a matrix of the second partial derivatives $d^2S/(dp_i\, dp_j)$. This gives indication on how much parameters influence each other.
SECM data interpretation: gives the distance of the closest point of the data fitted set to the surface in real and normalized coordinates. In the example the point right at the display in Fig. 105 has a distance of 5.53 µm to the surface.

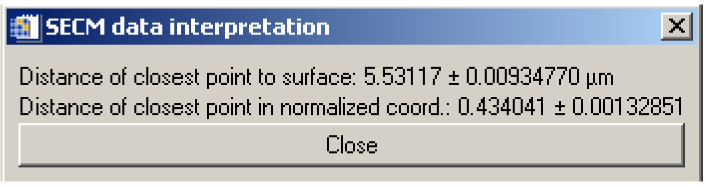


Fig. 110: Output of the menu *Display/ SECM data interpretation*.

Plot normalization: After the plot was fitted (and r_T and $i_{T\infty}$ are determined) the plot can be shown in normalized coordinates. Check the options in the window

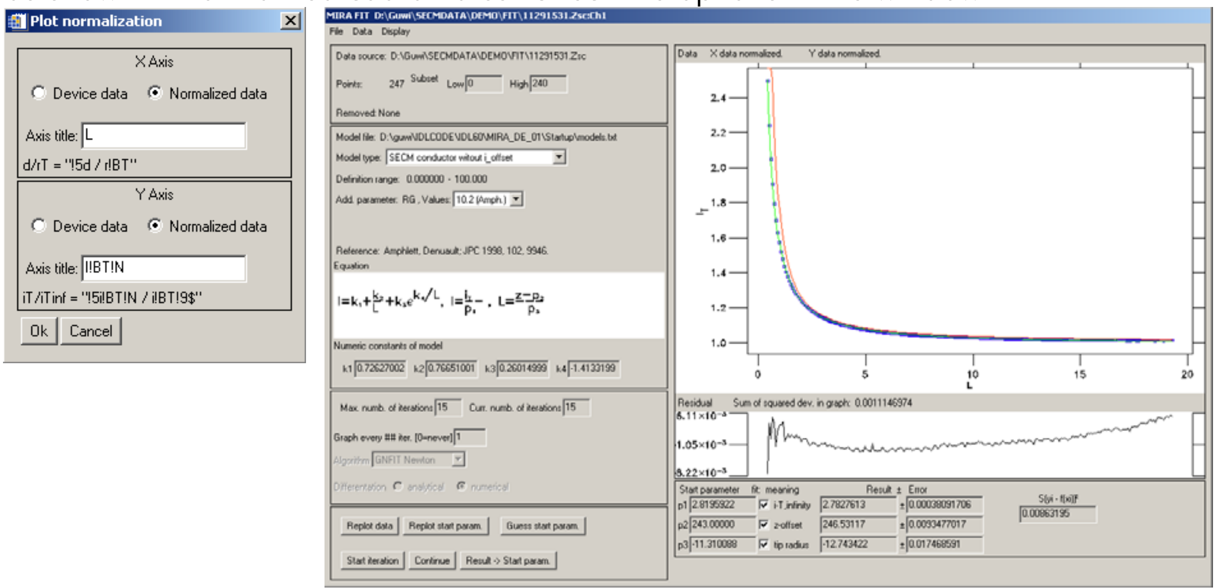


Fig. 111: Setting of the normalisation options (left) and resulting output (right). The title of the axis must be given with the formating notation of IDL if special characters and superscripts and subscript are used. As a guideline, the notations for d/r_T and $iT/i_{T,\infty}$ are given.

4 Multiplot

This configuration allows having a look at more than one plot at the same time (Standard initialization is given with 4 graphs for different data sets. → *Multiplot/Options/Change layout*). If you are not sure while loading the program either to choose *Single-* or *Multiplot*, you can change from *Single-* to *Multiplot* after starting working with the program. → *Single Plot/File/Start MULTIPLT*.

4.1 Elements of Multiplot

The general idea of multiplot is the following: Several data sets can be loaded into a filelist displayed on the left side of the Multiplot window.

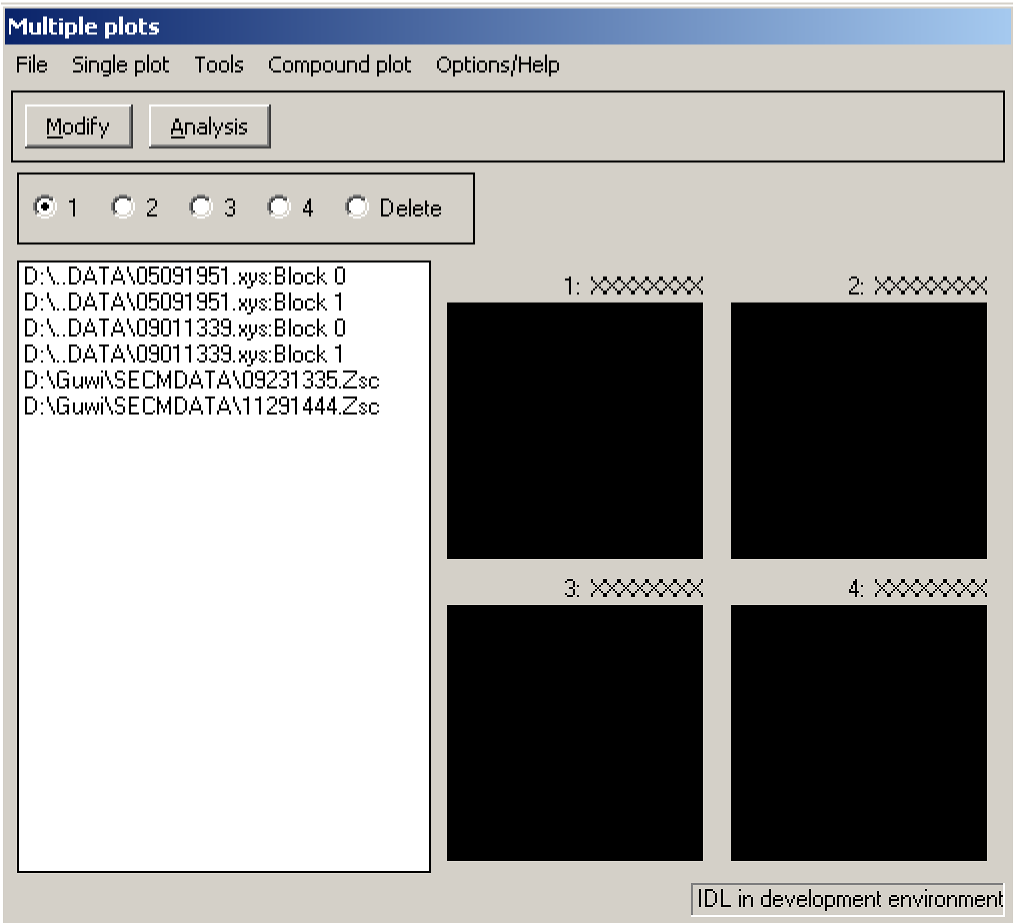


Fig. 112: Appearance of the *Multiplot* after loading some data sets.

