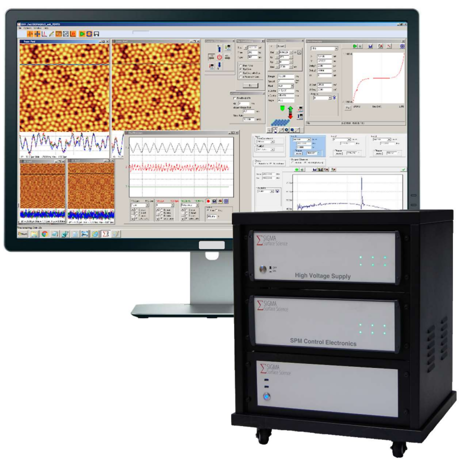

SXM

User Manual

SPM controller electronics for high resolution STM, AFM, qPlus® and Spectroscopy applications

Content

Features at a Glance

- SPM measurement modes: STM, STS, IETS, …
- AFM measurement modes: beam deflection NC-AFM, beam deflection contact mode AFM, qPlus® and related spectroscopy
- Feedback regulator modes:
  - STM: logarithmic or linear
  - AFM: mixed STM & qPlus, df-regulation, amplitude regulation
- Measurement and data analysis software
- True 24 bit AD/DA converters
- Fast 22 bit Z D/A converter
- Integrated Lock In Amplifiers
- PLL for NC-AFM
- Coarse motor control via software or joystick
- BNC/SHV connectors for optimum access to all signals
- STM & NC-AFM mode
- Single point and grid spectroscopy (I(U), df(U), df(z), I(z), Ext(U), dI/dU
- Individual spectra: create your own asci file and use it as a pattern for your individual spectra ➔ define the density of points according to the ROI of your experiment!
- Spectroscopy along a predefined line
- Software support for Femto-preamplifier
- Oscilloscope window for 3 cannels simultaneously (access to every ADC)
- FFT spectrum analysis via oscilloscope or Lock In amplifier
- Single spectroscopy outside the current scan range (within the maximum scan range)
- Lateral tip positioning via mouse control
- Z-control
- PLL with feedback loops for frequency shift, amplitude regulation and …
- STM feedback loops: logarithmic or linear
- Coarse motor operation via software or joystick
- Simple data format (like Scala)
- Basic analysis / image processing software
- Combined STM/AFM experiment (mixed feedback / “slider”)
- Lateral and Vertical Atom Manipulation
- Phyton & LabView interface…
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-

General Information

The Image Acquisition

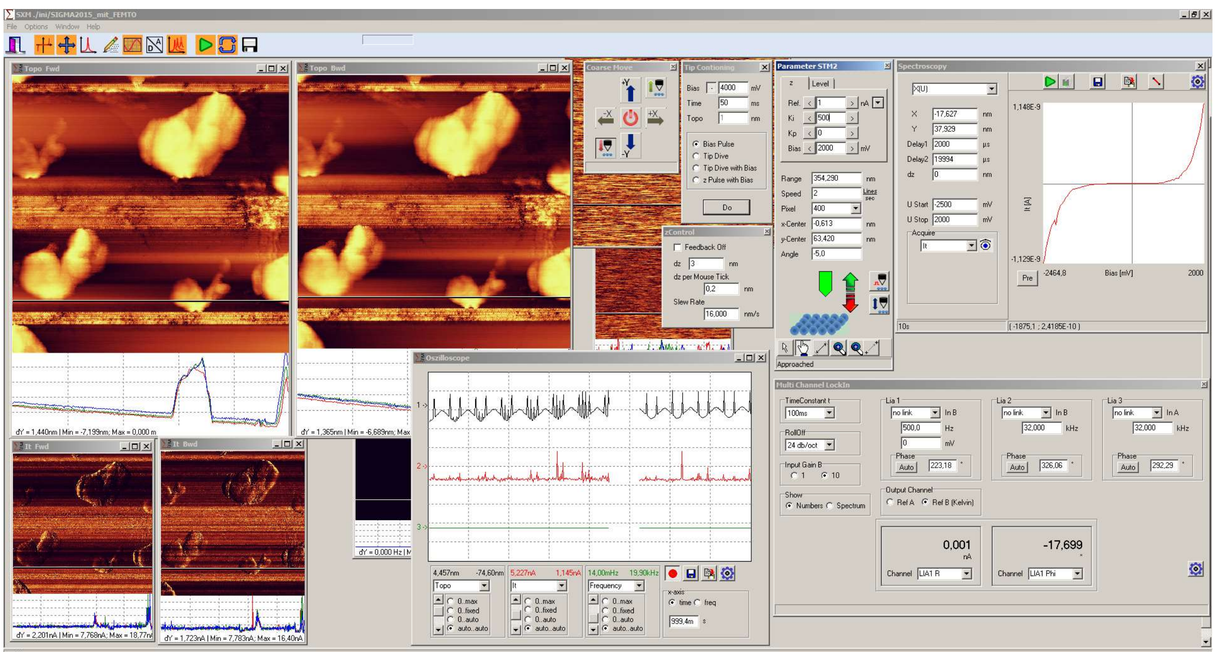
The SXM software is designed for various applications. It is initialization file based. All user settings are saved during work and reloaded when the program is opened again.

In order prepare the program for different applications (e.g. different experimental applications), the program can be stored in several directories with separate initialization files, or the “*.ini”-files can be saved to keep settings stored.

Note: all parameter inputs into the program have to be confirmed with ENTER. Wrong numbers, which can be detected automatically, are marked in red and comments explain what's wrong.

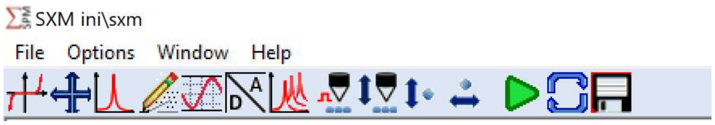
Double click on the icon Σ SPM on your desktop. Each start of program restarts the SPM-controller. Therefore, it is important that the power supply of the controller is switched “on” before the program is started.

When started, the last opened scan windows and the parameter windows are shown.



For everyday use, all necessary channels are already open. For special experiments, you can store the settings (sxm.ini) in a separate file (mysetup.ini) and call the program from the desktop with the option of this filename (case sensitive!): ' “...\sxm.exe” mysetup'.

Icons in the Main window



 : opens the window for settings of the spectroscopy

: opens the window for coarse motor control of sample and tip

: opens the PLL window for qPlus NC-AFM measurements (determination of resonance frequency, oscillation amplitude, quality factor, etc.)

: opens window for line- and grid-spectroscopy, for user controlled lateral tip positioning and for loading and execution of scripts

: opens the Oscilloscope window

: opens the window to get access to the D/A converters

 : opens the Lock-In amplifier window

 : opens the window for tip preparation (voltage pulsing, Z-pulsing, tip diving, etc.)

 : opens the window for manual Z-control of the tip

 : opens the window for vertical atom manipulation

: opens the window for lateral atom manipulation

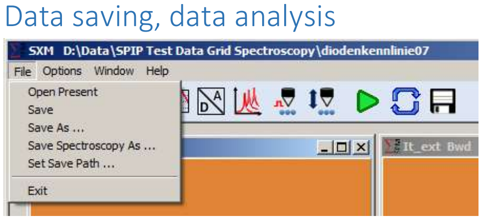
: start button to start a measurement (single scan)

: if both are pressed, the measurement (scan) is running continuously repeating

: results will be stored if pressed

Explanation of Functions:

Data saving, data analysis



Under the Index Tab “File” one gets access to different data saving options, to switch to the data analysis software “present” or to Exit the software

The data are saved in two formats: SXM file format and bitmap, that the following files are created:

- a base file (*.txt)
- and 2*N data files (*.bmp + *.int)
  (N ... number of acquired data channels, each saved as bitmap and as integer).

The file names ('*') consist of:

- a base name provided by the user (example: “S45B”)
- an automatically generated 2-digit number (example: “00”)
- the channel name written in the image windows (example: “TopoFwd”)
- the file extension.

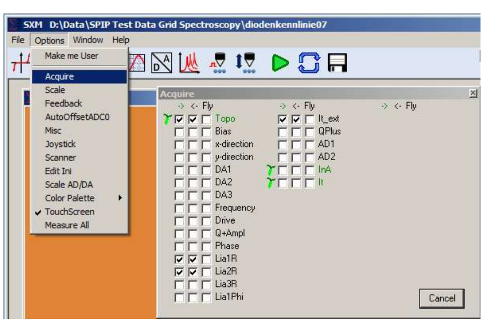
In the case that two channels called “TopoFwd” and “ItFwd” are acquired, the generated files are:

- S45B00.txt
- S45B00TopoFwd.int
- S45B00TopoFwd.bmp
- S45B00ItFwd.int
- S45B00ItFwd.bmp

Each click on the save button increases the 2-digit number by one (next file set: S45B01.txt, ...).

With the OpenLast function [File/OpenLast], the last saved image is opened in a new Present window. You can enable **AutoSave** with “Shift+left mouse button” on the Save button. The base name of the stored files can be given in [File/Save As].

Selection of channels (forward, backward and liftmode can be chosen) for acquisition

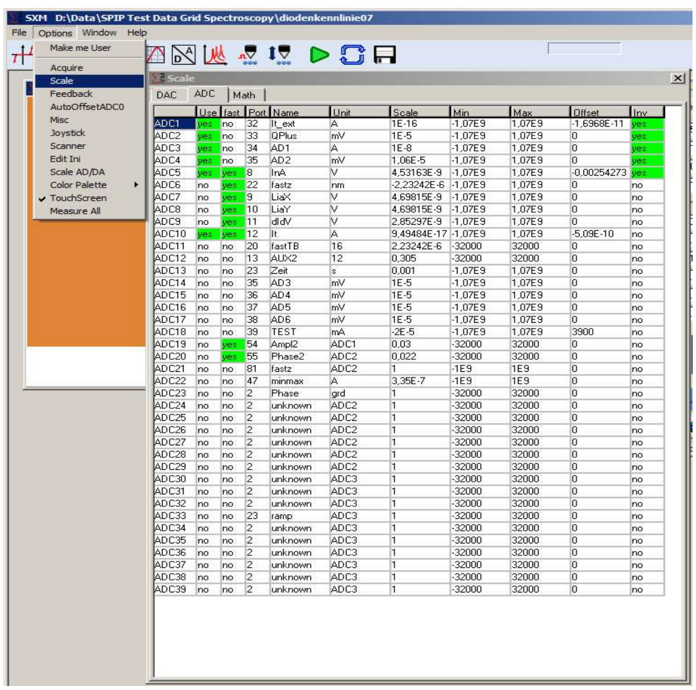


- This menu displays all channels that are selected as “used” in the Scale-Window. Each channel provides three selections which are displayed in rows.
- For each channel the forward and backward path can be measured as well as the signal obtained in “Fly”-mode (lift mode)

- in this example, the forward- and backward scan-data will be measured for the four measurement channels: Topography (Topo), phase-independent Lock-In 1 and Lock-In 2 signals (Lia1 and Lia 2) and the tunneling current (second current input: called It-ext)
- number of channels (here 21) can be modified by activation of A/D and D/A converters in the "Scale" window
- if the fly mode is activated by setting the ticking the box, the Parameter windows (for setting the measurement parameters) will show an additional index tab, called "fly"

Measurement Channels: Activation and Scaling of in- and output signals (D/A and A/D converters)

This window selects, which channels are active and can be taken as picture by the sxm-software, on which hardware channel is which program channel and it makes the relation between the numerical units of the digital SPM controller and physical units of interest for the user.



- in- and output channels can be activated/deactivated in the "Scale" window
- all activated channels will be listed in the acquire window (above)
- calibration/scaling of channels

Use if checked, this channel can be acquired with the software

Name name of the channel displayed in the head line of the windows and used for file names

Unit physical unit displayed at related positions in the program

Scale scaling factor between numerical units and physical units. This factor can be negative or positive. If the topographical image, for instance, appears inverted, one can place a negative scaling factor in order to invert its **visualization** in the SXM-program and the Present-program.

num. values	numerical values used in the back round of the sxm software

Min /Max	minimal num. value, for 16-bit signed integer variables, these values are +/- 32000. For the 32-bit integer variables, +/- 1e9 is chosen. Set to “0”, the output of the channels can be reduced to -10 V.. 0 V or 0 V ... 10 V. Even -2 V ... 10 V as needed for PI HV amplifiers is possible.

Max	maximal num. value

Offset	For certain uses the offset correction can be done here.

Invers   especially for z, it can be useful to have an “invers” option. If checked, the channel is inverted at the interface between hardware and software. This allows to define the operation direction of the piezo actuator in z-direction.

Calculation of scaling factors:

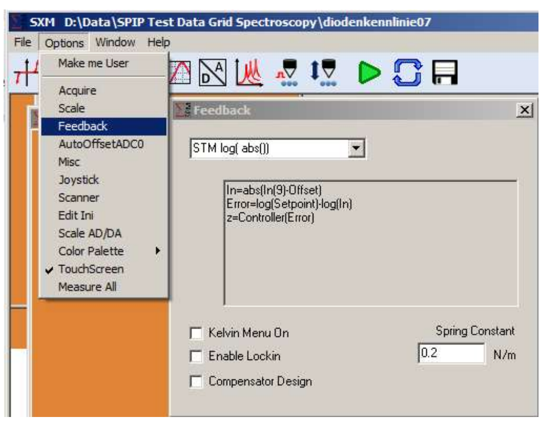
As all input channels and all output channels (except the lockin channels) are inverted, the equation for the scale factor is:

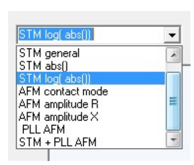
Phys. value = - scale factor * num. value

Example 1: The maximum voltage output of the DAC is 10 V and the related maximum num. value is 32000. Then, the scale factor is 0,3052 to obtain an output display in mV.

Example 2: The maximum voltage output of the DAC is 10 V and the related maximum num. value is 1e9. Then, the scale factor is 1,07e-5 to obtain an output display in mV.

Selection of the Feedback Mode





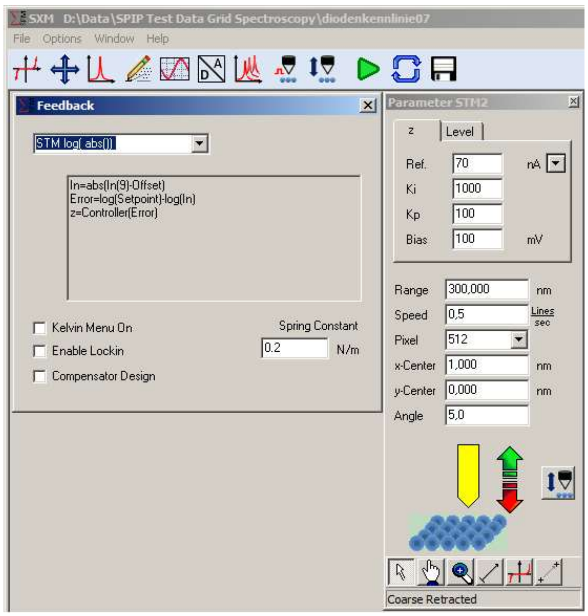
Selection of feedback mode (e.g. STM or AFM) as well as corresponding channels and algorithms for regulation

The following modes are included in standard software package:

- STM with linear feedback regulation (STM abs())
- STM with logarithmic feedback regulation (STM log(abs())
- PLL –AFM for qPlus

- Mixed Regulator (slider between log-STM and PLL-AFM): this mode was developed for fast change between STM and NC-AFM feedback by using a slider. Here both feedback regulators (STM and AFM) are active and calculate individually the corresponding feedback output. Both the regulator output can be mixed. By this, it is very easy to find the proper parameters for NC-AFM measurement when starting in STM mode with oscillating cantilever. If the slider is completely at the left side, we have a pure STM regulation and fully at the right side we have a pure NC-AFM regulation.

Example: STM Feedback Selection & parameters for STM



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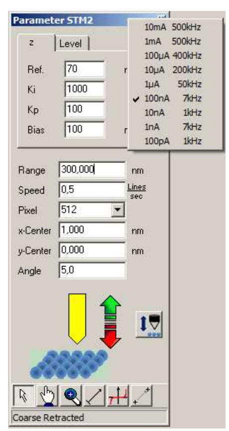
• because of the exponential dependence of the tunneling current on the tip-sample distance, the standard feedback for STM is the "STMlog(abs)"

• once the feedback mode is chose, the Parameter displays all basic parameters for the STM measurement



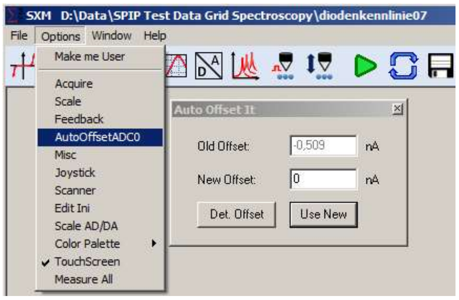
- **Ref:** setpoint for the tunneling current (here 70nA)
- In combination with a SIGMA SPM, there are 9 the pA range to very high amplifier can be switched corresponding maximum

current ranges for very small currents in currents of >10µA. The rage of the via software by selecting the value of the desired range.

- Ki: integral part of the PI feedback
- Kp: proportional part of the PI feedback
- Bias: gap voltage between tip and sample (for Sigma instruments the standard configuration is: voltage is applied to sample whereas the current is measured at the tip)
- Range: scan range in µm
- Speed: scan speed in lines per second. If the speed is selected higher than 10 lines per second, the on-line visualization of the acquired images might be switched off automatically.
- Pixel: All images are taken square like with N by N pixels resolution. The number of pixels effects the scan achievable speed and the achievable resolution of the images.
- **x-Center, y-Center:** in relation to the scan range, are the central coordinates of the acquired images with respect to the total provided range.

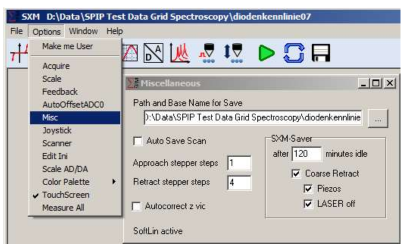
- Scan Angle: turns the scan direction. If the scan angle is 45 degree, the maximum scan range is reduced by a factor of $\sqrt{2}$

Elimination of Offset on feedback input channel



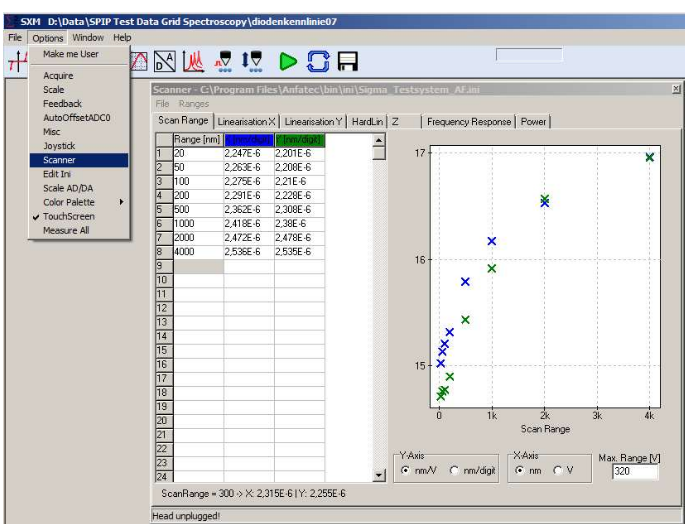
- if there is a DC -offset on the feedback signal (e.g. tunneling current It), this function enables to measure the offset and to subtract this value. This function is useful when working with very small tunneling currents in the pA range.