Currently none of the data sets is actually loaded and can be worked with. To load a data, it must be loaded into one of the graph windows. To do so follow the following scheme

1) Select the graph window by either clicking on the option box in the selection tool on the right side OR clock on the graph area itself.

2) Click on a data set within the list.

Once a graph window is selected you can continue clicking on data sets. They are then loaded into the graphic field. That is very convenient to get a fast overview on a large number of measured data files. By selecting another graph more than one data set can be inspected. Please note: Only the data set selected last is the present data set with which manipulations can be done. If *Single Plot* and *Multiplt* are active at the same time, the active data set is always loaded into *Single Plot*.

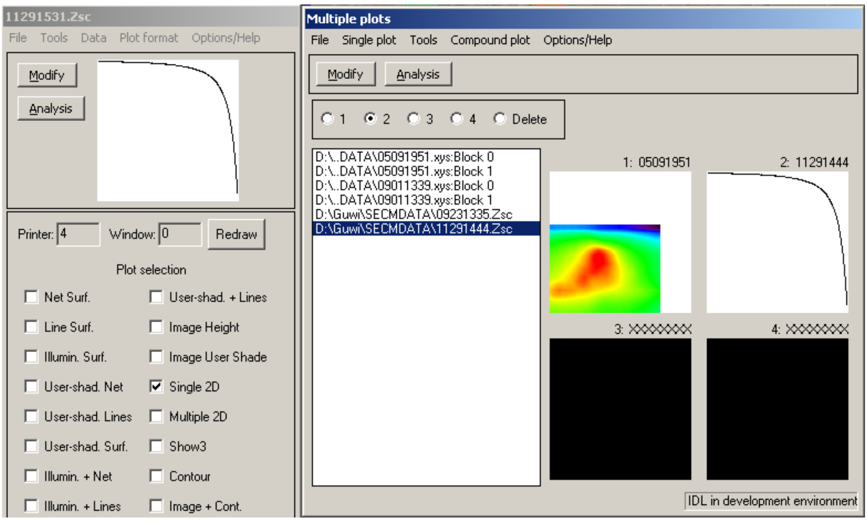


Fig. 113: *Multiplot* with two data sets loaded in graph 1 and 2. Only the data in graph two is the active data set (because 2 is selected in the selection tool and *Single plot* shows the 2D graph.

The active plot can be manipulated by the menu in *Multiplot* in a way very similar to Single Plot. User may also use Single Plot to make modifications to the graph display.

The display in *Multiplot* shows the pre-defined default plot for each data type. If formatting was changed, the changed format is shown if you click 2 times on the graph while the data set is highlighted in the file list of *Multiplot*. Often this display looks strange. But if they are plotted on normal sized windows, they look o.k.

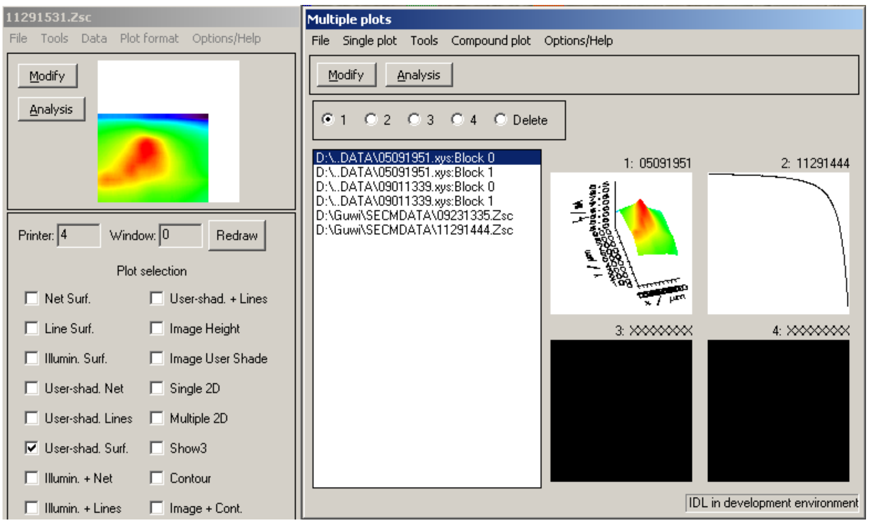


Fig. 114: *Multiplot* with two data sets loaded in graph 1 and 2. The plot type for data set 1 was changed in *Single Plot*. Clicking two times on graph region 1 in *Multiplot* displays the current graph in the graph field 1.

If a new data set is loaded into graph field 1, the old data together with all formatting informations are written to a temporary file. If this data set is loaded again later, the data will be recovered from that file.

By selecting "*Delete*" in the selection tool on the left and subsequently clicking on entries in the *File list*, the corresponding entry is deleted. Note that the last entry cannot be deleted in order to prevent en empty list. To do so load another data set and delete then the last entry of your previous selection.

Most options in the menu are the same as the ones which are explained in *Single Plot*. Here only those options are explained which are different to the *Single Plot*.

4.2 File

4.2.1 Add file to list

Selecting this menu item, you can select one or multiple file for reading into the file list. New files are appended at the end of the file list

4.2.2 Load from IDL binary

Here again you may select multiple files for loading.

4.2.3 File types

This function displays a spreadsheet with the initialisation data of each data set in the file list. It's main function is for debugging.

4.2.4 Change default path

-> *SinglePlot/File/Change default path*.

4.2.5 Selection of graphic format

-> *SinglePlot/Selection of graphic format*

4.2.6 Setup of windows printer

-> *SinglePlot/Setup of windows printer*

4.2.7 Print

-> *SinglePlot/Print*

4.2.8 Start SPM

SPM is a short cut of *Single Plot*. Starts *Single Plot*. If SPM is already active the command is quietly ignored.

4.2.9 Start batch interpreter

The batch interpreter is an important tool to increase the productivity when working with experimental data. It can perform typical operation with all data in the file list of *Multiplot* such as display on screen or creating a graphic file of a specific format. Batch interpreter can also be used to load a large number of files from a file list. Even sequences of operations can be performed by batch interpreter. Its main function in the author's group is to generate standardized printout for note books and archiving. Based on the printouts specific data sets can be selected for closer inspection.

The menu options within the batch interpreter are:

File/Load batch file:
This batch files allow for instance to load files from a list, make a printout of them and export the data to ASCII files. An example of a batch file is supplied in the installation path under ~/lib/example.bat. (You may need to change paths before running it).
File/Change default path
As described for *Single Plot*.
File/Selection of graphic format
As described for Single plot
File/Close/open log file
Batch interpreter keeps a log file where all operations are noted. Such a log file can be closed and a new can be opened. The log file is written to ~/scratch.
File/Exit
Returns to *Multiplt*.