Miscellaneous: data storing and automatic tip retraction

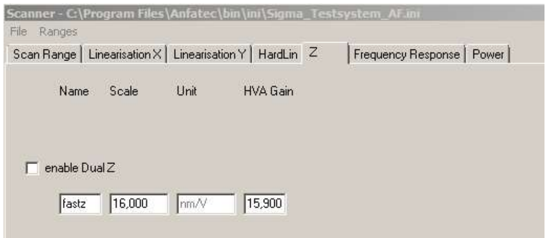


- definition of a path for data storing
- automatic stop of measurement after a certain time: in the example shown here, the measurement will be stopped after 120min. Afterwards the tip will be retracted and the laser light will be switched off.

Scanner calibration

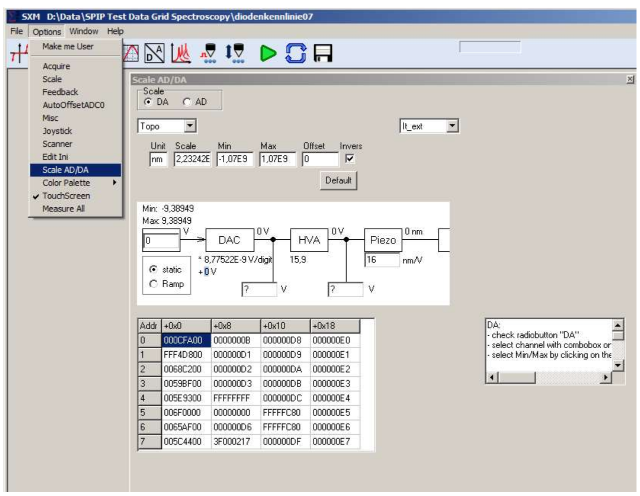


- besides the input of the sensitivity of the piezo (nm/V) for a small scan range, there is additionally the possibility to consider the change of the sensitivity as a function of the size of scan range (about 13-20%, depending on the piezo material). This is simple to increase the accuracy of the calibration.
- in the example shown at the left, 8 different sensitivities are used for the calibration. If this is not required, one can eliminate the values in the lines 2-8.

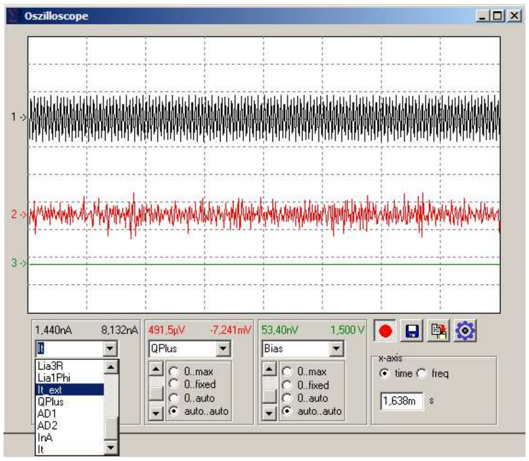


- for Z-calibration, simply enter the nm/V - value

Other possibility to change the calibration on the D/A and A/D converters



Oscilloscope window



- The oscilloscope 3 channels can be displayed and saved simultaneously (here, the signals It, qPlus and bias are displayed)
- Works like a real 3-channel-oscilloscope. Content, scaling type and offset of the three channels are selectable.
- easy choice of channel by using the picklist (see channel 1)
- the signals are either displayed as a function of time or the frequency components are displayed
- time/frequency base is adjustable (lower right)

Channel selection: is done from a drop down list, which shows only the available channels. The numbers above the channel selection are the scaling factor per vertical unit and the mean value

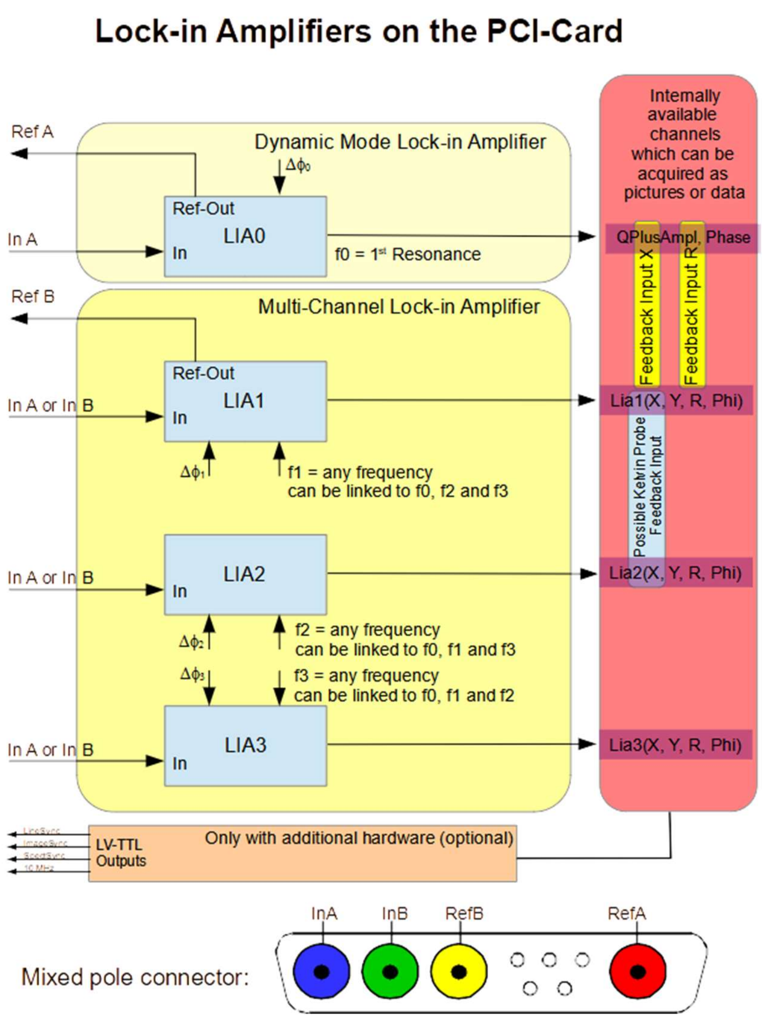
Vertical scaling types:

- **0..max** the scaling is set to maximum value of the channel
- **0..fixed** the maximum value can be changed by a slider appearing on the right sight of the scaling type selection
- **0..auto** the program calculates the the optimum, but takes always “0” as minimum
- **auto..auto** automatically scaled

Usage of the 4-Channel Dual-Phase Multi Channel Lock-in Module of SXM

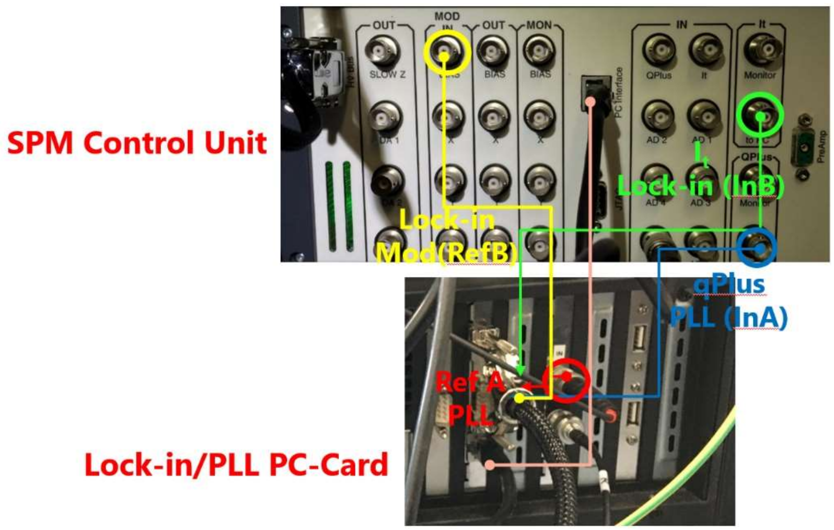
Scheme

- The SXM LIA module provides four digital lock-in units (**Lia0**, **Lia1**, **Lia2** and **Lia3)**. The first unit (Lia0) can also be used for PLL operation, e.g. for qPlus measurements.
- There are two input stages (**InA** and **InB**) which can be assigned to the individual lock-in units.
- There are two reference outputs with independent frequency selection (**RefA** and **RefB** with frequencies **f0** and **f1**).
- Lia0 can only be used with f0 and InA whereas Lia1, Lia2 and Lia3 can either use InA or InB as input and arbitrary frequencies as references.
- For both InA and InB two different input gains can be selected (1 and 10) with max. input amplitudes $10V_p$ and $1V_p$., respectively.
- For RefA an output gain in terms of output range can be selected ($0.1V_p$, $1V_p$ and $10V_p$).



Logical scheme of the MultiChannel Lock-in module (PCI card)

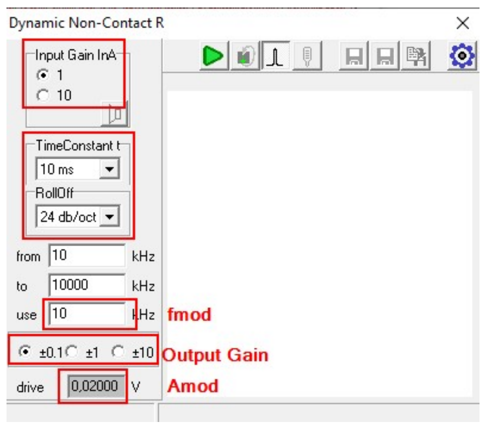
- There is an adaptor cable from the PC Lock-in card to four color-coded BNC cables (InA, InB, RefA, RefB).
- By default, the BNC connector '**It→To PC'** of the SPM Controller is connected to the InB. This connects the FEMTO STM or SPM Pre 4 preamplifier output to the input of the PC LIA. It digitizes the I_t (=tunneling current) signal and generates the Channel '**It_to_PC**' in the SXM software. Furthermore, it can serve as the input for any of the digital Lock-ins.
- By default, the BNC cable **RefB** of the PC LIA is connected to the **MOD→IN(BIAS)** BNC connector of the SPM Controller. This is the sine modulation voltage added to the Sample or Tip bias.



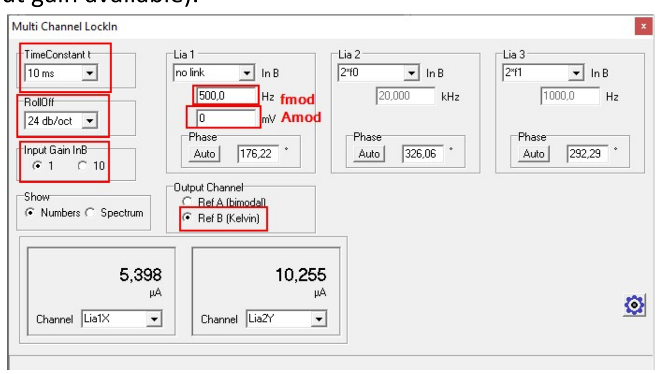
Setting up a Lock-in measurement

- Connect the oscillator output (typically RefB, RefA is more dedicated for PLL operation) to the target to be excited, e.g. bias of the STM tip for tunneling spectroscopy.
- Connect any of the Lock-in inputs (typically InB, InA is more dedicated for PLL operation) to the modulated and derived signal to be probed, e.g. tunneling current of an STM measurement.
- Set up modulation frequency, amplitude, input and output gain and filter settings according to your signal properties and measurement requirements.
- The common '**TimeConstant t**' can be set between 0.1ms and 5s, the **filter roll-off** to 6, 12 and 24 dB/octave.
- The **input gain** can be set to 1 or 10 (for small signals use 10).

RefA/InA:



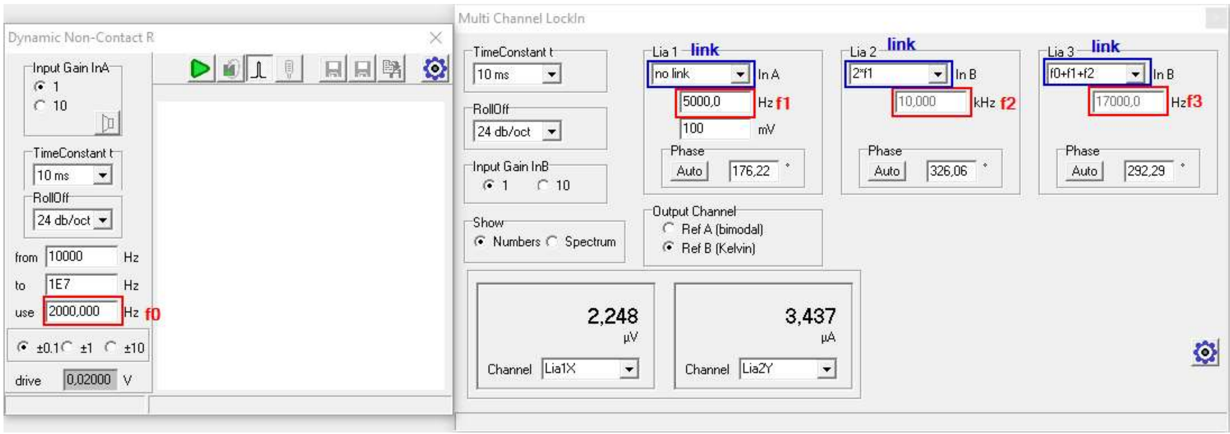
RefB/InB (no output gain available):

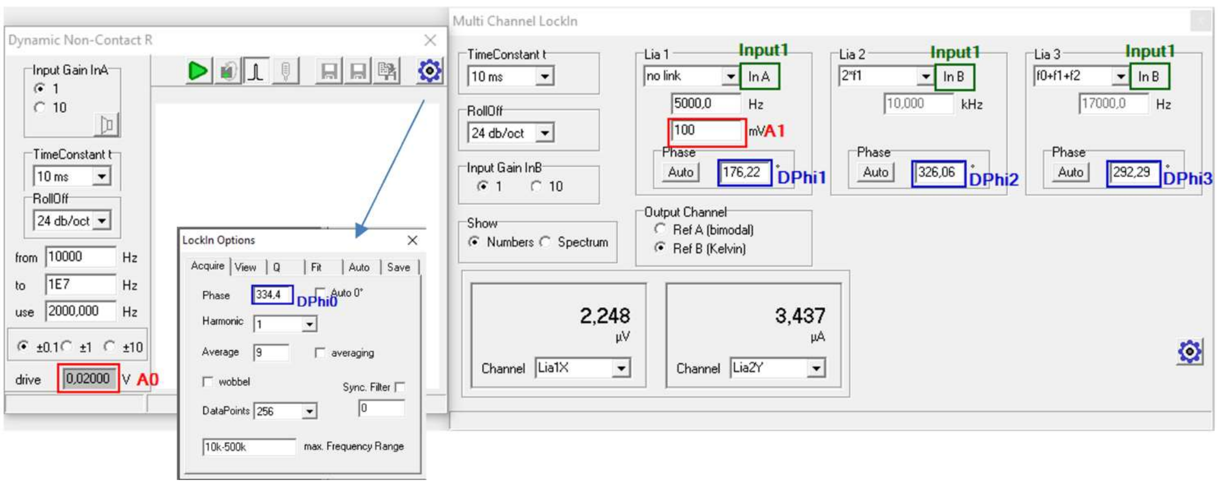


Please keep in mind that all amplitude values to be entered and measured are by means of **RMS**.

- The Lock-in measures a signal amplitude and phase with a narrow bandwidth given by the lock-in filter width at a given frequency which is called '**Reference frequency**' (labelled **f0, f1, f2, f3** for **Lia0, Lia1, Lia2, Lia3**, respectively) or mixing frequency.
- The reference frequencies f0 and f1 of Lia0 and Lia1 can be output with a sine oscillator at output RefA and RefB, respectively. f2 and f3 for Lia2 and Lia3 are only internally available.
- To set any of the reference frequencies just leave the link control input empty ('no link' will be shown) and enter the reference frequency into the corresponding frequency control below (see figure). For f0 it is the control 'use' in the DNC window. The reference frequencies can be chosen independently between 0.1Hz and 10MHz.

- To set a dependent measurement frequency just enter any linear combination of the other frequencies using the operators * , / , + or - (e.g. f2/3+5*f1-f1/f2). **Please make sure not to use the measurement frequency recursively, e.g. “2*f1” for f1. This will yield unpredictable results.**





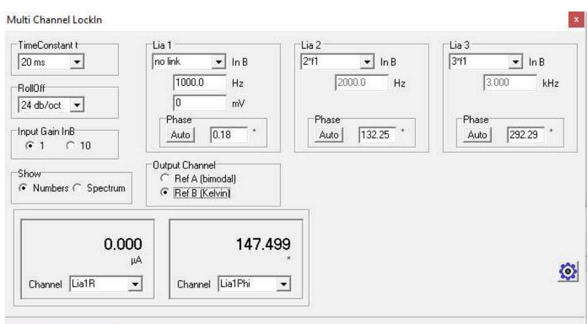
- The **amplitude** of the excitation sines A0 and A1 at the frequency f0 and f1 are set in the ‘DNC’ window (‘drive’) and below the f1 setting of Lia1, respectively (see figure) by means of RMS amplitudes.
- The **input signal** can be chosen between InA and InB by left-clicking on the Input1, Input2 and Input3 labels only for Lia1, Lia2 and Lia3. As described before, for Lia0 InA is fixed.
- If there is an **overload** on the corresponding input gain control will flicker red. Please be aware that a recovery of the Lock-in after an overload takes many time constants.

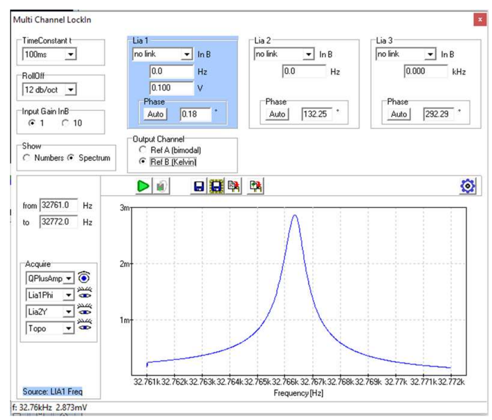
- The **phase** relations of the reference frequencies with respect to the input signals are set in the corresponding ‘DPhiN’ controls independently. DPhi0 can be set in the ‘Lockin Options’ of the DNC window. For DPhi0 it is necessary to disable ‘Auto 0°’ if the phase needs to be set manually (see figure above).

- For an **automatic setting of the phase** for a maximized in-phase signal a valid input signal needs to be present. With the 'Auto' buttons next to the manual input can be pressed for Lia1, Lia2 and Lia3 the auto phase mechanism is triggered. For Lia0 it is again little different: enable 'Auto 0°' in the 'Lockin Options' and press 'Enter' in the 'use' control for f0. This will trigger the auto phase mechanism.