Command/Make file list
Generates a file list from an input directory. The input directory can be selected using the path selection tool.
Command/Edit file list
Allows editing a file list formed by *Command/Make file list*. You enter a zero for those files that shall not be processed. Editing requires <***Enter***> when selecting the cell and <***Enter***> when confirming the change to the individual cell. Finally you confirm all changes. If you cannot see the full filename (with path), click on the cell, press <Enter> and scroll through the content of the cell. Recommendation: Use input path that contain only the data you want to process. This avoids somewhat inefficient editing of input files.
Command/Load file list
Selects a file with a file list. All data sets contained in the files listed in the file list will be loaded into *Multiplot*. It is not required that the list file is in the same directory as the data files.
Command/File filter
This selects or unselects certain data sets which are loaded in *Multiplot*. If there are for example all data sets generated in one day. You want to make a printout of all data sets except line scans that contain only 2 or 3 points (because they were interrupted because of wrong settings) you can do here. You can restrict printing to only 3D images or cyclic voltammograms etc.
Command/Print
A printout with the default settings of the currently selected graph format is generated for each data set contained in the *File List* of *Multiplot*. Graphic files are written to the current output path.
Command/Export
All data sets contained in *File List* of *Multiplot* will be exported to ASCII.
Help
Not active in the moment.

In order to complete the printout for the notebook, follow the step-by-step instruction in Chapter Auxilirary Tools at the end of the manual.

4.2.10 Start Combined Plot

This starts the window to produce combined plots, i.e. plots that marge information from several data sets such as overlay plots or surface plots, where the shading is taken from another data set.

→ Main Chapter Combined Plots.

4.2.11 Exit

Exits *Multiplot*.

4.3 Single plot

Single Plot only applies to the present data set only. When changing the present data set operations have to be performed again for the new data set.

4.3.1 Redraw

Pressing ***<Redraw>*** the selected plot will be presented in an extra window.

4.3.2 Full path

The full path of the data file is displayed (Fig. 115).

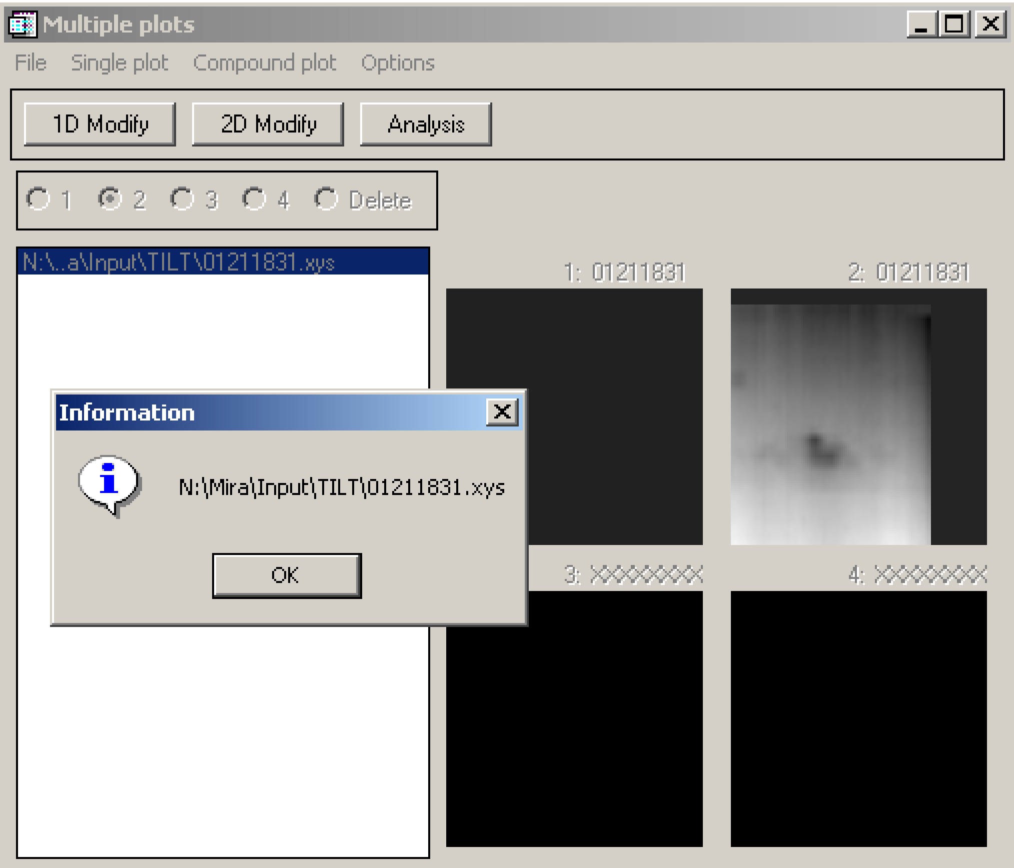


Fig. 115: Example for showing the path of a data set

4.3.3 Show header

→ *Single Plot/Tools/*

4.3.4 File

Save formatting
→ *Single Plot: File/Save Formatting*
Load formatting
→ *Single Plot: File/Load Formatting*
Save to IDL binary
→ *Single Plot: File/Save to IDL binary*
Export to ASCII
→ *Single Plot: File/Export to ASCII*
Print
→ *Single Plot: File/Print*

4.3.5 Data

Send data to Combined Plot
Transfers the present data set to the active set of Combined Plots
→ Combined Plot
Subsets
→ *Single Plot: Data/Subsets*
Resize array
→ *Single Plot: Data/ Resize array*
Arithmetics/X ~/Y ~/Z
→ *Single Plot: Data/ Arithmetics/X ~/Y ~/Z*
Data cutoff
→ *Single Plot: Data/ Data cutoff*
Rotate array
→ *Single Plot: Data/Rotate array*

4.3.6 Plot format

Handle volume data
Opens a tool to handle volume data. → *Single Plot: Handle volume data*
Create view
→ *Single Plot: Plot format/ Create view*
Plot dep. margin
→ *Single Plot: Plot format/Create view*
Plot region
Sets the limits of the plot region. This can be set here but will only affect Combined Plots. The position of the Single Plot is controlled only with the Plot-depending and hardware depending margins.
→ *Combined Plot: Example 2 - Create a Stacked Surface plot*
Skirt
→ *Single Plot: Plot format/Create view*
Axis rotation
→ *Single Plot: Plot format/Create view*
Scale user shade
→ *Single Plot: Plot format/Create view*
Light source
→ *Single Plot: Plot format/ Light source*
Symbol
→ *Single Plot: Plot format/Symbol*

2D Line Color
Sets the color for lines and symbols in 2D Plots. Than can be used to distinguish data sets in Combined Plots. A graphical selection tool opens with the color palette of the currently selected palette.
Font system
Allows selection of the font and font system. →*Single Plot: Format/Plot System*.

4.3.7 Axis/X ~/Y ~/Z

→ *Single Plot/Plot format/Axis/x ~/Y ~/Z*

4.4 Tools

XLoadct
The color table is selected. The new color is used for all subsequent graphs. The data sets that were treated before are saved together with the color table that was active when the processing was made.
Xpalette
The color table is edited. The new color is used for all subsequent graphs. The data sets that were treated before are saved together with the color table that was active when the processing was made. Pleas note, that the edited color table is used for graph output. The new color table will not be available if *Multiplot* is loaded gain.
iSurface
The current data set is used and *iSurface* is called (*Single Plot: Tools/iSurface*). Works only for 3D data sets.
iSurface (shaded)
The current data set is used and *iSurface (shaded)* is called (*Single Plot: Tools/iSurface (shaded)*). Works only for 3D data sets.
iContour
The current data set is used and *iContour* is called (*Single Plot: Tools/iContour*). Works only for 3D data sets.
iImage
The current data set is used and *iImage* is called (*Single Plot: Tools/iImage*). Works only for 3D data sets.
iPlot
The current data set is used and *iPlot* is called (*Single Plot: Tools/iPlot*). Works only for 2D data sets.

4.5 Options + ?

4.5.1 Change layout

Change the number of graph fields and the size of the graph fields. Defaults are 2x2 and 128x128 pixels.

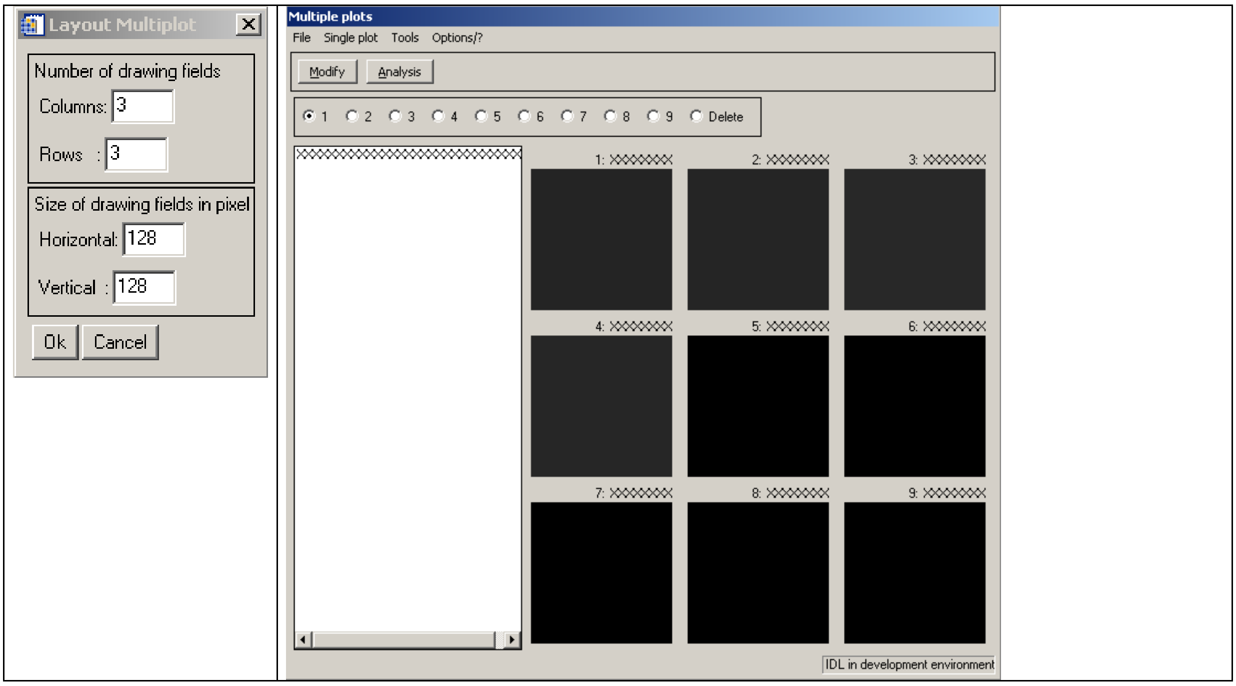


Fig. 116: Layout of *Multiplot*. Here the setting of a 3x3 layout with 128x128 pixels for each graph is shown. The right shows the resulting layout of *Multiplot*.

4.5.2 Save layout

This saves the current layout. This layout will become the new default layout when *Multiplot* is started again.

4.5.3 Load INI file

→ *Single Plot: Options/?/Load INI file*

4.5.4 Save INI file

→ *Single Plot: Options/?/Save INI file*

4.5.5 Information about MIRA

→ *Single Plot: Options/?/Information about MIRA*

4.5.6 What's new in MIRA VM 1.0

→ *Single Plot: Options/?/What's new in MIRA VM 1.0*

4.5.7 Manual about MIRA

→ *Single Plot: Options/?/Manual about MIRA*

4.5.8 RSI Manual about iTools

→ *Single Plot: Options/?/RSI Manual about iTools*

4.6 Menu Modify

The functions of this menu apply to the active data set and they are identical to the one in *Single Plot*.

4.7 Analysis

The functions of this menu apply to the active data set and they are identical to the one in *Single Plot*.

5 Combined Plot

Combined Plot allows generating graphs containing information of more than one data set. For 2D data sets these are overlay plots. Combined Plots of 3D data sets are designed primarily to deal with shear force SECM data. For instance the topography is shown as a surface or contour plot and the Faradaic current is shown as a false color scale of the surface or as an overlaid image of the contour plot. Another application are time sequences were the same region was imaged several times. The same number of data points must exist in all data sets. You should be proficient in making plots of individual data sets. This manual cannot cover all possible combinations and complications. Contact the author for specific requests.

In order limit the possible ways of arranging and manipulating the data, the following general steps must be followed: Prepare and format the individual data sets in Multiplot or Single Plot. Then transfer the formatted data set from Multiplot to Combined Plot. If you need to change formattings, do so in Multiplot than transfer the data set again (The old version will be overwritten).

Some formattings (rotation angle of axes, margins around the plot) are taken from the first data set (shown in drawing area 1 in Combined Plot). There is limited possibilotiy to change those settings in Combined Plot. The changes should be made in Multiplot and then the data set transferred to Combined Plot. However, with this all settings you might have done in Combined Plot are overwritten! There are two settings that are conveniently made in Combined Plot:

- Combined Plot: *Plot format/Plot region* (needed for stacked surfaces)
- Combined Plot: *Plot Format/Stacked Surf. common settings*. (needed for stacked surfaces)

Both will be explained in Example 2.

After all data sets are transferred, you can produce the Combined Plots. Printing to files follows the same principles as elsewhere in MIRA. The procedure is detailed here for combined surface plots and stacked surfaces. For other plots the suggestion should be followed analogously.

5.1 Example 1: Creating a combined Surface plots

- Load the required data sets into Multiplot
- Start Combined Plots from Multiplot: *Data/Start combined plot*.
- Select the data set that is the topography. Select the data subset, rotation etc. Modify the formatting of the axis in Multiplot or Single Plot.