Acquisition of Lock-in data

- The Lock-in output is handled as ordinary measurement channels in SXM. They are labeled LiaNX, LiaNY, LiaNR and LiaNPhi for In-phase, Quadrature, Magnitude and Phase of Lock-in N=1,2,3 or 4. They can be used for imaging, spectroscopy, manipulation, oscilloscope etc.
- In the Multi Channel Lockin window there are two different modes available for displaying the lock-in data:
  '**Numbers**' shows two numeric displays of real time values of any channel (also non-Lock-in channels). This is useful for phase and amplitude adjustments. The physical units can be selected by left- or Shift-left clicking on the unit string. '**Spectrum**' allows to sweep the frequency of the currently selected reference. It can measure and display four arbitrary channels as a function of frequency. Click on the Lia1, Lia2 or Lia3 section to set the corresponding frequency as sweep source (see figure).

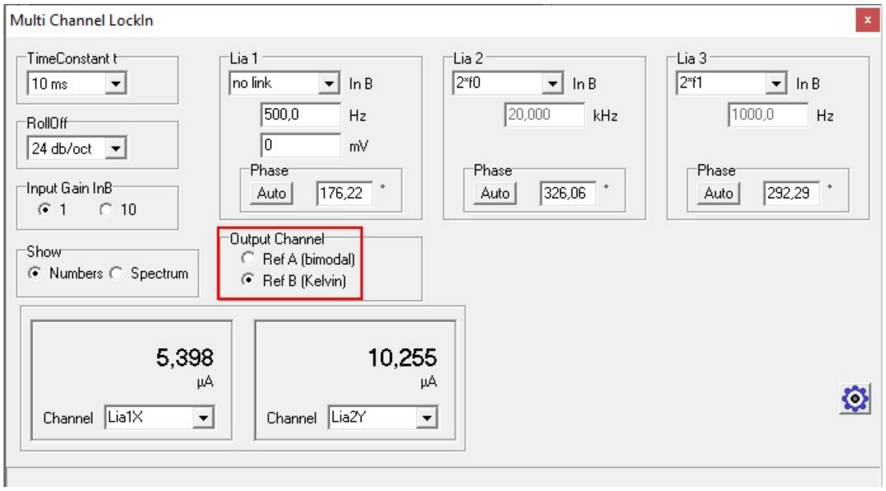




'Numbers' (left) and 'Spectrum' (right) modes

Output Channel selection

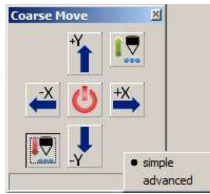
- The of the frequency f1 in the Lia1 section can be switched with the Output Channel control (see figure).

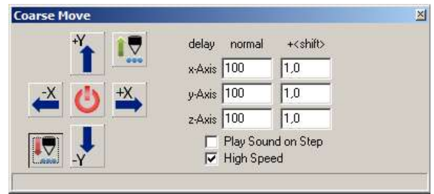


Setting **'Ref B (Kelvin)**' causes the sine wave at frequency f1 to be output at RefB in parallel to the output on RefA currently set in the DNC window. Setting '**Ref A (bimodal)**' causes the sine wave at frequency f1 to be added to the output on RefA currently set in the DNC window. This allows, e.g., for a bimodal excitation of an oscillating sensor.

- Switching behavior: if for both 'Drive' in the DNC window and the amplitude f1 control in the Multi Channel Lock-in window valid non-zero values are entered in Ref B – mode RefA will output the amplitude 'Drive' at frequency f0 and for RefB the amplitude given in section Lia1 at frequency f1. If switching to Ref A – mode then RefB will be zeroed and RefA will output the sum of the oscillators running at f1 and f2. This allows for bimodal excitation. Switching back to Ref B – mode will zero RefA and output oscillation f2 at RefB again.

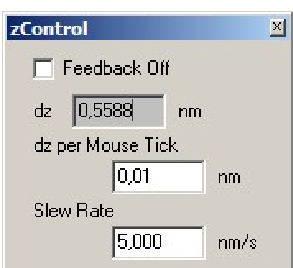
Coarse motor control



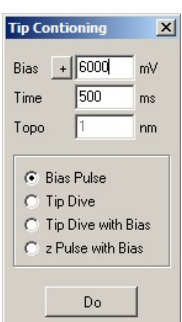
- easy coarse motor control by software (left) or via remote control (right)
- in SIGMA SPMs, the sample can be moved laterally in ±X and ±Y direction and the tip vertically
- by pressing the right mouse button on the Coarse Move window one gets access to advanced setting (number of steps, voltage)
- in case of an Omicron VT STM, the tip will be moved in ±X, ±Y and Z whereas the sample is fixed
- coarse motor operation is thus possible via VPN connection (e.g. from home)

Manual Z-control of the Tip



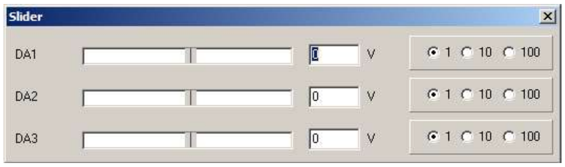
- The Z-control can be used to retract/approach the tip manually, e.g. for atom manipulation (e.g. picking up an atom) or for tip preparation (tip wetting)
- For this, the feedback will be switched off and the current Z distance between tip and sample can be changed by dz (via mouse operation or via numerical data input)
- the distance will be changes with a defined velocity (slew rate)

Tip preparation



- the tip can be modified by voltage pulsing with active feedback regulation (applying a voltage “bias” for a defined time interval “time”) or by diving the tip into the sample by a defined path lengths “topo”
- furthermore combinations of voltage pulses and tip diving is possible

D/A converter, DC outputs



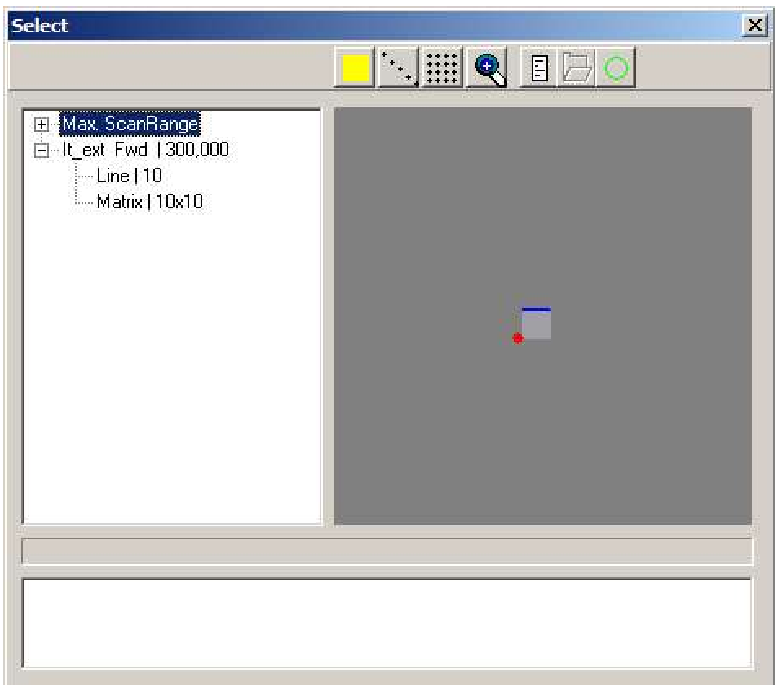
- the SIGMA SX Controller has three 24bit D/A converters for free use
- Within the window the output voltages for each D/A converter can be set by using either the slider or by numerical data input

The Select Window

The select window covers the following functions:

- Choose a point position for the point-spectroscopy
- Zoom into the current scan area
- Run user defined scripts in the currently selected scan area
- Observe the current tip position in the totally available scan area
- Moving the tip

When the select window is opened, it shows an entry "Max.ScanRange" (maximum scan range). The grey screen represents the totally available scan area. The current tip position inside this scan area is displayed as red dot.



Observing the tip position

If the entry "Max.ScanRange", "CurrPosition" or one of its sub-entries is activated (selected), the red spot shows the current tip position inside the total scan area during the scan or any kind of spectroscopy.

Open the entry "Curr.Position" to display the numbers behind each sub-entry X, Y and Z (example: "X| *2.355*"). These numbers are the value of the current position in the currently selected physical units (here: µm). They are updated during each scanner movement.

Move the tip within the maximum scan range

- Click on the icon
- Click with the left mouse button somewhere you want to place the tip.
- A cross appears
- Click with the right mouse button → select "Go in X and Y"
- Afterwards, the tip (represented by the red dot) moves to the cross
- Now many actions can be executed, e.g. vertical manipulation (via Z-control window), tip preparation (via tip preparation window), spectroscopy, or others

Move the tip in the scan area

- Click in any data channel window and 'drag&drop' the image into the image part (right) of the select window. Then, this window is shown there (as bitmap in the same way, it was displayed on the screen before) and its scan range as well as its centre position are stored with the image. On the left side below the entry "Max.ScanRange" appears an additional entry in the list. So, a list of former images is generated
- Click on the icon
- Click with the left mouse button somewhere you want to place the tip.
- A cross appears
- Click with the right mouse button → select "Go in X and Y"
- Afterwards, the tip (represented by the red dot) moves to the cross
- Now many actions can be executed, e.g. vertical manipulation (via Z-control window), tip preparation (via tip preparation window), spectroscopy, or others

Zoom

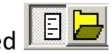
Click with the left mouse on the icon to activate the function "zoom". Use the mouse to zoom into the image in the select window.

At any time later, one can go back to the old scan ranges by selecting their images from the list on the left side and might repeat the zoom at a different position.

Reset scan range to former parameters

After a zoom into an image and a new scan, one can go back to the old scan range selection. One selects the related entry so that it gets blue and clicks with the right mouse button on it. Choose "Use Parameter" to reset the values of *Range*, *x-Center* and *y-Center* in the parameter window.

Run user defined Scripts

- The select window allows to run user-defined scripts.
- A script is loaded with the button “load last script” 
- Once the button is pressed the icon changes and the folder icon is activated  and the program loads automatically the last used script.
- By pressing the folder icon  a dialogue box is opened and a script can be opened
- Start the script with the button 
- Script language is similar to Pascal

<u>Example script 1:</u> reading the current bias voltage

```
begin

ClrScr; //Deletes the visible data on the select screen

GETCHANNEL(-1); //reads the current offset value (AUX8) result (variable c) in physical units (mV)

writeln('Bias = ',c); //writes the value of c in the display

c:=c;

SETCHANNEL(1,c);

WAIT(2);

end.
```

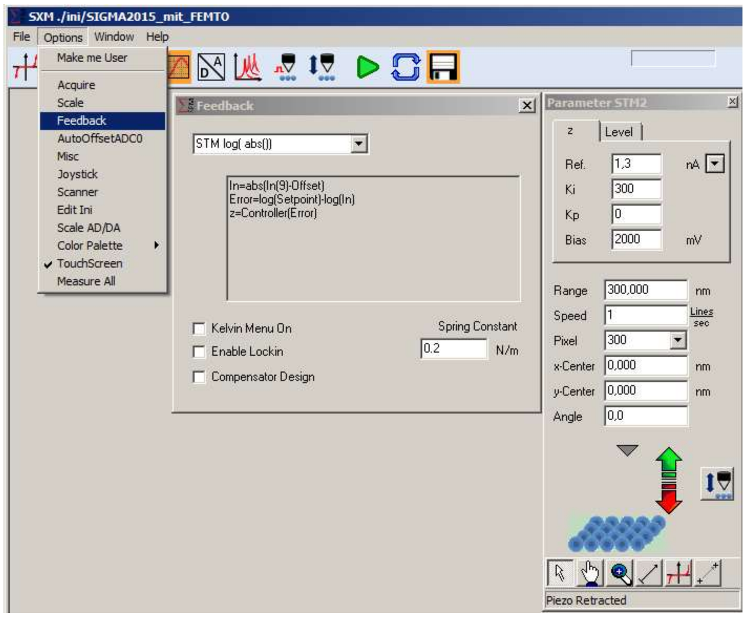
<u>Example script 2:</u> scanning a matrix of 3 x 3 images, each 300nm scan range and the distance between the images is 600nm

```
begin

// Move('Approach',2); // approaches tip

Wait(1);

// set parameters that are equal for all images:

FeedPara('Ki',1000);

ScanPara('Speed',20);

//ScanPara('AutoSave',1);

ScanPara('Range',300);

// variable x is center position in X

// variable y is center position in Y
```

```
// units are as defined for X and Y scan (here: µm)
x:=-600;   // start center position in x-direction for 1st image
y:=-600;   // start center position in y-direction for 1st image
d:=600;              // distance between images
for i:=1 to 3 do begin
  for k:=1 to 3 do begin
    writeln('Pos [',x,', ',y,' ]');
    ScanPara('X',x);
    ScanPara('Y',y);
    ScanImage;
    ScanImage;
    y := y + d;
  end;
  x := x + d;
end;
 end.
```

Setting up a STM measurement

- insert the STM tip and the corresponding sample into the STM head
- open the parameter window
- select the feedback mode for STM ➔ STM log(abs()) (or alternatively “STM abs()”)

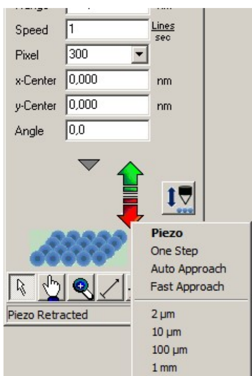


- set the feedback parameters tunneling current, bias voltage (0-10V) and Ki (typ. 20-150) (Kp is nearly always 0)
- Typical starting parameters for STM measurements:
  - HOPG: Bias: 100-250mV, Tunneling Current: 0.5nA, Ki: 100
  - Au(111): Bias: 100-600mV, Tunneling Current: 0.5-3nA, Ki: 100
  - Si(111) 7x7: Bias: 2-3V, Tunneling Current: 0.5-1nA, Ki: 100
- Checking and elimination of offset on the tunneling current (via Options/AutoOffset ADC0)
- Approach the tip via coarse move window to the sample. Use a long distance microscope or a CCD camera for observation of the vertical and lateral tip/sample position. Do not to crash the tip into the sample.
- Center the tip by setting the X- and Y-center values to 0
- Enter a value for the scan range
- Choose the desired resolution for imaging (>300 is a good value) either by picking a value or by numerical data input
- Set the scan speed (depending on the scan range, 1 line/second is a good starting value)
- The scan angle can be adjusted later during the measurement in order to minimize the slope in scan direction to enable faster scanning (alternatively enable auto leveling)

Approaching the tip

- Start automated Approach by pressing with the right mouse button on the red arrow and selecting “Auto Approach”
- “Auto approach” means:
  - the piezo is retracted fast
  - The steppers move “Approach steps” forward (approach steps are defined in the miscellaneous window).
  - The feedback approach the tip with the user defined speed until the front position – 10 % is reached.
  - This auto-approach stops whenever a single data point is above the given setpoint value.

Additional information:



- When the right mouse button is executed on the red arrow (pointing downwards), the following options will be shown: “Piezo”, “one step” and “Auto Approach”.
- The bold written one is the standard option performed when the left mouse button is used on the approach knob.
- “Piezo” means: only the measurement piezo is stretched into direction of the sample until the setpoint is reached. If no setpoint current is detected, the tip will stay in the fully extended position.
- “One Step” means: A vertical coarse step is executed and afterwards the piezo will be extended until a setpoint is reached. If no setpoint current is detected, the tip will stay in the fully extended position.

Retracting the tip: When pressing on the green arrow (pointing upwards), the tip is retracted. In order to view the selected option, use the right mouse button on the retract knob. The picture left shows, that the retract button can be used to retract the piezo only (“piezo”). This option is used for soft-retract, if any sensitive feedback parameter or even the sample position has to be changed.

As standard, “10 µm” is selected. When the retract button is used in an approached situation, the piezo is retracted first. Then the coarse motor is used to retract 10 µm. When inside the selection menu the “100 µm” is chosen, the system retract 100 µm.

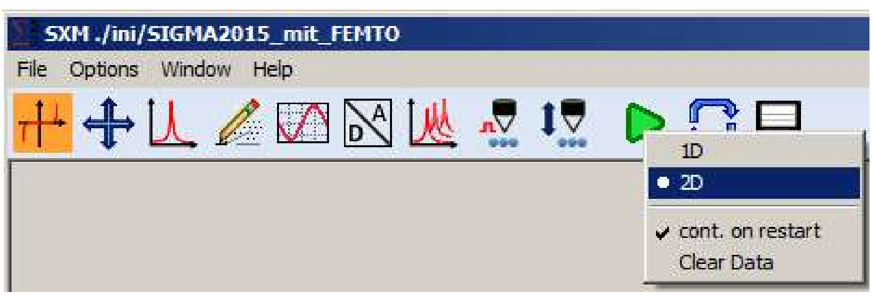
Tip colour:

Red	Almost retracted	The tip is the last 10 % of the possible positions, and cannot retract further.
Green	Central positions	The tip is approached and hold in a central range between 10 % and 90 % of the possible z-values.
Yellow	Most extended position	The tip is extended more than 90 % of its maximum possible

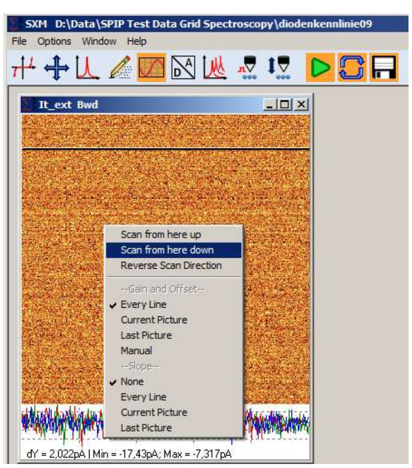
		extension. If this colour occurs during scan, it is possible to loose the tunneling contact.
Lime Green	Any	If the tip moves very fast in the time slot, its position is detected, the difference between its maximum and minimum extension in this time slot is shown in lime green.

Starting the Acquisition and Scanning (after tip approach)

- Before starting the scanning process, you can change the scan mode when you click with the right mouse button on the scan button of the Main Menu bar.
- The appearing window shows:
    - 1D line scan at the first or current line
    - 2D 2-dimensional scan
    - cont. on restart: when checked and you stop the scan, the scan restarts at the line at which it was stopped.



- Start the measurement (Scanning) by pressing in the Main Menu Bar. If both are pressed, the measurement (scan) is running continuously repeating.
- Once the measurement was started and the data are displayed in the channel windows, the right button of the mouse can be used to click into the measurement channel window for several options like reversal of the scanning direction or others.



Scan from here up and **Scan from here down:**
usage: during the image acquisition or in order to start image acquisition *function:* uses the current mouse position to determine "here" and starts to scan from this position upwards or downwards. The function does not change or check the setting "cont. on restart".

Reverse Scan direction:

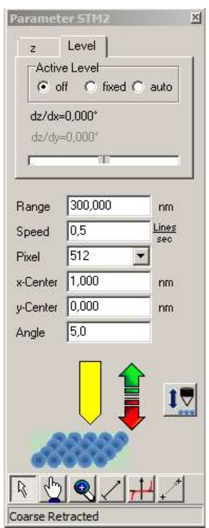
usage: during the image acquisition

function: changes the scan direction from downwards to upwards or vice versa.