- In Combined Plot: Set the number of data sets to be combined (2 is the default). If a value different from 2 is selected, use ***[Refresh]*** to rebuild the Combined Plots form.
- In Combined Plot: Select the draw area 1 to receive the next data set by clicking on the draw area or using the radio button at the button of the window (Fig. 117a).
- In Multiplot: Make sure the data set is formatted and selected as the active data set. Select Multiplot: *Single Plot/Data/Send Data to Combined Plot*.
- The data set will appear in the draw area 1 of Combined Plot (Fig. 117b).
- In Combined Plot: Select the draw are 2 by clicking on the draw area or using the radio button at the button of the window.
- In Multiplot: Select the data containing the electrochemical currents.
- In Multiplot or Single Plot: Format the data set with respect to the desired user color scaling → *Single Plot: Plot format/Scale user shade*
- In Multiplot or Single Plot: Make sure an identical subset has been selected as in the data set transferred to draw area 1 in Combined Plot.
- In Multiplot: Transfer the data set to drawing area 2 by selecting *Single Plot/Data/Send Data to Combined Plot*
- In Combined Plots: Select ***Combined Surf.*** in the option field on the right side and press ***[Redraw]***. A plot appears where the topography of the surface is made by the data in drawing area 1 and the color shade is a false color representation of the data in dataset 2 (Fig. 118).
- The color scale can be surpressed if in Multiplot the drawing of the z-axis of the second data set is surpressed → *Single Plot/Axis/z.*

a) b

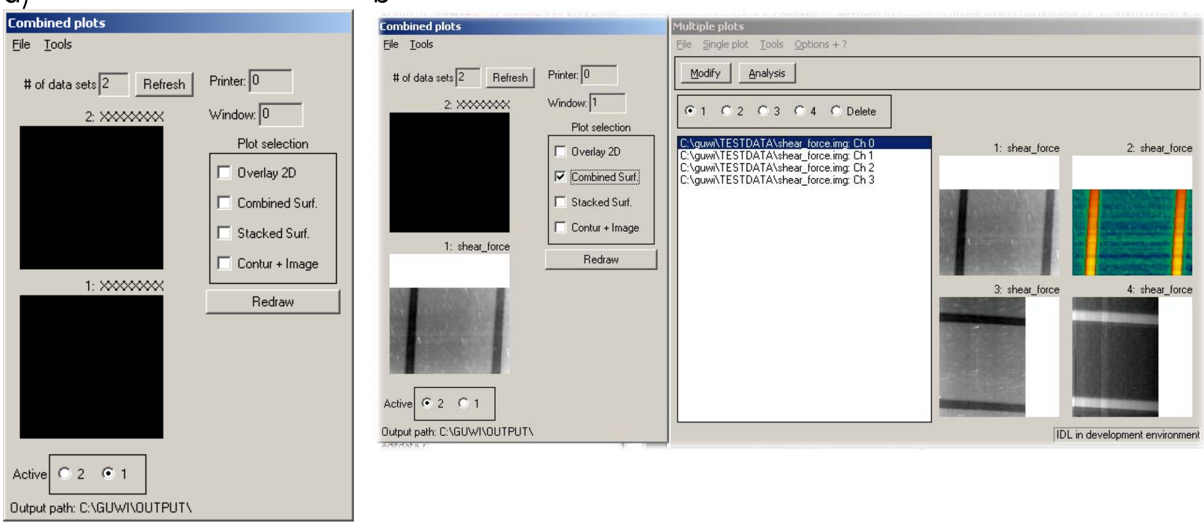


Fig. 117: Combined Plot form. a) Appearance after start, draw area 1 will receive the next data set. b) The first data set has been received into draw area 1 and will be used to construct the topography of the combined plot (or the contour map). Its information will be used for the x and y axes. The next data set will be received in draw area 2 (indicated by the radio button below the draw area.

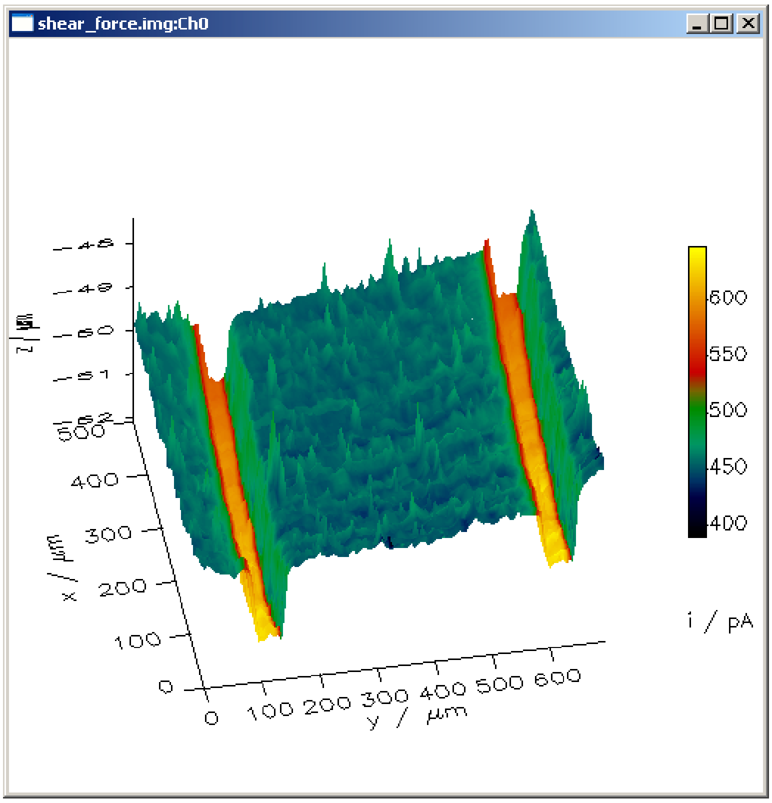


Fig. 118: Example of a combined plot from a shear force image (supplied in the demo data set). The topography is shown on the z scale in µm. The current is shown as false color with the scale to the right.

5.2 Example 2: Create a Stacked Surface plot

Stacked surface plots can be used for instance to represent shear force data or a sequence of images or different properties recorded at the same sample location. More than 2 data sets can be combined.

5.2.1 General background: placing multiple plots on a page

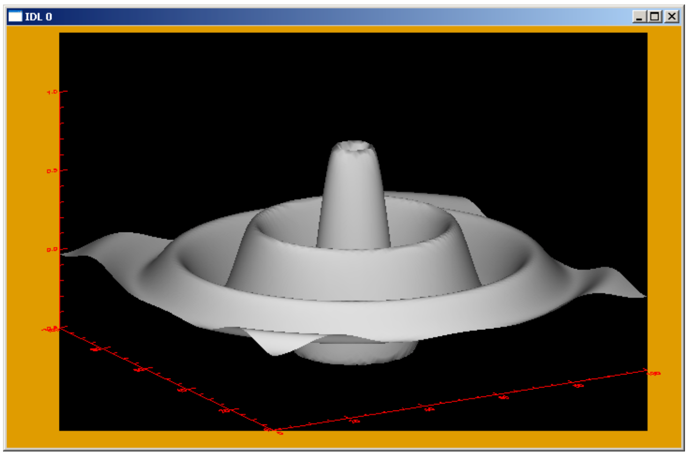


Fig. 119: Definition of the Plot window (black rectangle) and the margins (orange). The plot region comprises the Plot Window (Black) plus the axes and annotations.