Gain and Contrast: changes the gain and the contrast of the used colour range during the scan. Maximum and minimum are taken automatically in *Every Line* or from the whole *Current Picture*. In case of *Current Picture*, all values available from the 1st scanned (might be the uppermost or the lowermost line in an image) to the currently scanned line (visualized with a black or yellow line) are evaluated. In case of *Last Picture*, maximum and minimum of the last acquired image are taken to calculate the contrast.

Slope: subtracts either a linearly fitted line from each scan line (*Every Line*) or a fitted plane through the whole currently acquired image from the 1st to the currently scanned line (*Current Picture*). One can also use the calculated slope from the last image (*Last Picture*) or disable the slope correction completely (*None*).

Plane Correction during imaging (Level Tab)



The main change is the leveling of the sample plane versus the scanning plane during image acquisition. This leveling is neutral to the z-output of the feedback. It consists of two coefficients 'dz/dx' and 'dz/dy', which describe the tilt in x- and in y-direction, respectively. During the scan, when the scan generator provides a step in x-direction, the resulting step dz calculated from 'dz/dx' is added to the z-output. The same is done for the y-direction.

Level is visible as extra tab in the parameter window. It has three different states:

Off disables the level function. Even if there are numbers available from the last scan, these values are not used for the tilt correction. One can click with the left mouse button into one of the coefficients and provide a number for later use.

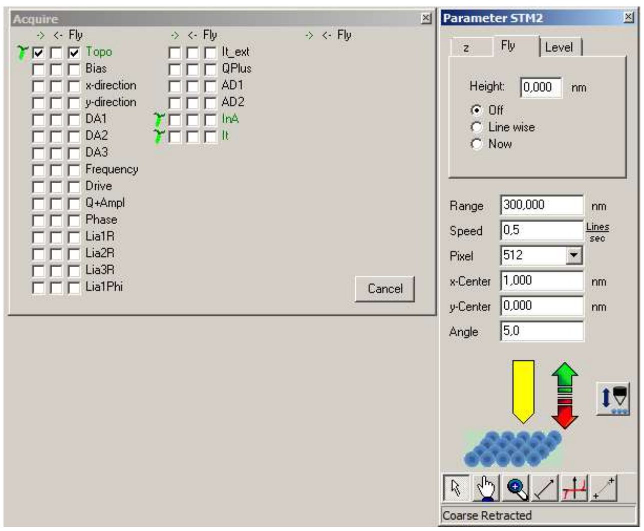
Note: when the program is started, ***Off*** *shows the last used values, but does not use them. It is useful to click into the values and set them to zero before one switches to Auto.*

Fixed allows the manual adjustment of the sample plane. It is thought for fine adjustment or for the case, when a single line scan is used for the plane evaluation. One selects the direction bz clicking into the displayed value 'dz/dy' or 'dz/dx'. The slider allows to change the value continuously. Alternatively, the number can be printed in the edit box.

Auto reacts on “Image ready”. When a picture is completed, the plane of this image is calculated based on the last (displayed) coefficients 'dz/dx' and 'dz/dy'. The new coefficients are displayed. The next image is taken with corrected plane. As long as Auto is ON, this procedure is repeated after each completed image.

The **coefficients** are calculated degree. The given number presumes that the scaling in x- , y- and z-direction correct.

The Fly Mode (normally used in NC-AFM)



Fly modes are used to image the surface a 2nd time in a different height. If the flight is intended, one has to check at least one of the 3rd column check boxes in the acquire menu (Options\Acquire) with the name Fly. Then, an additional tab appears in the parameter window.

Off scans over the surface as if 'Fly' is not intended. Even, if there is a number given as height, this number is not used. (Don't get irritated: the images with the name ".... Fly"do not disappear and their last data are shown during scan. But when saved, these images are empty.)

Line wise equals the former 'Fly mode'. Each scan line is taken once as topography. After backward trace, the tip is elevated the "Height" above the surface and the same topographical line (including all detected topographical variations) is scanned a second time in this height. **Important: Negative value of Height = retract.**

Now is intended for the scan of a complete plane above the surface without tracing the real topographical variations. It is important, that the surface has been leveled with the Level function properly, before this mode is used for scanning. When "Now" is selected, the tip is lifted immediately, and not released to feedback until **Now** is switched OFF again.

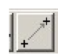
IMPORTANT: Don't forget to switch Now OFF, when the image is ready. Drift might cause a collision of the tip with the surface, because the feedback is OFF!!!

When a planar scan in a 'Height' is intended above the surface, but no complete picture should be taken in advance, we suggest the following procedure:

- go to “line scan” by right mouse click into the scan knob. This enables a function, that scan only the first line of a picture.
- Chose the scan angle 0° (In original settings, this scans the y-direction.). Open the Level-Tab and the oscilloscope window. Chose 'Fixed' in the Level-Tab.
- Start the line scan by clicking into. The first y-line is scanned repeatable.
- Use the slider or the Edit window to adapt the leveling coefficient 'dz/dy', until the plane vanished.
- Rotate the scan direction to 90° (x-direction is scanned). Adjust the leveling coefficient 'dz/dx'.
- Go back to 2D scan mode. Use **Now** to lift the tip and start to scan.

Drift Correction

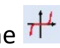
Serves to compensate a constant relative lateral drift between tip and sample by adding a velocity vector to the X- and Y scanning voltages.

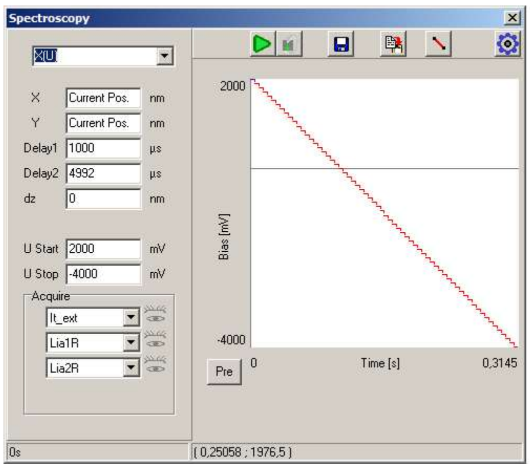


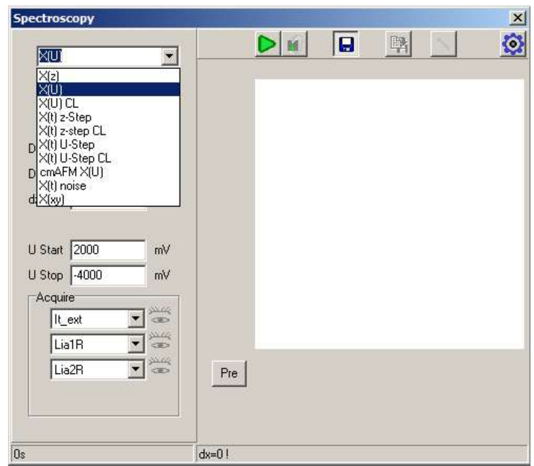
- Activate the Drift correction by pressing on the icon in the parameter window.
- Click with the left mouse button on a characteristic feature in one of the measurement channels (while scanning).
- Once you see the feature again, click again on this feature.
- Afterwards the drift is calculated automatically and the drift compensation is activated
- This procedure can be repeated to reduce the relative drift further.

Spectroscopy

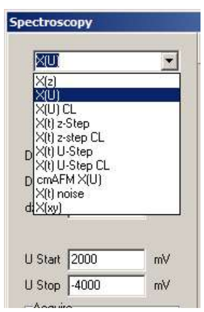
Spectroscopy parameter setting

- Open the window “Spectroscopy”, either via Window/spectroscopy or by pressing the  icon in the main menu bar





- The spectroscopy allows to acquire a wide range of spectra. As there are many different possibilities to collect data, some typical spectroscopy types (data acquisition versus tip-sample distance or data acquisition versus bias voltage) are predefined.



- The pick box allows to select the desired spectroscopy mode:
  - **X(z)** Z-spectroscopy: Signals are measured as functions of the tip-sample distance (z-output is swept); e.g. df(z) or It(z)
  - **X(U)** V-spectroscopy: Signals are measured as functions of the applied voltage between tip and sample (bias is swept); e.g. I(U), dI/dU, d2I/dU2, df(U), etc.
  - **X(t) z-Step:** feedback test ➔ provides a jump at the output “Z”
  - **X(xy):** for lateral atom manipulation

- **Distance Spectroscopy (X_s)**
  - the tip moves with scan speed to the acquisition point
  - wait “delay 1”
  - the feedback is switched off

  - z-movement over dz
  - data acquisition with “delay 2” between the single data
  - feedback is switched on

- **I-U-Spectroscopy (X_U)**
  - the tip moves with scan speed to the acquisition point
  - wait “delay1”
  - the feedback is switched off
  - z-movement over dz
  - data acquisition with “delay2” between single points
  - feedback is switched on
- **Contact Mode Conduction Measurements in dynamic Mode set-up (CM X(U))**
  - the tip moves with the scan speed to the acquisition point in the current feedback mode
  - wait “delay1”
  - the feedback is switched to Contact Mode based on the last settings in contact mode
  - wait “delay1”
  - data acquisition with “delay 2” as point delay (voltage is swept according to settings)
  - the feedback mode is switched back to the former feedback mode

Main parameters:

X, Y coordinates of the data acquisition (changed with “select”)

U1 (dz1) start voltage of spectroscopy ramp (start distance in case of X(z) spectroscopy)

U2 (dz2) end voltage of spectroscopy ramp (end distance in case of X(z) spectroscopy)

Delay 1 time before 1st data point, see time scheme of spectroscopy

Delay 2 time between data points, see time scheme of spectroscopy

dz distance to be retracted/approached after feedback loop was switched off, e.g. to increase/decrease the signal in case I(V) spectroscopy (negative values for retract!!)

 starts the spectrum acquisition. The spectrum is also taken, if you zoom into a new frequency range.

 if both are checked, the spectrum acquisition is repeat, until this knob gets released again.

 Saves the spectrum with the next valid number (to activate: shift + press on save). The number can be reset to zero by changing the base name of the file with “Save as” or by using the entry [SpectOpt] → NextNumber = 0

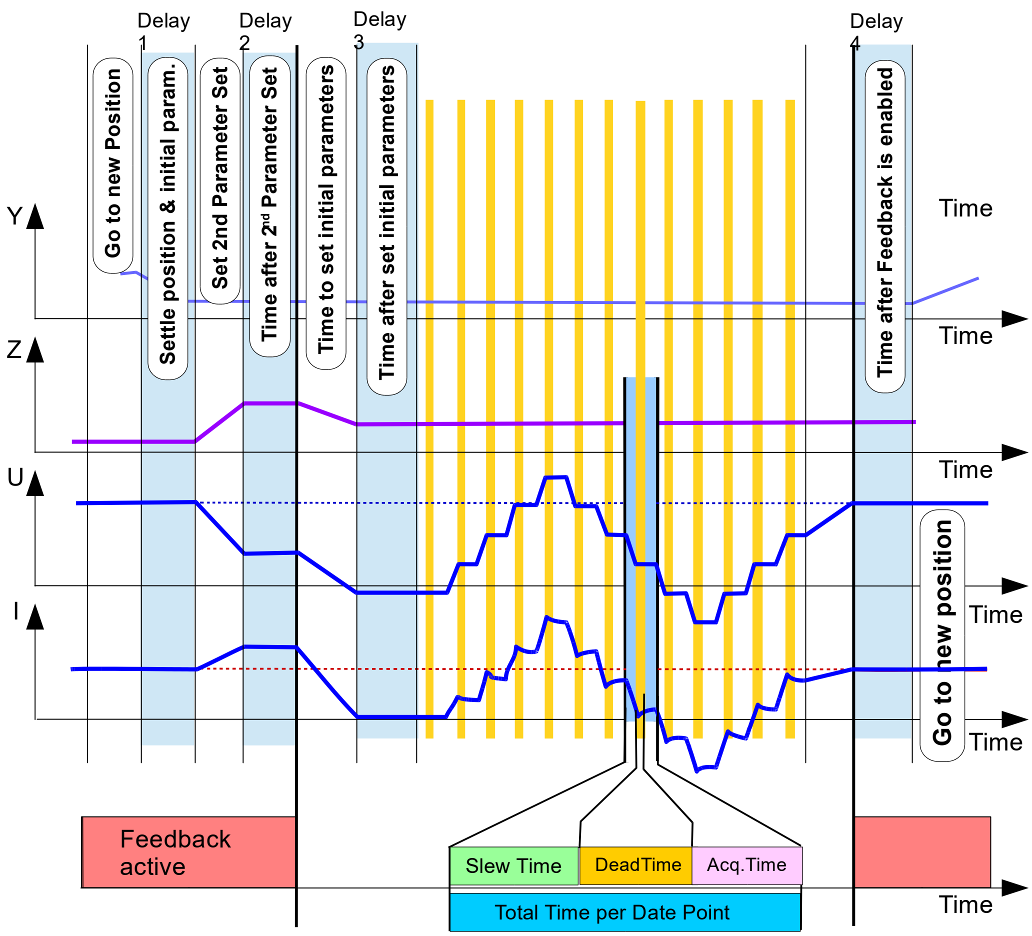
 Copies the data to clipboard.

 Linear fit

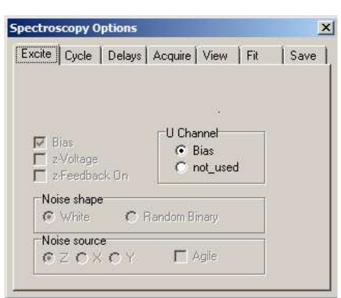
 Opens a sub-menu to get access to many more spectroscopy parameters and options

Channel selection: Here, the channels to be acquired can be selected. For standard I(V) spectroscopy, choose It (tunneling current) in STM mode, and the channel Lia1R and Lia2R for the corresponding (dI/dV and d2/dU2 signals). The data will be displayed after measurement. Only one channel can be displayed at the time. To show the other channel press on the “eye”-icon.

Time scheme of spectroscopy:



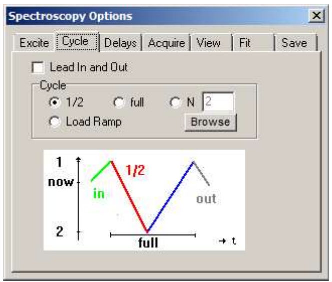
Further Spectroscopy options



Excite:

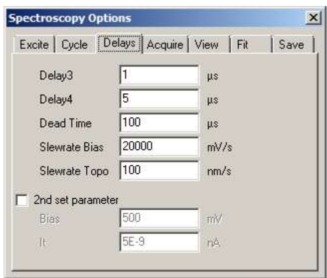
When a pre-defined spectroscopy is chosen (e.g. I(U)), this window shows, which variable is swept during spectroscopy.

When the customized spectroscopy is selected, the user can choose the variable to be swept, here.



Cycle

- *Lead In an Out* if "On", the sweep starts at the value set or detected at this moment
- *Cycle* ½ cycle measures from value 1 to value 2. The full cycle measures from value 1 to value 2 and back. N cycle repeat the full cycle N times. With "Load Ramp" a user defined ASCII ramp can be loaded (first column: Z values; second column: V values → Feenstra mode can be realized by the corresponding ASCII ramp).

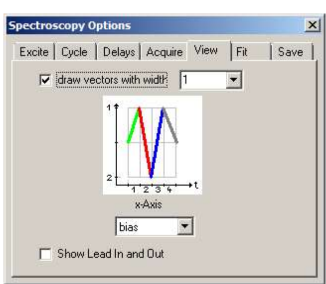


Delays

- See explanation of times and slew rates in the Time Scheme above
- In case of standard spectroscopy (X(U) and X(z)), the second parameters set are feedback parameters, that will be executed at the place of spectroscopy before the feedback loop is switched off for the spectroscopy.
- In case of X(x,y), the 2nd parameter set are the parameters for lateral atom manipulation

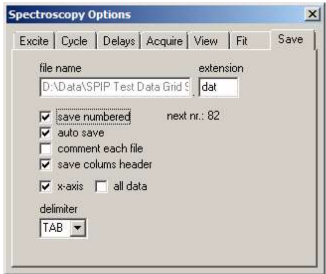
Acquire

- *Data Points* number of points in the spectroscopy curve (half-cycle).
- *Channel(s)* defines the number of acquired channels. Which of the available signals is displayed in the channels, can be chosen in the Acquire-part of the spectroscopy window.



View

- defines the way the data are displayed on the screen.
- With "Draw vectors" enabled, the data points are connected with lines of the provided width. Otherwise, each data point is drawn as dot with the width as size/diameter.
- drop down selection at x-axis allows to select the data that are used as x-axis



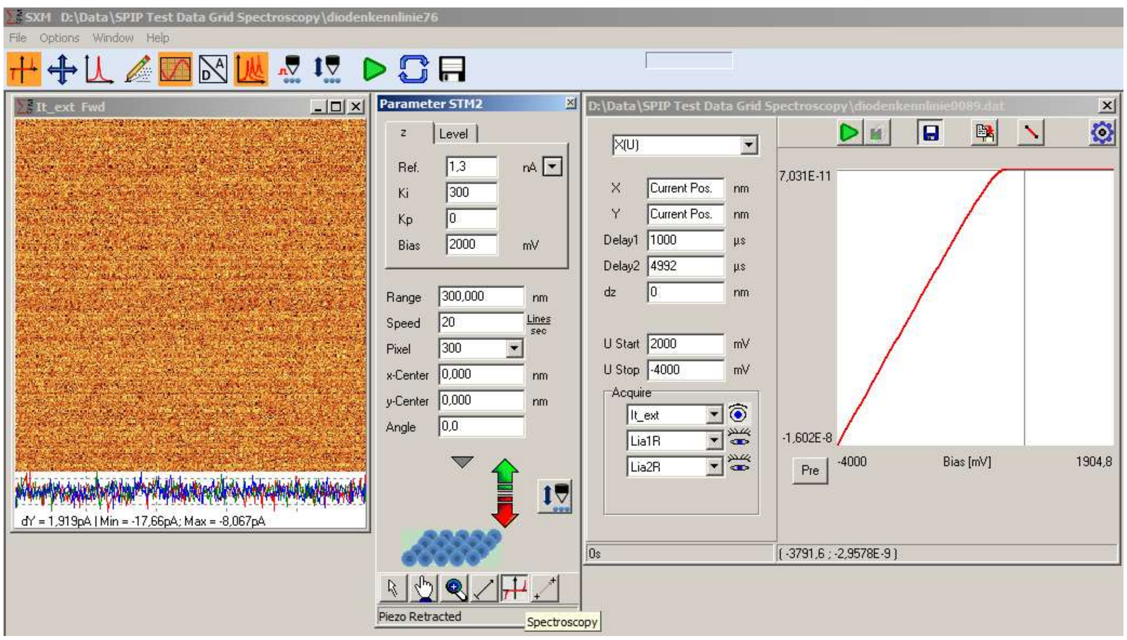
Save

- enables the user to set the file parameters for the ASCII export of the data

Carrying out the spectroscopy

Single Point spectroscopy

- activate the single point spectroscopy by pressing on the icon spectroscopy  in the parameter window

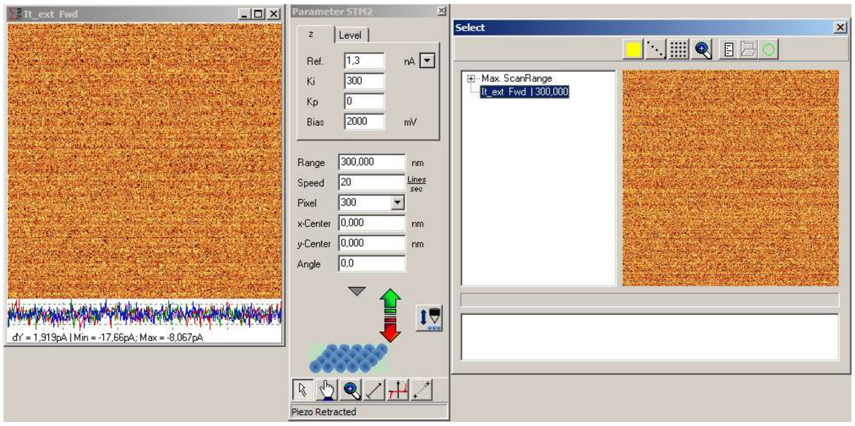


- activate the single point spectroscopy by pressing on the icon spectroscopy  in the parameter window
- position the mouse cursor in the measurement channel window (active scan window) and click the left mouse button to carry out the spectroscopy on the position of interest

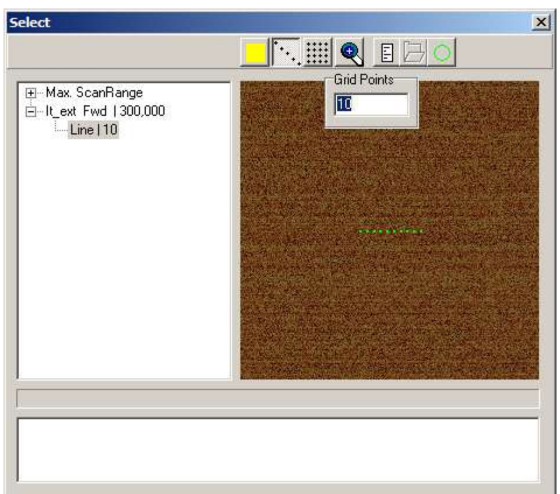
Spectroscopy along a line

- open the select window (window/select)
- activate “drag and drop into script window” by pressing on the icon  in the parameter window

- once activated, pull (per drag and drop) the measurement channel window of interest into the select window
- the measurement channel is now copied and displayed in the select window



- activate the line spectroscopy in the select window by pressing on the icon
- once the line spectroscopy is active, an additional text line appears in the left part of the select window

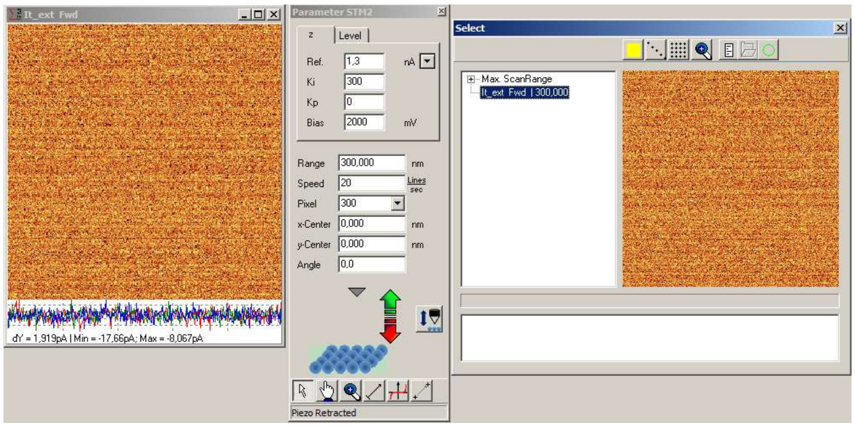


- press on the text "Line|10" to open a sub-window for entering the number of spectroscopy curves to be taken along the line
- define a line (length and orientation) with the mouse by pulling the line in the data channel (select window)
- once the line is aligned properly across the atoms of interest, the spectroscopy can be started with the start button in the spectroscopy window

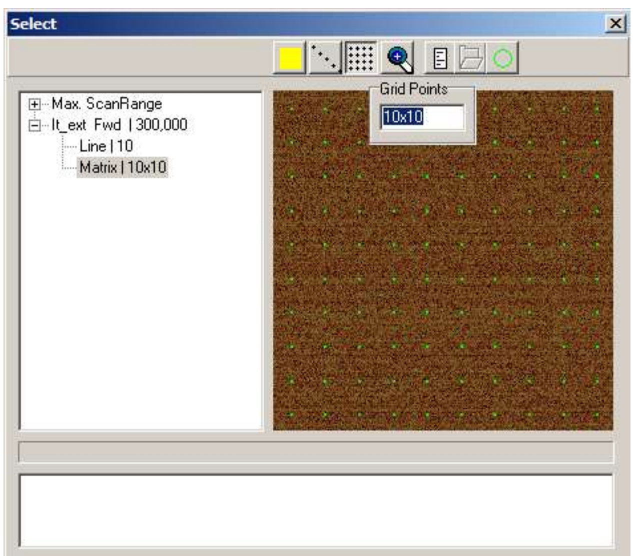
Grid spectroscopy

- open the select window (window/select)

- activate “drag and drop into script window” by pressing on the icon in the parameter window
- once activated, pull (per drag and drop) the measurement channel window of interest into the select window
- the measurement channel is now copied and displayed in the select window



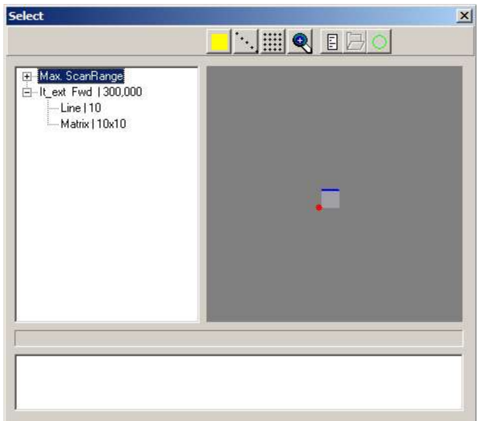
- activate the grid spectroscopy in the select window by pressing on the icon
- once the line spectroscopy is active, an additional text line (“Matrix|10x10”) appears in the left part of the select window



- press on the text “Matrix|10x10” to open a sub-window for entering the number of spectroscopy curves to be taken (Matrix: X, Y)
- once the matrix is defined properly, the spectroscopy can be started with the start button in the spectroscopy window

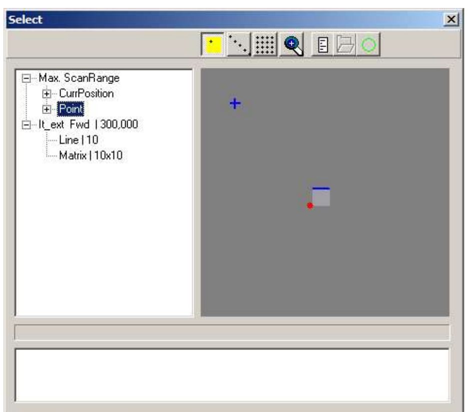
Spectroscopy outside the current scan range but within the total scan range

- this is often used if spectroscopy has to be carried out to clean/recover the tip by spectroscopy in order to avoid contamination of the clean surface of interest
- open the window select (window/select)



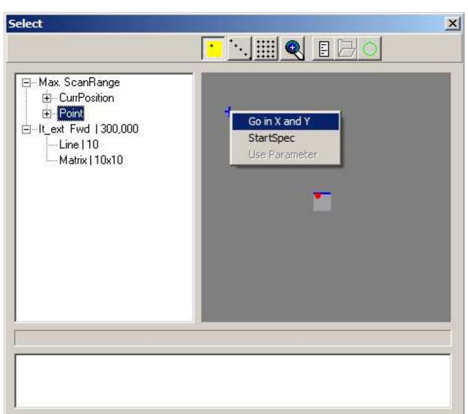
Click on the text field “Max ScanRange”

The whole image at the right shows the maximum scan range and the current scan range in the middle



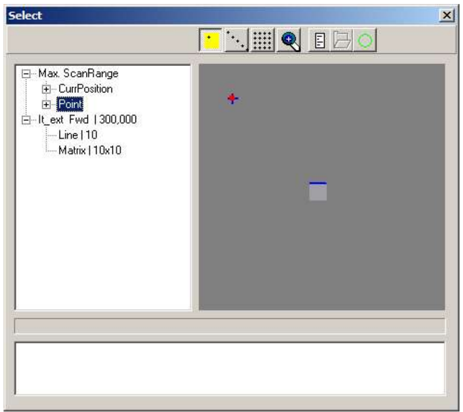
Press the icon for single point spectroscopy and tip positioning

Define a position with by placing the cursor somewhere in the maximum scan range (or in the current rang if wanted). Define this position with the left mouse button. Afterwards the position is represented by a cross.

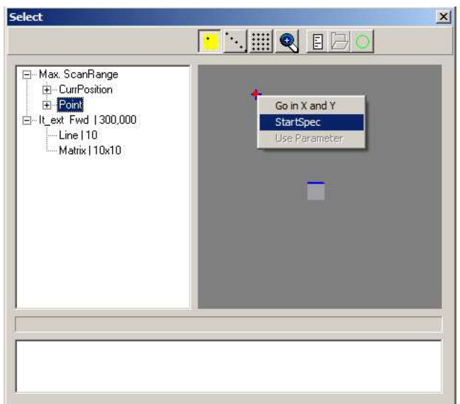


With the right mouse button select “Go in X and Y”

Afterwards, the tip (tip is represented by the red point) moves to the new position (with active feedback regulation and with scan speed)



Tip has reached the goal position when the red point has reached the cross.

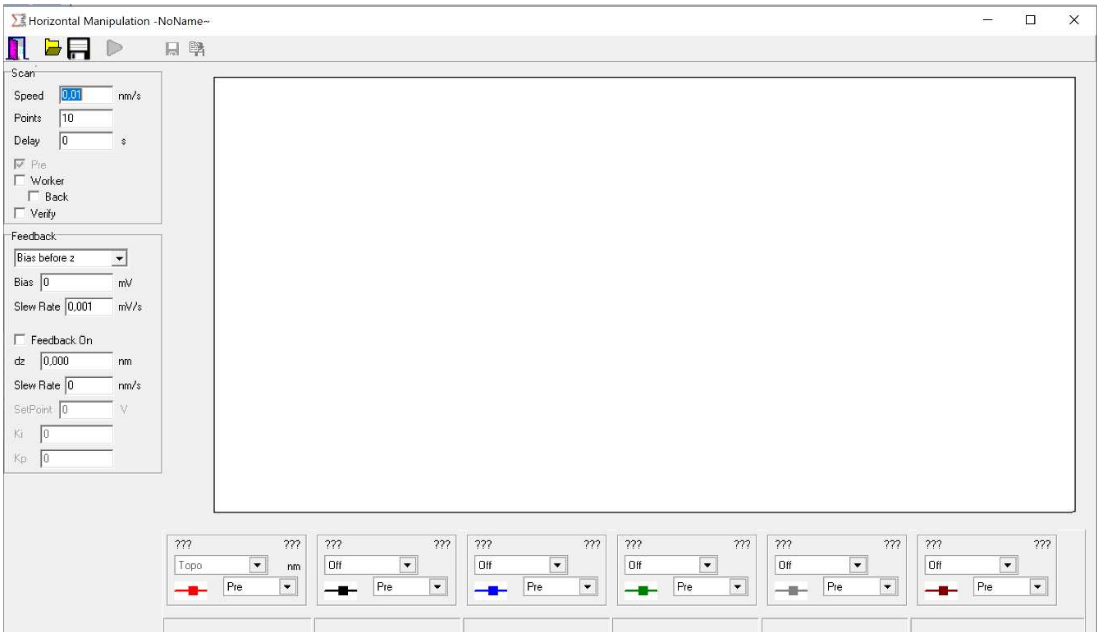


○ Start spectroscopy via right mouse button or via  start button in the spectroscopy window

In the same way the tip can be laterally positioned either in the active scan range or within the maximum scan range, e.g. for manipulation experiments.

Lateral Manipulation

- Open the window for horizontal manipulation by pressing the icon



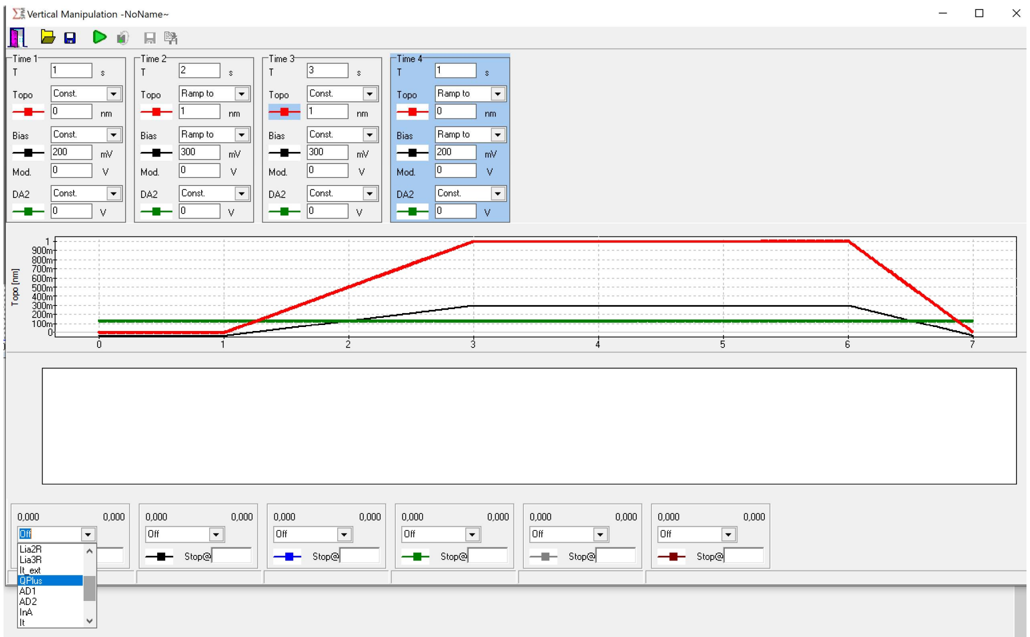
- Set the feedback parameters for atom manipulation (second parameter set in the Delay-window under spectroscopy options); here 10mV and 100nA
- activate the lateral atom manipulation by pressing on the icon spectroscopy in the parameter window
- use the left mouse button to define (drag and drop) a path for the manipulation (definition of a vector between pick-up point and lay-down point). Here, the length of the manipulation path is 203,8nm
- after definition of the path, the manipulation can be carried out by start button in the spectroscopy window
- During the manipulation process the data channels can be displayed and saved via Oscilloscope window. The empty display will display the measurement channels that are of interest for this experiment.

  Select your signal of interest from the drop-down menu (click). The maximum number of channels is limited to 6 channels.

- Once the parameters for the lateral manipulation are defined, the recipe can be store by pressing on the icon
- The routine will be carried out after pressing the icon .

Vertical Manipulation

- Open the window for vertical manipulation by pressing the icon



The software supported vertical atom manipulation allows for definitions of vertical actions, e.g. to pick up an atom or to dehalogenate a molecule, ….

The procedure would be that the tip will be at first placed at a certain location at your sample, e.g. above a single atom or a molecule. Once the tip has reached this position it will stay there. Now, with the vertical manipulation tool, a procedure can be defined that will be carried out at this position. The software allows for definition of several time windows and actions that shall be carried out within this time window. For each time segment the tip-sample distance(topo), the bias voltage or the output of the DA2 can be e.g. suddenly changed or ramped to a new value, or the values can be kept constant. In principle all 3 outputs can be changed simultaneously.

The upper display in the manipulation window with the red, green and black lines is illustrating the actions that needs to be carried out.

The empty display below will show the measurement channels that are of interest for this experiment. Select your signal of interest from the drop-down menu (here "QPlus"). The maximum number of channels is limited to 6 channels.

Once the routine and the channels are defined, the recipe can be store by pressing on the icon

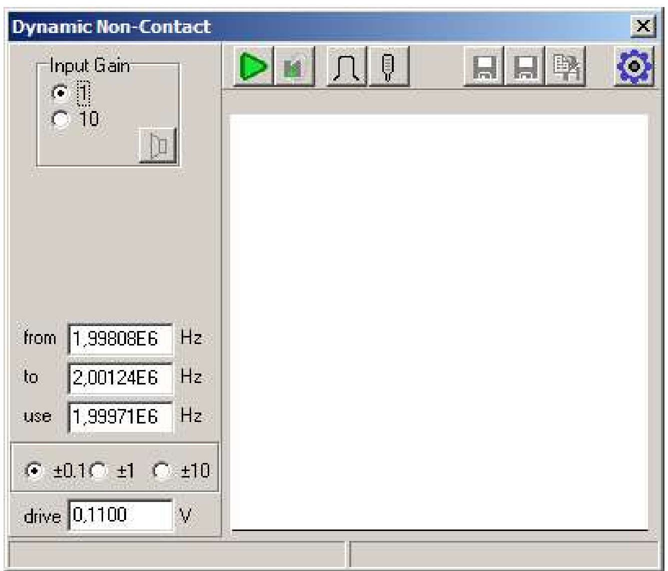
The routine will be carried out after pressing the icon .

An additional time segment can be added by clicking on one time window, e.g. clicking on "Time 4". After clicking on the segment, the segment gets a blue background. Now press simultaneously "insert" and "+" at your keyboard of your PC and a 5th time segment will appear.

The PLL

The DNC window (Phase Locked Loop for Dynamic Non-Contact AFM Mode)

- Select the "PLL AFM" feedback under "options/feedback"
- DNC window is the main window for the settings of the cantilever oscillation
- Here, the frequency response of the cantilever can be measured, the oscillation will be set (frequency and amplitude) and the measurement bandwidth is set
- Open the DNC window by pressing the  icon in the main menu bar, or via Windows/DNC



Parameter:

- **Input gain:** is a hardware switch for the input amplification on the PCI lockin amplifier. It affects the available range for the T-B signal:
  - gain = 1: - 7 V ... 7 V
  - gain = 10: - 700 mV ... 700 mV
- **from:** start frequency for frequency sweep (to find the resonance)
- **to:** end frequency for frequency sweep (to find the resonance)
- **use:** selected frequency for PLL NC-AFM measueremnt
- **Output gains:** ±0.1; ±1 and ±10
- **drive:** excitation amplitude

Menu bar

- starts the spectrum acquisition. The spectrum is also taken, if you zoom into a new frequency range.

    - Repeated spectrum acquisition if booth are pressed. When the “continuous” feature is enabled in the “Acquire” tab of the DNC options window, all spectra are integrated. Otherwise, this feature allows to use the spectrum acquisition as spectrum analyzer.