In order to produce stacked surfaces, you should understand how IDL places plots on a printing page (e.g. the draw area of a graphic window or the page of an EPS file.).

Figure 119 shows a 3D surface plot. The orange background is the page (e.g. the drawing area of the window). The black rectangle is called the "Plot Window" which should not be confused with the window as defined by the operating system. The Plot Window contains the actual data points (excluding the axes and annotation). For surfaces plots the Plot Window is still rectangular and may contain part of the axes. The area including the axes is called "Plot region". Plot Windows and Plot Regions are given in normalized coordinates of the lower left and upper right corner, i.e. as fractional numbers between 0 and 1. In addition plot positions are manipulated by the margin keyword that controls how much space is available for tick marks and axis labels, e.g. the width of the orange margins around the black rectangle on Fig. 119. Margings are given in multiples of character width. This can be difficult to predict. It is advisable to play width this parameter, if the default settings do not produce a satisfying output. This can happen because the character width also depends on the output device. The properties of margins plot regions and plot windows are not independent from each other. They also affect how background colors are assigned during drawing. The Plot Window will always be drawn in the background color of the currently selected color table.

5.2.2 Use of plot regions for stacked surface

MIRA uses normally in single plot the margins to control the plot positions. The plot region is always left to its default, i.e. (0,0) - (1,1).
For stacked surfaces this is not sufficient and for each surface the plot region must be set in order to place the plots one atop the other. In order to align the z axes of different plots in one vertical line restrictions apply. For the first data set, the horizontal and vertical limits of the plot regions are used. For the other data sets the user can only modify the lower vertical limit of the Plot Region. The horizontal limits and margins are taken as identical to the first data set. The height of the plot affects the way the graphic transformations are made and has to be again identical to the first data set (you may not use the entire range of the z axis if you would like to give the plot a flat appearance).

In order to produce a good appearance one would like to place the stacked surfaces as close as possible above each other but avoid overdrawing one surface by the other. Unfortunately, the black rectangle in Fig. 119 will always be filled by the (opaque background color and cannot be fully used by two plots. Figure 120 shows a stacked surface plot with the two drawing regions indicated by transparent rectangles. Careful inspection of the lower left corner of the upper image shows that the plot was just clipped a little bit by the lower, although the actual surfaces are still far from overlapping. You should also change the format of the plot window or output size to file to have a portrait orientation (larger vertical size).

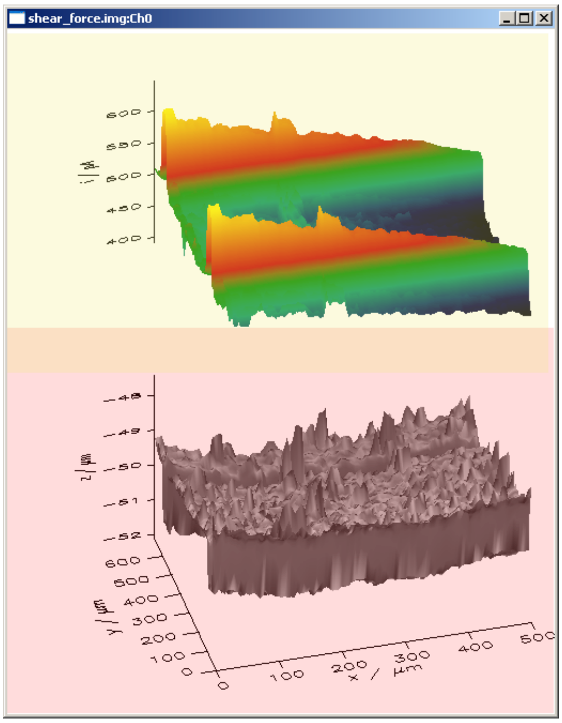


Fig. 120: Plot regions for a stacked surface plot. In the example the plot regions were (0, 0)-(1, 0.57) for the first plot and (0, 0.43)-(1, 1) for the second plot.

5.2.3 Fine adjustment of plot regions

Selecting the plot regions might not be easy and therefore MIRA can make suggestions upon request using Combined Plot: *Plot format/Stacked surf. common settings* (Fig. 121). The color tables provided by IDL do not have identical background and line colors. The first 2 options make sure that the background and line colors of the first plot are also used by the other plots. These options should be left in almost all cases. The option to remove exists because in rare cases it might be that the background color appears (unintentionally) in the plot itself.
The size of the labelling of the z axis follows the same idea. It uses the settings of the first plot for all plots. (Remember, if you reload the first plot, that will change the settings for all other plots).
The last option makes IDL to suggest plot regions for all plots. They can than be refined by using ***[Redraw]*** and setting the plot region limits individually with the tool Combined Surface: *Plot format/Plot region* (Fig. 122). The first selected surface plot, (i.e. the one used for the stacked surface will be highlighted. The regions can be adjusted

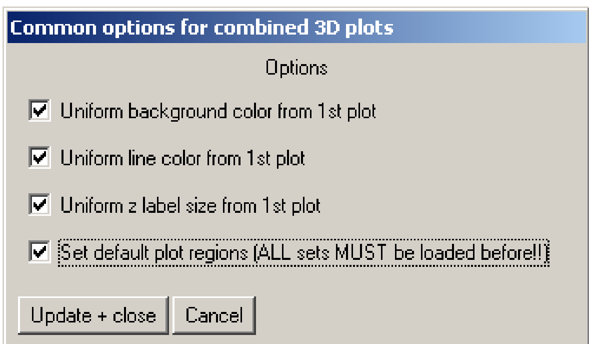


Fig. 121: Tool for setting common background colors and suggesting plot regions.

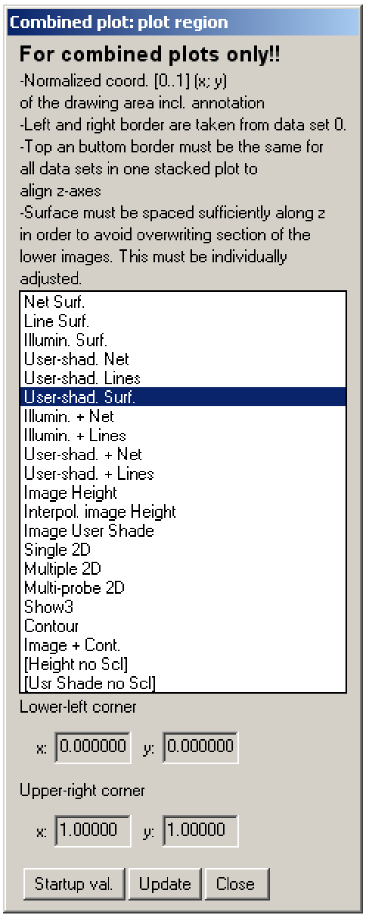


Fig. 122: Tool for selecting the limits of the plot regions individually. It will affect only stacked surfaces. For the first data set all fields are editable, for the other data sets only the lower limit of the plotting regions is editable. The other values are copied from the first data set.