- if this icon is not pressed, the bandwidth is set to the maximum bandwidth of 40kHz (around the use frequency)

- If is pressed, the icon changes to and at the left additional parameters for the PLL settings appear (time constant and RollOff)

- = **“Thermal Noise Spectroscopy”:** used to determine the thermal noise spectra of the cantilever and can be used to determine the force constant based on the method of Mr. Sader. When the feature is selected, the excitation of the cantilever is switched off automatically. The displayed data are a Fourier transform of the input signal acquired vs. time. The best result is obtained, if many of these Fourier transforms are integrated. The integration is enabled with the “continuous” feature in the “Acquire” tab of the DNC options window and automatically repeated spectrum acquisition

    - Saves the spectrum with the next valid number.

- Allows to “save as” under a new name or directory.

    - Copies the data to clipboard.

- Opens an options window, where data storage, view and acquisition options can be changed.

Bottom text line

- The quality factor is shown in the lower left corner of the DNC window once a resonance was measured

- Frequency, amplitude and phase of the current cursor position will be displayed in the lower right corner of the DNC window

Options for the DNC window

    - Open the options by pressing on the icon

<u>Acquire:</u>

When the spectrum of the cantilever oscillation is acquired, the frequency is swept in N steps (N = **DataPoints**), while the amplitude is measured. As the SPM lockin has always 25 µs time constant, a better filtering or an adjustment of the bandwidth can be achieved by averaging a certain amount (given in **Average**) of subsequently acquired values at the same frequency.

Another possibility to improve the signal to noise ratio is to average subsequently acquired spectra. If **Continuous** is selected in the *Acquire* tab and the repeat knob is ON, spectra are acquired continuously and averaged automatically.

It is possible to adjust the **Phase** offset between outgoing excitation (REF-OUT) and measurement signal (T-B or IN). In case **Auto Zero** is selected, the phase offset will be automatically set to zero when the working frequency is selected in the DNC window.

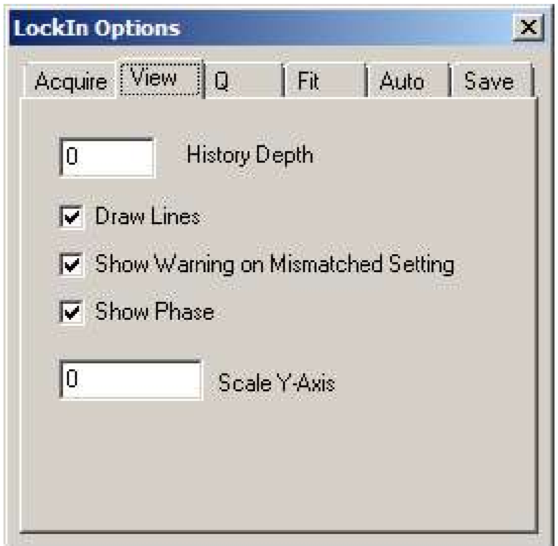
For some applications, another than the 1st **harmonic** might be used as feedback input.

If the expected peak is so small, that the single frequencies might not exactly meet its values, it is possible, that one does not find the peak in a large range spectrum. For this case, the function "**Wobble"** allows to sweep the excitation between the values of neighbored data points so that every excitation frequency is used during acquisition.

If the vertical adjustment position on the photo detector is more than 30…50 mV away from zero, it is useful to switch to ac coupling. "**Input AC"** coupling works for all frequencies above 1 Hz, which means for all cantilevers. This ac coupling is available when the hardware version of the AMU2.x board is higher than 2.3 or equals "2.3". For the version 2.3, one needs to set the ac coupling option manually in the *sxm.ini*.

"Sync Filter" is a special feature available from PROM-Code version 26h in the AMU2.6 cards. The feature enables a faster evaluation of the amplitude signal related to the operations frequency. The amplitude is taken after 1/f, already. This feature increases feedback speed. For cantilevers with high resonances, the noise is increased. The reaction time of the feedback system reduces from 100 µs down to 50 µs. The sync filter is enabled with the entry [scanner] SyncFilter=1 in the sxm.ini.

The default value for the spectrum (right mouse button click inside the white area of the spectrum + topmost line in the **frequency range** listing) can be changed here as well.



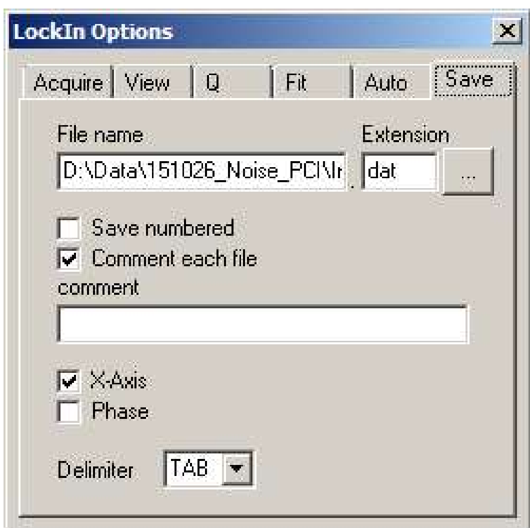
VIEW:

The spectra data might be drawn as single points or **vectors**. One can set the input gain of the lockin in a range that leads automatically to wrong amplitude values (too high internal amplification). This is detected in the hardware by an overflow. When **"Show Warning on Mismatched Setting"** is selected, the field around the *input gain* gets red on overflow.

"Show Phase" enables the display of the phase signal during spectrum acquisition.

It is possible to show the current and a certain number of previous spectra in the same screen. When the **History Depth** is set to zero, only the current spectrum is shown. When "1", the current plus the last spectrum are shown.

As default, the y-axis of the spectrum is scaled automatically to the last acquired spectrum. If one likes to change this, one has to put a vertical scaling factor into **Scale Y-Axis**.



SAVE:

The data can be stored in an ASCII file. The **file name** shown here is the complete path and file name of the last saved file.

The file **extension** can be chosen here costumer specifically.

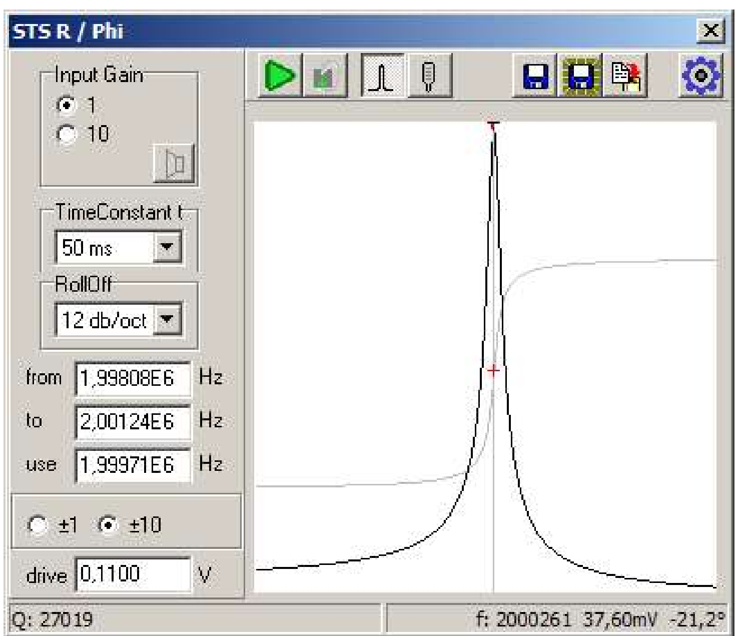
If **save numbered** is ON, one click on the *save button* will save the current data with the same name but count the last number of the file name upwards. The number of the next file is shown behind.

If comment each file is ON, the comment providable in the edit line below.

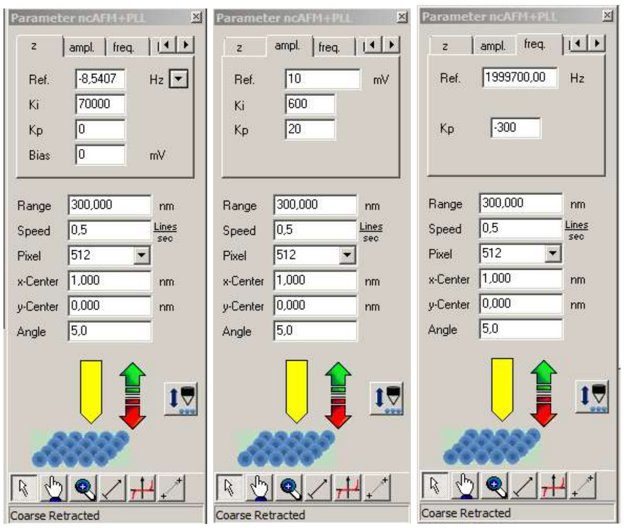
The **x-axis** and the **Phase** are stored only in the data set, if selected here. Single rows are delimited by the character provided as **delimiter**.

Measurement of the Cantilever resonance and setting of oscillation parameters

- Select the "PLL AFM" feedback under "options/feedback"
- Open the DNC window by pressing the icon in the main menu bar, or via Windows/DNC
- Press the icon ➔ it changes to
- Set a TimeConstant and the RollOff for the PLL. 5ms and 12dB are good values for the first measurement. In a second run the time constant can be increased for a better S/N ratio (in the example shown below 50ms was used)
- Set the start and end frequency for the frequency sweep. Make sure that the expected resonance frequency will be covered by this range.
- Enter an amplitude for the excitation frequency. 0.1V is a good start value. (Attention: if the curve is measured close to the surface a tip crash can happen for huge oscillation amplitudes!)
- Press to start the spectrum acquisition. Depending on the TimConstant, the acquisition of a spectrum may take several 10^{th} of seconds. The spectrum will be displayed after the full spectrum was measured (please be patient). The spectrum is also taken, if you zoom into a new frequency range. The spectrum acquisition can be stopped by pressing again on the start icon.
- **Zoom in:** Once the first spectrum is measured, click with the left mouse button into the spectrum and move the mouse to the right with pressed button. A red line at the top edge of the window indicates the selected frequency range. When the mouse button is released, the spectrum in the new range is acquired automatically.
- **Frequency selection:** click once with the left mouse button. The lateral mouse position is used as "use" frequency, the vertical mouse position is used as new amplitude setpoint.



- Inside the spectrum, a vertical grey line appears which visualizes the chosen position and a red cross on this line shows the selected setpoint for the feedback. If the user changes the setpoint now manually, this cross moves along the line to the new position.
- Use the right mouse button to display former frequency selections and a default range over the full spectrum.
- Once the resonance was set up, the amplitude of the cantilever oscillation can also be set in the “PLL-NC-AFM” parameter window (“Ref.” value under the tab “ampl.”)



Setting up a qPlus measurement

General information

NC-AFM in UHV

In UHV the standard NC-AFM operating mode is the ‘Constant Amplitude Frequency Modulation mode’. The resonance frequency is modulated by the interaction forces while the probe is scanned in X and Y close to the surface. The shift of the resonance frequency from the free resonance $\Delta f(x,y)$ is measured with a phase locked loop (PLL) which locks to the resonance frequency and controls the oscillation frequency. The oscillation amplitude is always maintained at a fixed value by an amplitude controller.

Setting up this mode involves finding the free resonance frequency of the sensor, its phase with respect to the electronic circuitry phase, its mechanical properties by means of quality factor and finding proper parametrization of amplitude and phase control loops.

NC-AFM scheme of SXM

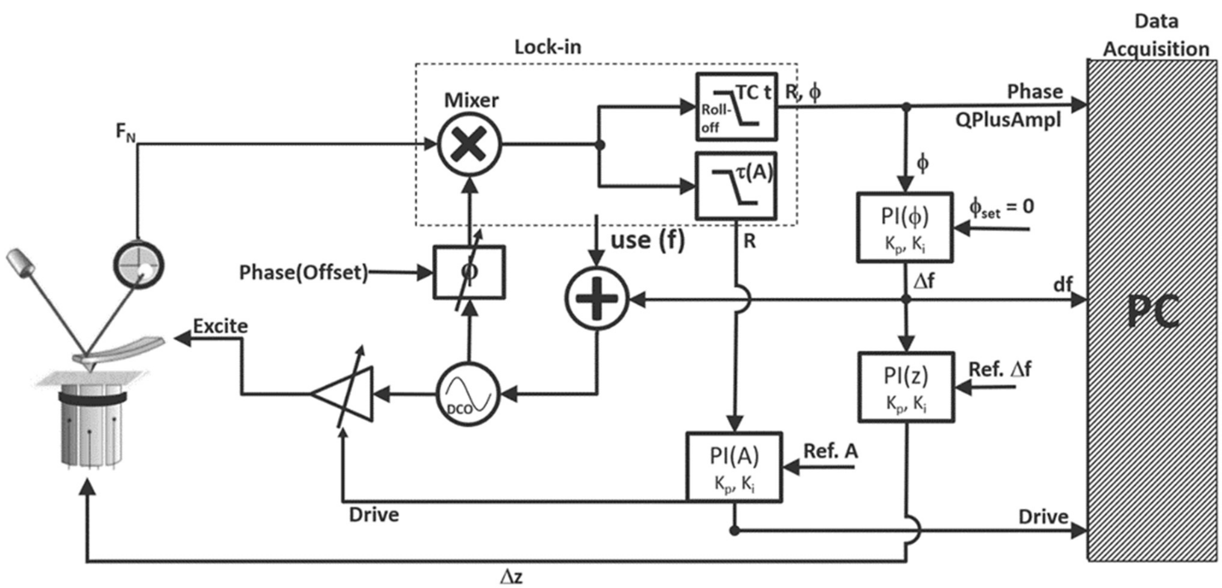


Fig.: Control scheme of the NC-AFM operation mode for SXM

DCO: Digitally Controlled Oscillator

TC: Time Constant

PI: Proportional/Integral regulator

Ref.: Setpoint of respective feedback loop

(naming taken from SXM software interface)

General Notes

- All controls or readings of sine wave amplitudes in SXM are by means of Root Mean Square (RMS), i.e. $\text{amplitude}_{\text{peak-to-peak}} = 2*\sqrt{2}*\text{amplitude}_{\text{RMS}}$.
- All input controls need to be confirmed by pressing 'Enter'.
- All Ki and Kp parameter values are by means of arbitrary units and derived from their software internal representations.

Preparing the controller for qPlus measurements

Cabling & SPM preparation

- Connect BNC cable from FEMTO HQA-15M-10T (old version: Physimetron A6504-B) Charge Amplifier '**OUT'** (Omicron: QPlus Pre→'**ω-out**') to the '**IN→QPlus**' input SPM Controller. It digitizes the QPlus signal and generates the Channel '**QPlus_ext**' in the SXM software. The signal galvanically isolated from the preamp is '**IN A**' of the Lock-in card (blue BNC).
- Connect the red BNC cable ('**Ref A'**) of the PC LIA to the '**IN'** BNC connector of the galvanic isolation card with the two BNC sockets.

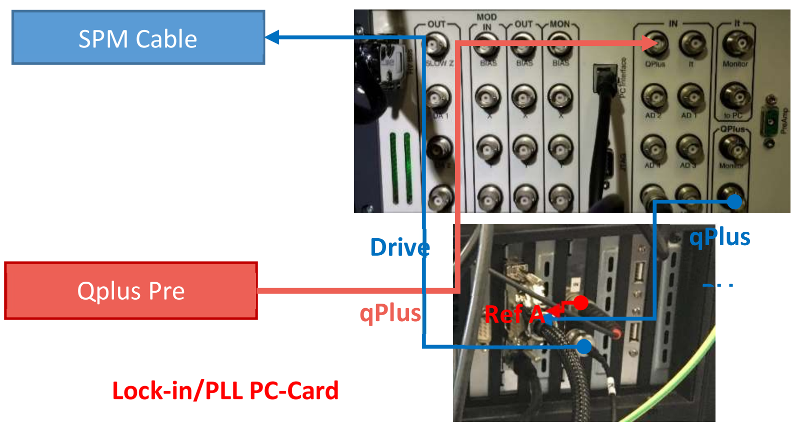
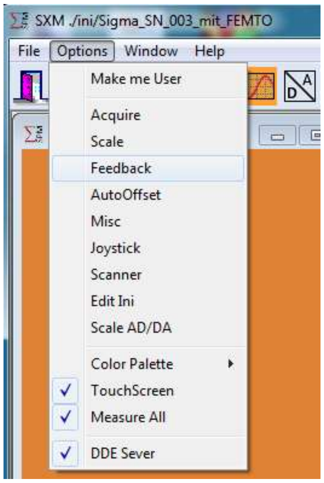


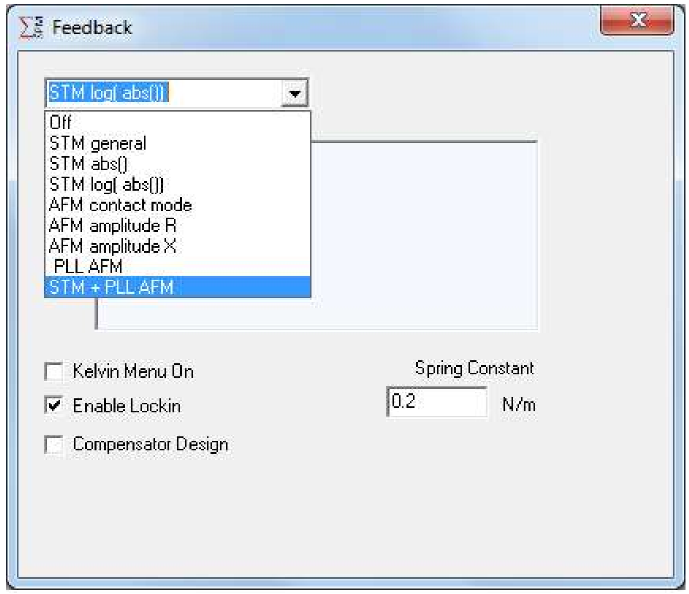
Fig. 1: QPlus cabling SXM

- Connect the BNC cable '**R'** of the SPM cable (Omicron: '**Excite**') to the **OUT** BNC connector of the galvanic isolation card with the two BNC sockets. This is the sine modulation voltage added to the tube scanner ring electrode for the mechanical qPlus excitation.
- Connect the blue BNC cable ('**IN A'**) of the PC LIA to the blue '**QPlus→to_PC**' BNC connector of the SPM Control unit. This is the input signal for the amplitude lock-in and the PLL.
- Insert the qPlus sensor and sample and approach the qPlus tip under optical control with the CCD camera as close as possible to the sample

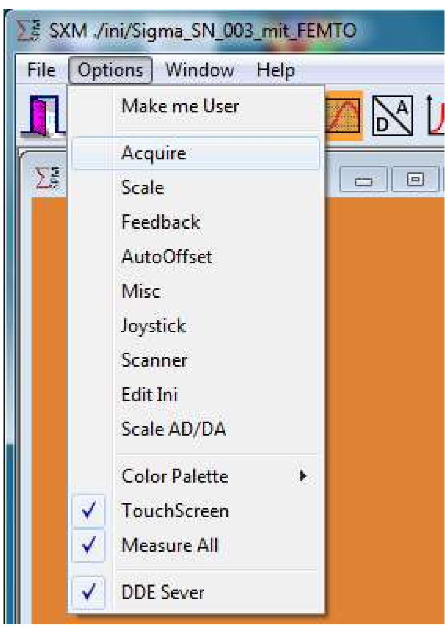
Software: select the measurement mode and measurement channels

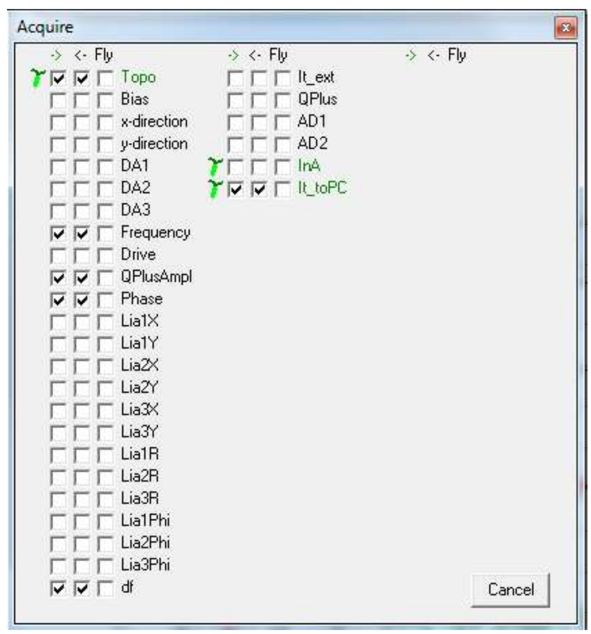
- Select the feedback mode for qPlus ➔ “STM+PLL AFM” (or alternatively only “PLL AFM”)





- Select the channels to be acquired under “Options/Acquire”





Useful channels for qPlus measurements are:

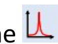
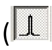
df:	frequency shift
Topo:	topography signal
QPlusAmpl:	oscillation amplitude of qPlus sensor
Phase:	phase signal
It_toPC:	tunneling current (only in case of conductive samples)
Frequency:	frequency of qPlus sensor

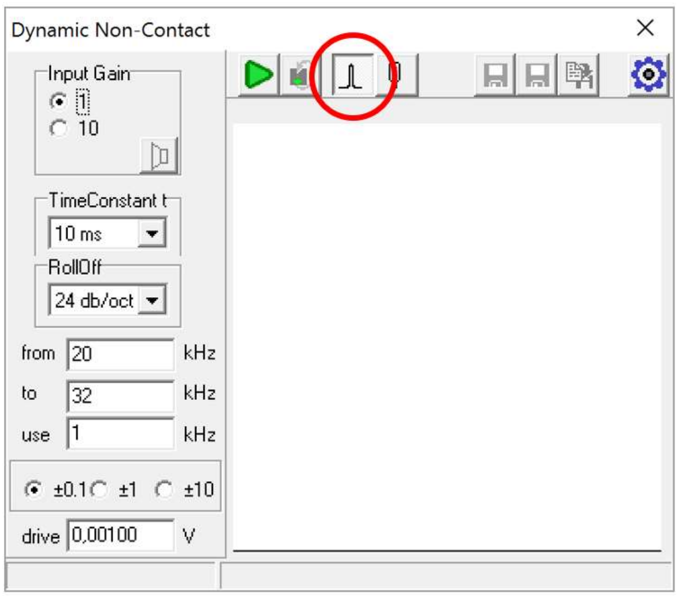
Drive: excitation amplitude for qPlus oscillation

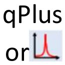
Minimum required channels: “df” and “Topo”

- Open the “parameter” window

Finding the resonance

- Open the “DNC” window (Dynamic Non-Contact) Oby pressing the  icon in the main menu bar, or via Windows/DNC and set-up the oscillation
- Click the “bandwidth” button to small bandwidth () until the parameters “TimeConstant” and “RollOff” will be displayed



- To find the (free) resonance frequency of the sensor $f_{res,free}$ an excitation sine voltage is applied to the excitation actuator of the AFM (e.g. the tube scanner ring electrode for the mechanical qPlus excitation). The corresponding module is found in the ‘DNC’ window (‘Window’ menu or  button) The sine wave frequency is swept across a frequency range given by the ‘**from**’ and the ‘**to**’ value at a ‘**drive**’ amplitude in the DNC window (**Main menu→Windows**):

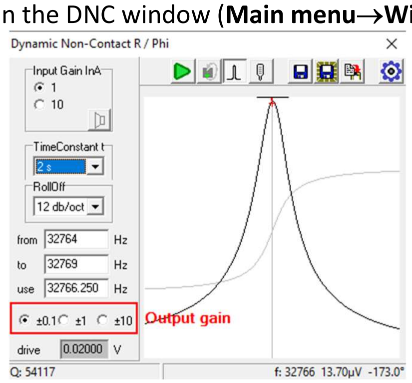


Fig. 3: DNC Window

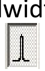
Please note: there are three different '**Output Gains**' (±0.1, ±1, ±10) which allow to adapt the digital resolution of the sine D/A output to the desired analog output amplitude to minimize anharmonic distortions. The '**drive**' amplitude is entered by means of **RMS** voltage whereas the '**Output Gain**' describes the maximal peak values in [V_p]. If a new '**drive**' amplitude is entered the '**Output Gain**' will automatically adjust. However, the gain can still be changed manually.

Please note: there are two input gains for the sensor signal input at '**IN A**':

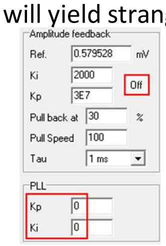
Gain 1: -7V < input signal level < +7V

Gain 10: -0.7V < input signal level < +0.7V

For best performance choose the highest gain possible without overloading the input stage. In case of an overload the '**Input Gain InA**' user interface element will flash red.

Please note: the amplitude of the sensor signal is measured with a lock-in amplifier. It can run at maximal bandwidth  (25µs time constant, bandwidth button set to 'wide') or in bandwidth control mode  (bandwidth button set to 'narrow') . Only the latter mode should be used. In this mode the lock-in time constant and roll-off (typical: 12dB/oct) are set by the corresponding controls of the DNC window. The measurement time per frequency point which determines the speed of the sweep is automatically aligned to the time constant

Please note: before running a sweep make sure that '**Parameter→Amplitude Feedback→On/Off**' is set to '**off**' (Amplitude feedback loop disabled) and '**Parameter→PLL→Kp,Ki**' are both zero (PLL off). Otherwise running a frequency sweep will yield strange results.



- Typically, for an unknown sensor first an overview sweep is performed with many frequency points:
  - ⇒ Select '1' for '**Input Gain InA**'.
  - ⇒ (Make sure 'narrow' bandwidth is selected) Select '10ms' for '**TimeConstant t**' and '**RollOff**' 12dB/oct.
  - ⇒ To select the frequency sweep range enter its start value at '**from**' and its end value at '**to**', e.g. 20kHz to 30kHz for a qPlus sensor.
  - ⇒ The excitation amplitude for the excitation actuator is set with '**drive**'. For a Polar/Infinity SPM typical starting values are 1-2mV at low temperature, for Omicron SPMs 10-100mV.
  - ⇒ From the '**LockIn Options**' menu (gear symbol) go to the '**Acquire**' tab and select 2048 '**DataPoints**'. The large number of frequency point is necessary to find also large quality factor resonances. '**Average**' should be set to '1' (i.e. one time constant integration time/frequency point).

⇒ Start the sweep by pressing and wait for it to finish. The time scale for a full sweep is **t_{sweep}** ≈ **TimeConstant t * DataPoints**. (**Hint**: the sweep can be interrupted any time by pressing the green triangle again.)

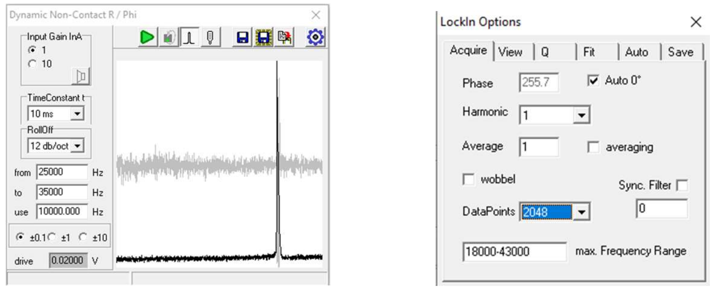
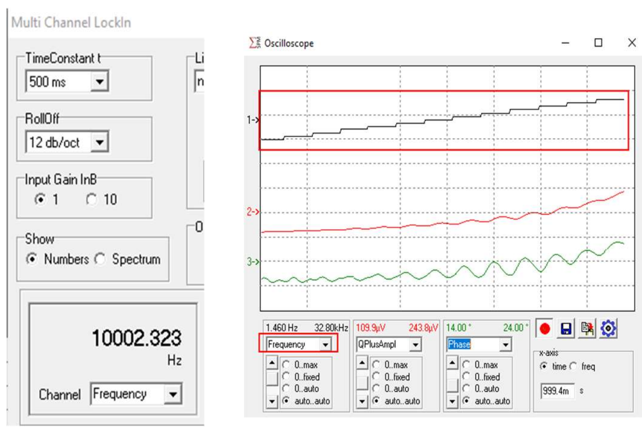


Fig. 4: Initial frequency sweep

Please note: the progress of the sweep is not shown during the sweep. If the progress should be monitored (e.g. for long sweeps) the channel 'Frequency' can be selected in the 'Oscilloscope' at appropriate time scale for a graphical display or the channel 'Frequency' can be selected in the MultiChannelLockin window in numerical display mode at proper resolution.



⇒ Once the sweep is finished the resulting amplitude curve will be displayed. If '**Show Phase**' is enabled in the '**LockIn Options→View**' tab also the phase curve will be displayed.

⇒ To zoom into the curve left-click close to the left side of the (typically very narrow) peak into the curve display area, keep left mouse button pressed, draw to the right side of the peak (a green bar range indicator will be shown at the top of the curve display) and release the left mouse button. A new curve is started immediately on release. Alternatively, start and stop frequencies can be entered manually (see above).

⇒ Since for the next iteration the number of frequency points can likely be reduced stop the sweep by pressing the green triangle again, reduce the number of points (e.g. 256 points, see above) and start the sweep again.

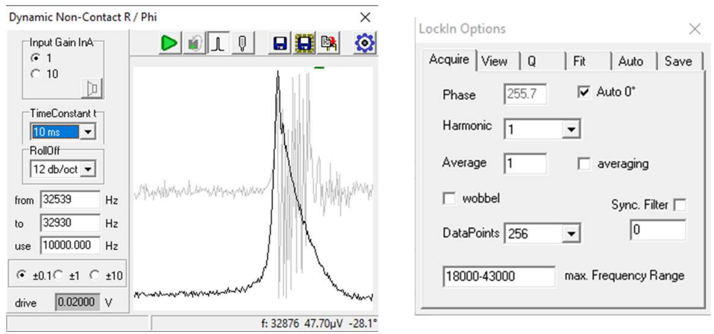


Fig. 6: Second sweep with reduced #DataPoints

⇒ If a finite peak width can be identified for the resulting curve click onto the position of the peak. In the lower left of the status line an estimated quality factor is shown and the 'use' frequency will be set to the clicked position.

⇒ Set the '**TimeConstant t**' closest to quality factor/resonance frequency. This allows for a proper settling time for the final frequency sweep.

⇒ Repeat the steps for zooming-in with the final curve width covering appr. 1/3 of the frequency axis.

⇒ Determine the accurate resonance frequency and quality factor with a left mouse click to the peak position.

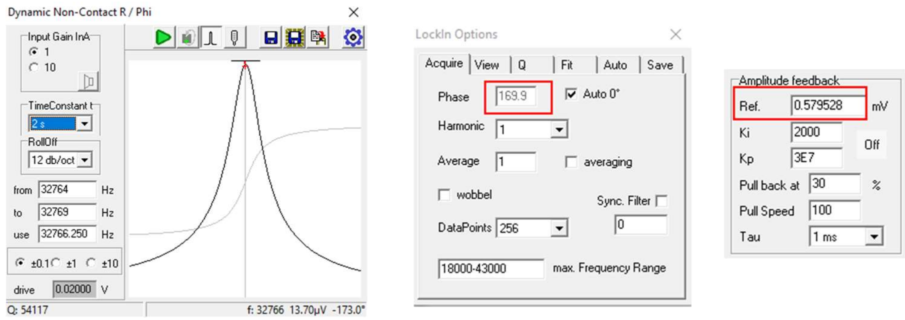


Fig. 7: Finale sweep at suitable parameters

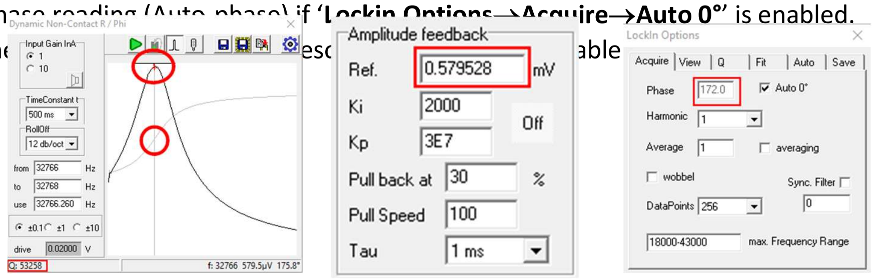
Please note (see fig. 7 above): Left-clicking into the spectrum region of the DNC window will initiate multiple automatic activities:

⇒ the frequency at the click position will be transferred into to '**use**' control, i.e. the center frequency of the PLL

⇒ the amplitude at the click position will be transferred to the '**Parameter→Amplitude Feedback→Ref.**' control, i.e. the setpoint of the amplitude control loop.

⇒ the phase offset (=phase shifter) of the PLL will be automatically tuned to yield zero phase reading (Auto phase) if '**Lockin Options→Acquire→Auto 0°**' is enabled.

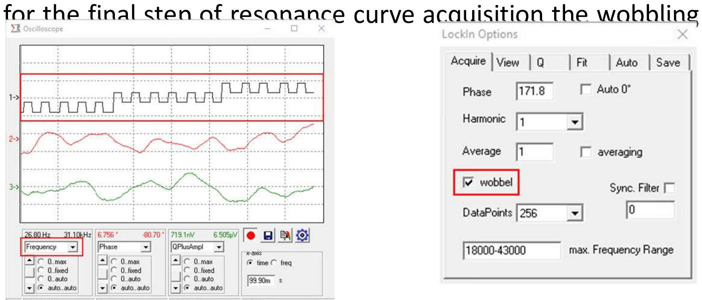
⇒ the [illegible] esc [illegible] able



⇒ Set the '**TimeConstant t**' to a value >1/bandwidth(PLL regulator), e.g. 2ms.

Please note: If '**Lockin Options→Acquire→Auto 0°**' is enabled a change (automatic or manual) of '**DNC→use**' will always trigger an Auto-phase. If this is not desired, e.g. for just a modification of the reference frequency disable '**Auto 0°**'.

Please note: The initial sweep can be performed faster if '**Lockin Options->Acquire->Wobbling**' is enabled. In this case on each (center) frequency step the frequency is flipped between ±half the frequency step size. This method allows to catch intermediate frequency also for small number of frequency point. It is in particular useful if the resonance frequency is unknown and the quality factor is large. However, for the final step of resonance curve acquisition the wobbling should be turned off.



Setting up the amplitude feedback loop

- To set up the amplitude feedback loop (AFL) ‘**DNC→use**’ should already be set to the free resonance frequency $\mathbf{f_{res}}$ and the probe retracted from the surface to a safe distance. The PLL should be off by setting its Ki, Kp to zero. The AFL should also be toggled to ‘**off**’ with ‘**Parameter→Amplitude Feedback→On/Off**’.

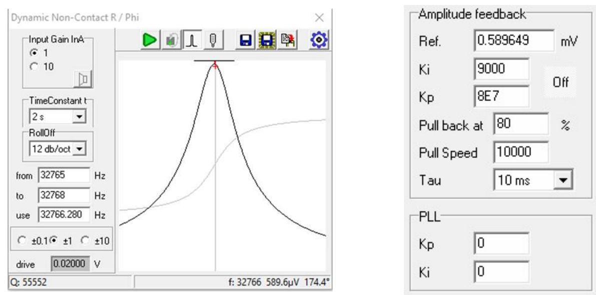


Fig. 9: Switch off Amplitude loop and PLL

- If the AFL is switched off the sensor is excited at a fixed frequency (‘**use**’) and fixed excitation (‘**drive**’). This is called ‘Constant Excitation’ mode and useful for setting up the AFL.

> **Please note**: Once the AFL is switched on the ‘**drive**’ excitation is switched off and the excitation output amplitude is controlled by the AFL.

- Enter a setpoint value for the AFL into ‘**Parameter→Amplitude Feedback→Ref.**’. A good starting point is $1nm_{pp}$ for QPlus sensors (Tribus: $6mV_{RMS}$, Omicron QPlus Pre 4: $64mV_{RMS}$) and $10nm_{pp}$ for NC-cantilevers (VT-AFM with I_{tot}=2V and 130mm cantilever length: $82mV_{RMS}$).
- Set starting values for ‘**Parameter→Amplitude Feedback→Ki, Kp**’. As a rule of thumb Kp ≈ 10^4*Ki. Starting values for Ki can be estimated from Q derived from the resonance sweep: Ki ≈ $5*10^8/Q$ and thus Kp ≈ $5*10^{12}/Q$ at output gain ±1V.

> **Please note**: When changing the output gain of the AFL Ki and Kp also need to be adjusted. E.g., when changing from gain ±1V to ±0.1V both Ki and Kp need to be multiplied by 10.

- Set a bandwidth for the AFL low-pass filter ‘**Parameter→Amplitude Feedback→Tau**’: $\tau \approx Q/(100*f_{res})$.

> **Please note**:
>
> ⇒ ‘**DNC→TimeConstant t**’ will alter the bandwidth of the phase for the PLL (phase regulator input) and the Phase and Amplitude measurement channel (not amplitude regulator input) in the SXM software.
>
> ⇒ ‘**Parameter→Amplitude Feedback→Tau**’ will change the bandwidth of the input signal for the AFL only. Effects of ‘**Tau**’ can only be observed in the ‘**Drive**’ channel or in the feedback response of the AFL to input amplitude changes. See also fig. 2.

- Activate the AFL by toggling '**Parameter→Amplitude Feedback→On/Off**' to '**on**'. The AFL is running properly if 'QPlusAmpl' moves to the '**Parameter→Amplitude Feedback→Ref.**' and 'Drive' settles at a constant value, both fluctuating slightly.

- The next step is only needed if accurate settings for the AFL are needed or if the AFL is suspected to create distortions. Otherwise continue with setting up the PLL (see below). Proper Ki and Kp parameters for the AFL can be derived from the step response of the AFL.
  - ⇒ Start the AFL with suggested 'Rule of thumb' parameters: Toggle the '**Amplitude feedback On/Off button**' to '**On**' and monitor '**QPlusAmpl**' and '**Drive**' channels with the software '**Oscilloscope**', e.g. at 1s per division.
  - ⇒ Modify '**Parameter→Amplitude Feedback→Ref.**' by ±10% (e.g. toggle between 5.4mV and 6.6mV) to create a step in the setpoint of the AFL.
  - ⇒ Optimize '**Parameter→Amplitude Feedback→Ki, Kp**' to obtain a rectangular shape of QPlusAmpl vs. t going from one setpoint to the other.
  - ⇒ '**Drive**' should also reflect the changes of the setpoint but may also exhibit overshooting at the steps. Avoid a too strong (saturating) overshooting and watch the noise on '**Drive**' which is amplified by Kp.
  - ⇒ Once good absolute values for Ki and Kp are found remember the ratio of Ki and Kp. The speed of the AFL can now be controlled by increasing (faster)/decreasing (slower) Ki and Kp while maintaining their ratio (rule of thumb).