5.2.4 Optimizing a stacked surface plot

The following steps describe how to produce the data of Fig. 120 into an optimized version (Fig. 123).

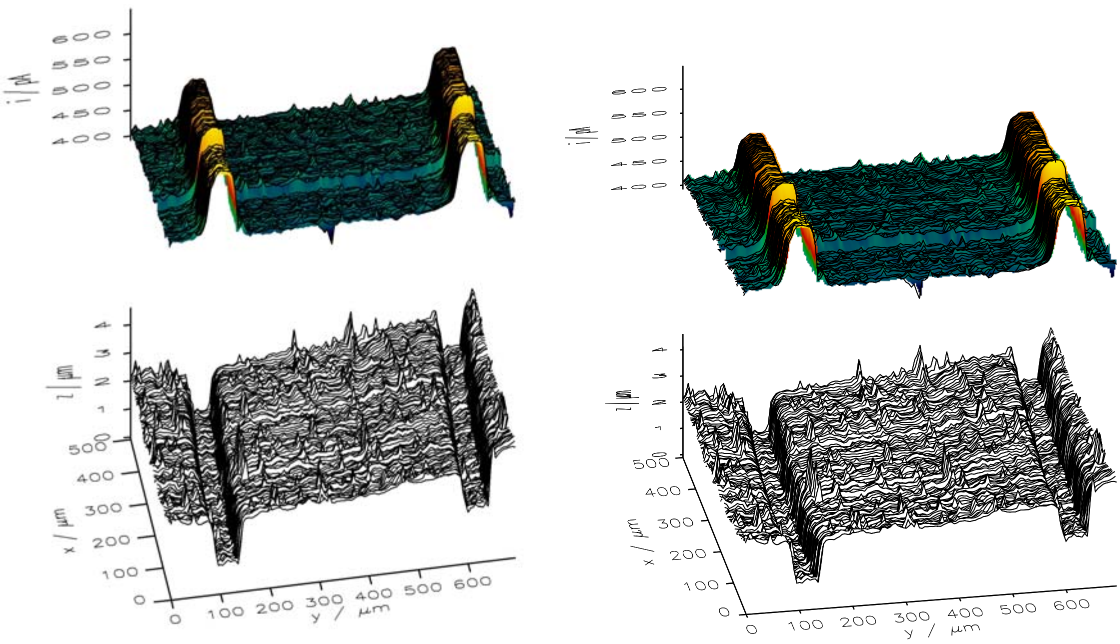


Fig. 123: Optimized stacked surface (left as jpg and right as eps).

- Load the required data sets into Multiplot. It is supplied as demo data set ([Installation path]\demo\SHEAR_FORCE\shear_force.img)
- Start Combined Plots from Multiplot: *Data/Start combined plot*.
- Start Single plot for convenient formatting.
- Select the data set that is the topography (first list entry) in Multiplot. Make the following modification in Single Plot: Select line plot as plot type. Use *Data/Arithmetics/z axis*. Set C = 52 to shift the data range (z/µm) from -52 to -48 to the range 0 to 4. Rotate data set by 90°. Set the axis rotation angles to 70° and 10°. Set in *Plot format/Axis format/z* the character size factor to 1.6. In Multiplot or Single Plot: Select the color table (Single Plot: *Tool/XLoadct* select B-W Linear).
- Select another data set and switch back to the topography data (this step makes sure that a temporary data file with the formatting information is created).
- In Combined Plot: Set the number of data sets to be combined (2 is the default). If a value different from 2 is selected, use ***[Refresh]*** to rebuild the Combined Plots form.
- In Combined Plot: Select the draw area 1 to receive the next data set by clicking on the draw area or using the radio button at the button of the window (Fig. 117a).
- In Multiplot: Make sure the topography data (first entry) is selected as the active data set. Select Multiplot: *Single Plot/Data/Send Data to Combined Plot*.
- The data set will appear in the draw area 1 of Combined Plot (Fig. 117b).
- In Combined Plot: Select the draw are 2 by clicking on the draw area or using the radio button at the button of the window.
- In Multiplot: Select the data containing the electrochemical currents (2nd list entry).
- In Multiplot or Single Plot: Select the color table (Single Plot: *Tool/XLoadct* select Blue/Green/Red/Yellow). Rotate the array by 90°. Select *User-shad. + Lines* Format the data set with respect to the desired user color scaling → *Single Plot: Plot format/Scale user shade.* Select register tab Line by line, select the option *Plane fit vertical to x axis* (important after the rotation!). Select *Use scan average*.
- In Combined Plot: *Select Stacked Surf.* .
- In Combined Plot: *Plot format/Stacked Surf. common settings*. Click on all options (Fig. 121), ***[Redraw]***.
- In Combined Plot: *File/Select plot format*: make the screen output to 512 wide and 640 high; ***[Redraw]***.
- In Combined Plot: *File/Select plot format*: select JPG, make the output to 1536 wide and 1920 high. Make the output file (*File/Print*).

Known problems For EPS a portrait plot aspect ratio only be obtained if the plot region horizontal values are changed for instance to 0.15 to 0.85.

There is the option of further processing graphic files with graphic programs like Coral Draw or Adobe Photoshop. This allows changing the background, adding labels and moving the plotting areas closer together.

6 Auxiliary tools

6.1 MIRA_VM_01.XLS

The MS Excel file *MIRA_VM_01.XLS* is supplied in the root of the installation. It can be copied to any path on your machine. You are free to modify the code in it. The code is made in VBA.

The purpose of this tool is to generate output of many data files for a quick overview and documentation. This printout is optimized for laboratory notebooks and is designed as a graphical directory. It may look as the following page.

The *MIRA_VM_01.xls* worksheet is optimized for interaction with *MIRA_VM_01*. <u>It will not function with older versions of MIRA.</u>

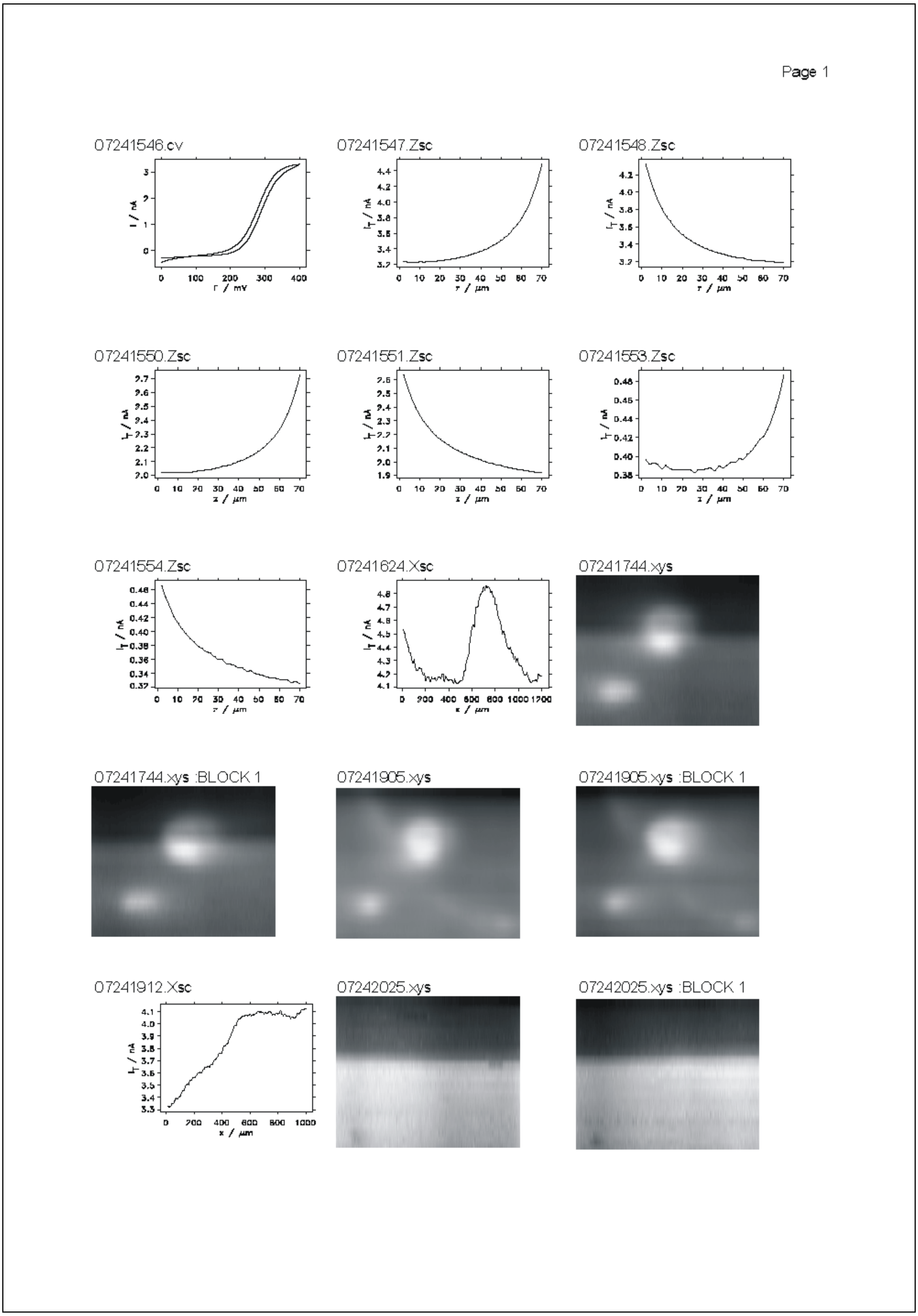


Fig. 124: Printout generated from mira.xls

6.2 Generating a lab book printout with MIRA_VM_01 and MIRA_VM_01.xls

The first part consists in loading all the data files into the file list of *Multiplot*. There are different ways to do this. They are described in the following section

1. Empty the input directory or create a new empty subdirectory of you preferred input directory. Load your all your measurement data files into the input directory or the new subdirectory.

2. Empty your output directory.

3. Start MIRA. In the startup section select *Multiplot* and your preferred INI-file.

Now you can either proceed with steps 4 or 8 or 10. Combination of the different loading methods are possible as well.

4. Start the *Batch Interpreter* from *Multiplot File/Start* batch interpreter.

5. In the *Batch Interpreter* select *Command/Make file list*. Select the path, where your experimental data files are located. Confirm the settings by <***Ok***>. Select a name and a path for the file list to be generated. Recommendation: Use the input path to store the file list with the experimental data.

7. In the *Batch Interpreter* select *Command/Load file list.* Select the file list you have just created. All files in this file list will be loaded into *Multiplot*.

Proceed with step 13.

8. Load files into *Multiplot* with the menu *File/Add file* to list or *File/Load IDL binary*. Note that you can select multiple files. Files can be loaded from different directories.

9. Start the *Batch Interpreter* from *Multiplot File/Start* batch interpreter.

Proceed with step 13.

10. If Single Plot is running, you can load data from Single Plot with File/Open file, File/Load IDL binary or File/Import ASCII.

11. Transfer the data to *Multiplot* by File/Add to MULTIPLT list.

12. Start the *Batch Interpreter* from *Multiplot File/Start* batch interpreter.

Proceed with step 13.
13. From the *Batch interpreter* select the graphic file type from *File/selection* of graphic format. Select the output directory in *Batch interpreter File/Change default paths*.

14. From *Batch interpreter* select *Commands/Print*. You will be asked for the name of an output file list. This list will contain the full name (including path) of the graphic files and a descriptive short name of the data file (e.g. image.xys_Block:1). This file will make the further work much easier. It can be placed anywhere. If you do not want to make such a file, select <***Cancel***> in the file selection box. A printout will be generated for each file and each data block in multi-image files. The printout will be made to your output directory.

15. Start MS Excel and load the file MIRA_VM_01.XLS provided in the installation directory of MIRA_VM_01. Confirm <***Makros aktivieren***> or <***Activate macros***>.

16. On the Excel worksheet press <***Clear old content***>.

17 On the Excel worksheet press <***Read file list***>, a file selection tool appears. You should select the output file list, which was created in step 14. The file list will be loaded. The file list appears underneath the three buttons in column E. In column D you have one entry of the name of the list file.

You may load more list files. They will be appended to the current list file.

18. On the Excel worksheet press <***Import graphic files***>. All graphic files will be imported and formatted. Postscript files will be displayed only as empty frames.

19. Make a printout using the printers installed on your computer. Only columns A to C will be printed. The printout should look like Fig. 124.

The printout is optimized for European A4 paper size. To change the size of the columns to adapt for US letter size go within the Excel on Excel/Macro/Visual basic editor. Go to the very top of the program listing. You find there 2 lines

Const col_width# = 29#
Const picture_width# = 153#

Increase the values 29 and 153 to fit to your paper size.
Repeat steps 15-19 until you are satisfied with the result.

Note: Imported PostScript files will only produce meaningful printouts if sent to a PostScript printer. If you are unsure whether you have a PostScript printer, consult your computer administrator.

Advice: If you have a PostScript printer, this should be the preferred file type. It can, of course, only be used if you have a PostScript printer available.

The whole sequence of steps 1-18 may take something like 3 minutes for 100 files. Printout of course depends on you computer, the performance of the printer and the type of connection from your PC to the printer.