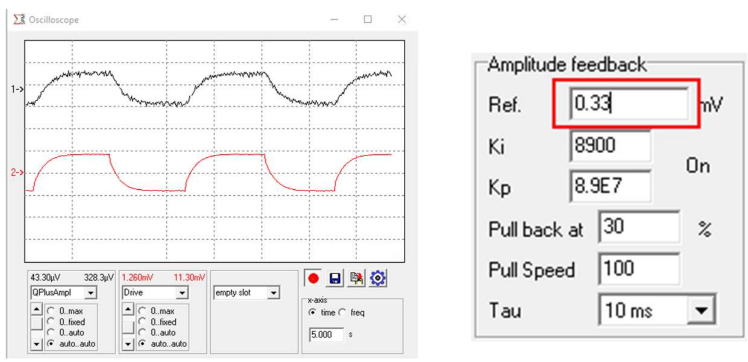


Fig. 10: Toggling the amplitude setpoint while optimizing Ki, Kp

Setting up the Phase Locked Loop

- To set up the Phase Locked Loop (PLL) '**DNC→use**' should already be set to the free resonance frequency $\mathbf{f_{res}}$ and the probe retracted from the surface to a safe distance. The AFL should be running at reasonable conditions. The PLL should be off initially with its Ki, Kp at zero.

Please note: the PLL has two tasks:

⇒ Ensure that the sensor is always excited at its current resonance by tracking its phase.
⇒ Determine the frequency deviation Δf from the free resonance frequency.

Please note: the PLL has always a setpoint of 0°. It is essential that the PLL is started at '**use**' = $f_{res,free}$ and Phase = 0°. Otherwise, Δf won't be a valid measurement and instabilities can occur.

- Set a bandwidth for the PLL low-pass filter '**DNC→TimeContant t**': $t \approx [10*BW(P_{LL})]^{-1}$ with $BW(P_{LL})$ the target bandwidth of the PLL (rule of thumb). Too large time constants will induce loop oscillations of the PLL.
- Auto-phase the PLL:
  - Make sure '**DNC→Lockin Options→Acquire→Auto 0°**' is enabled.
  - Monitor 'Phase' with the software 'Oscilloscope' and its numerical value.
  - Put cursor into '**DNC→use**' control and simply press 'Enter'. This triggers the auto-phase mechanism.
  - If 'Phase' is not very close to 0±0.5° repeat pressing 'Enter'. If 'Phase' is too noisy auto-phase will not yield good results. In this case temporarily set '**DNC→TimeContant t**' to a much larger value (this will reduce the noise) and do the auto-phase. After success put '**DNC→TimeContant t**' back to its previous value.
  - Alternatively, the phase offset can be entered manually into '**DNC→Lockin Options→Acquire→Phase**' if '**Auto 0°** is disabled.

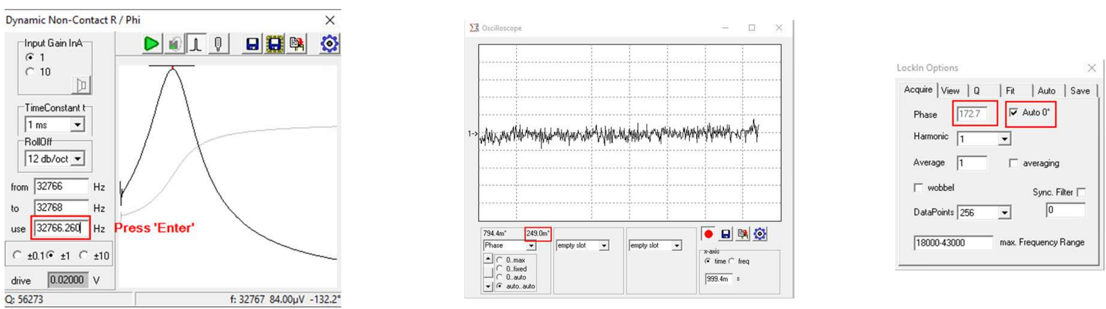


Fig. 11: Auto-phase procedure

- Set starting values for '**Parameter→PLL→Ki, Kp**'. Both must be negative. As a rule of thumb Ki ≈ 100 to 1000*Kp. Starting values for Kp are between -50 and -200, thus Ki ≈ 10^4 with Kp = -100. This will already activate the PLL. Please check if the 'df' channel is now at zero. Otherwise

Please note: Bandwidth of the PLL

The PLL has a bandwidth with which it reacts to changes of the phase. In case of scanning a surface the resonance frequency of the sensor and thus the detected phase change with a speed given by the scan speed and the corrugation of the sample. In constant df feedback mode it is mandatory to adjust the bandwidth of the PLL accordingly. Kp (and less pronounced Ki) determine the bandwidth of the PLL. For the SXM the bandwidth in the case of Ki =600*Kp is roughly given by:

$$BW(PLL) = 0.02*Kp+1E\text{-}5*Kp^2 \quad \text{or} \quad Kp = \sqrt{(1E6+1E5*BW(PLL)^2)}-1000$$

check the phase offset once more (see above) or in case of an instable oscillation try to modify ‘**Parameter→PLL→ Ki, Kp** ’.

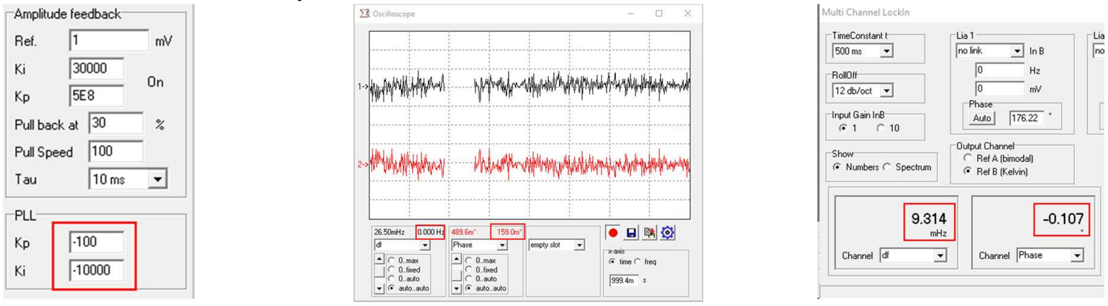


Fig. 12: Check if df and Phase are zero when starting the PLL

- The next step is only needed if accurate settings for the PLL are needed or if the PLL is suspected to create distortions. Otherwise continue with setting up the Auto-approach/topography measurement (see below).
  Proper Ki and Kp parameters for the PLL can be derived from the step response of the PLL.
  - ⇒ Make sure ‘**DNC→Lockin Options→Acquire→Auto 0°**’ is disabled.
  - ⇒ Monitor ‘**df**’ and ‘**Phase**’ channels with the software ‘Oscilloscope’, e.g. at 5s per division.
  - ⇒ Toggle the current ‘**DNC→use**’ frequency about ±1Hz around f_{res} to create an artificial frequency (equivalent to phase) step and watch the response in the software ‘Oscilloscope’.
  - ⇒ Optimize ‘**Parameter→PLL→Ki, Kp**’ to obtain a fast decay to 0° of Phase(t) without overshooting going from one frequency to the other.
  - ⇒ ‘**df**’ should be shaped rectangular and overshooting should be avoided as well.
  - ⇒ Once good absolute values for Ki and Kp are found remember the ratio of Ki and Kp. The bandwidth of the PLL can now be controlled by increasing (faster)/decreasing (slower) **|Ki|** and **|Kp|** while maintaining their ratio (rule of thumb). Please be aware that also the ‘**TimeConstant t**’ filter might need adjustments.

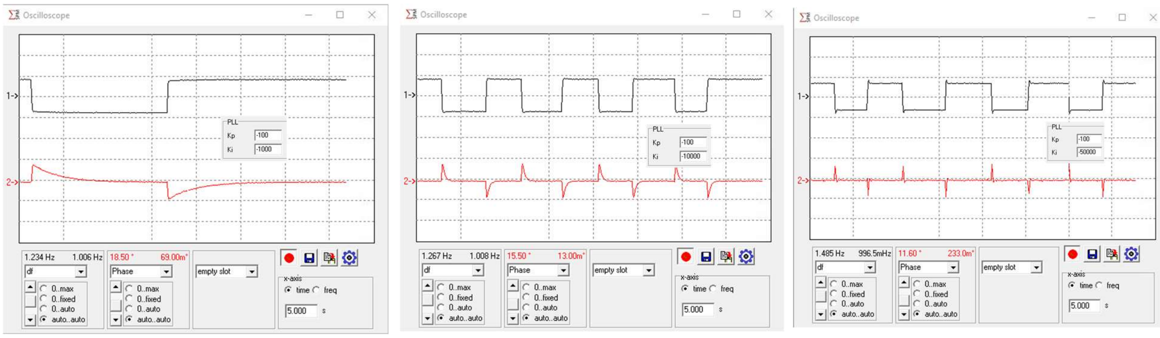


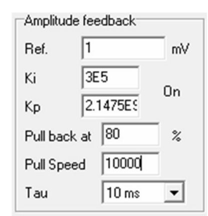
Fig. 13: Optimization of Ki at fixed Fp=-100. Left: slow adaption of phase for Ki=-1000, Center: reasonably fast phase decline at Ki=-10k, Right: Fast adaption of phase but overshooting for both phase and df at Ki=-50k.

> **Please note**: In FM NC-AFM the bandwidth of the demodulator (here: PLL) significantly determines the noise. In FM NC-AFM the phase noise and thus df noise more than linearly decreases with the reduction of the demodulation bandwidth. Of course, the scan speed needs to be adapted to the demodulation bandwidth.

> **Please note**: if for some reason the oscillation of the sensor collapses, e.g. due to a tip crash, the PLL can no longer lock to a certain frequency since no real phase is detectable. In this case typically the df drifts to arbitrary values and the drive significantly increases. To overcome this state retract the tip, reset '**Parameter→PLL→Ki, Kp**' to zero and back to the previous values. The PLL should now be locked again. Approach the tip at a different position at larger probe-sample separation (less negative df) since the surface area is likely damaged.

Tip Protection

- To protect the tip from crashing the tip protection continuously monitors the amplitude of the sensor (channel '**QPlusAmpl**'). If the amplitude falls below the given threshold 'Pull back at' (given in percent of the amplitude setpoint) then the tip will be retracted at speed '**Pull Speed**' (nm/s). Typical thresholds are 30%-80% (depending on noise and required sensitivity) and '**Pull Speed**' 10000 nm/s.
- To switch off the Tip Protection set '**Pull back at**' to 0%.



- **Please note**: the tip protection is not fast enough to avoid small tip crashes. However, it can prevent large dives of the probe into the surface for a longer time span, e.g. during unattended measurements.

Auto-approach and scanning in constant Δf-mode

- Once AFL and PLL are running and optimized the probe can be approached to the surface either in Auto-approach mode or, if already close to the surface, by enabling NC-AFM Δf-feedback.
- In the 'Mixed Mode' (STM and AFM topography feedback possible) switch the slider fully to the AFM side.
- Auto-approach: enter the Δf setpoint into the '**Parameter→Topography feedback→Ref.**' control. Typical values: QPlus -1Hz (1nm_{pp} amplitude) / Cantilever AFM -5Hz (10nm_{pp} amplitude).
- Leave '**Parameter→Topography feedback→Kp**' at zero (typically not used).

- '**Parameter→Topography feedback→Ki**' should be set to a value allowing the tip to cross the whole range of the z-scanner within ~5-10 seconds (rule of thumb). For a good signal-to-noise of df this is 1E6 to 2E6 at '**Parameter→Topography feedback→Ref.**' = -1Hz. The approach speed scales inversely proportional to the (negative) df setpoint and proportional to Ki.

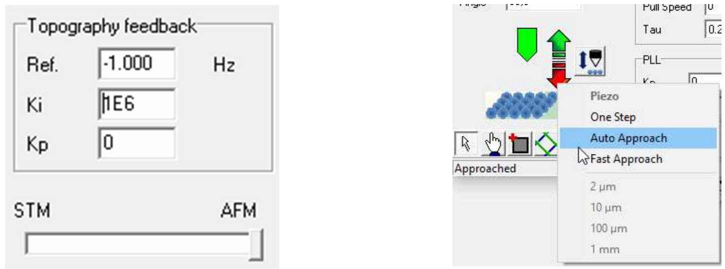
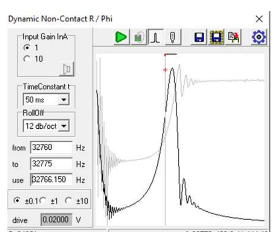


Fig 14: Typical Auto-Approach settings and start of auto-approach

- Initiate the Auto-approach by right-clicking to the red arrow of the tip z-position graphics (Fig.14) and selecting 'Auto-Approach'. Repeat if tip has moved to fully extended position. If the tip is already close enough just select 'Piezo' of the same menu.

> **Please note**: While the probe auto-approaches the surface please check for the '**df**' in the retracted state with the software oscilloscope. Sometimes changes in the mechanical coupling of the sensor during a coarse motor step might occur changing phase relation. In this case '**df**' does not return to zero if the tip is in retracted state. In this case a new resonance sweep and setup of the 'use' frequency is

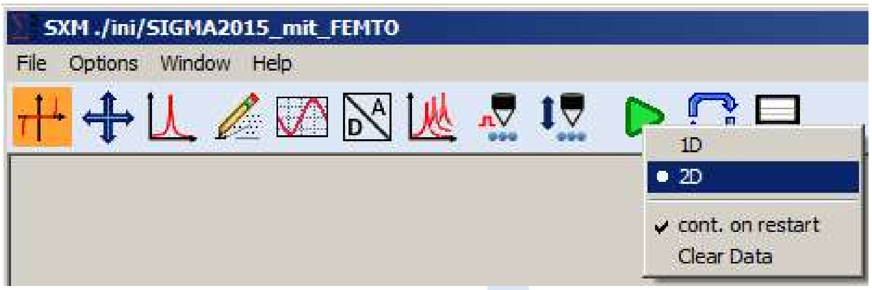
Troubleshooting:



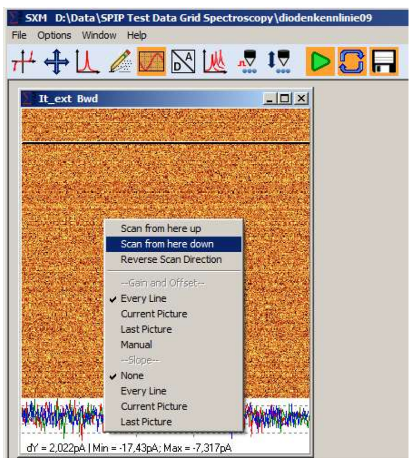
- Resonance Sweep: at starting frequency there is a residual decaying amplitude:
  - ⇒ Diagnosis: 'use' frequency is close to resonance. The sensor is excited and its amplitude is decaying while the sweep is started
  - ⇒ Solution: Set 'use' to an off-resonance frequency before starting the sweep.
- Resonance Sweep: the resonance curve has a lot of oscillations at its high frequency side. The resonance curve is shifted to higher frequency.
  - ⇒ Diagnosis: The sweep was performed too fast.
  - ⇒ Solution: Increase 'TimeConstant t' to a value matching the sensor's quality factor.
- Oscillating PLL: df is oscillating strongly even though Kp and Ki are set properly.
  - ⇒ Diagnosis: the phase detector time constant might be too large. It was not set to a shorter value after performing a resonance sweep
  - ⇒ Solution: shorten the time constant in the DNC window w/r to the PLL bandwidth (see section 7).

Starting data acquisition

- Before starting the scanning process, you can change the scan mode when you click with the right mouse button on the scan button of the Main Menu bar.
- The appearing window shows:
  - 1D line scan at the first or current line
  - 2D 2-dimensional scan
  - cont. on restart: when checked and you stop the scan, the scan restarts at the line at which it was stopped.



- Start the measurement (Scanning) by pressing in the Main Menu Bar. If both are pressed, the measurement (scan) is running continuously repeating.
- Once the measurement is started and data are displayed in the channel windows, the right button of the mouse can be used to click into the measurement channel window for several options:



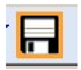
- **Scan from here up** and **Scan from here down:** *usage:* during the image acquisition or in order to start image acquisition *function:* uses the current mouse position to determine “here” and starts to scan from this position upwards or downwards. The function does not change or check the setting “cont. on restart”.
- **Reverse Scan direction:**

usage: during the image acquisition

function: changes the scan direction from downwards to upwards or vice versa.

- **Gain and Contrast:** changes the gain and the contrast of the used colour range during the scan. Maximum and minimum are taken automatically in *Every Line* or from the whole *Current Picture*. In case of *Current Picture*, all values available from the 1st scanned (might be the uppermost or the lowermost line in an image) to the currently scanned line (visualized with a black or yellow line) are evaluated. In case of *Last Picture*, maximum and minimum of the last acquired image are taken to calculate the contrast.
- **Slope:** subtracts either a linearly fitted line from each scan line (*Every Line*) or a fitted plane through the whole currently acquired image from the 1st to the currently scanned line (*Current Picture*). One can also use the calculated slope from the last image (*Last*

Picture) or disable the slope correction completely (*None*).

- Enable auto storing 
    - when the floppy disc icon is highlighted (hold “shift” and click simultaneously on the icon), all data are automatically stored:
        - scanning/imaging routine
        - atom manipulation results curve
        - spectroscopy results (point, line, grid)
    - when the floppy disc icon is not highlighted, single mouse click on this icon will store only imaging channels up to actual moment of scanning. All others (atom manipulation, spectroscopy, etc.) and also all future data of the image will not be stored, or must be stored individually.

Scripting

General Syntax

The general style is Pascal:

- There is no case sensitivity.
- The program starts with **begin** and stops at **end.**.
- **( )** - brackets are used in mathematical formulas.
- Strings are enclosed in **' '** (**" "** is also working).
- Decimal separator for floating point numbers is a point: "**.**".
- Each command is completed with a semicolon: "**;**".
- Available mathematical operations: **+ - * / ^**
- **Available mathematical functions: TAN, SIN, COS, ARCTAN, SGN, ABS, LN, LOG, SQRT, SQR ..**
- Available relational operations: **= > < <>**

Variables & Assignments

Variables up to 8 characters long. The data format of all variables is real.

Example for variable usage: **A := A + 1.2;**

Command Overview

Command	Meaning
Beep	Play a sound
ClrScr	Deletes the visible data on the data screen
CCDScan	Takes a spectrum with the optical spectrometer Spec64
DNCPara(n,*v*)	Sets the n-th parameter of the DNC window to the value *v*
DNCStart	Record a Frequency Spectrum
Execute('filename')	Executes another script *./script/filename.scr*
FeedPara('*t*', *v*)	Sets the parameter *t* for the feedback to the value *v*
FileName ('name1')	Defines the name of the data storage file as ./data/*name1.txt*
for .. to .. begin	Loop definition
GetChannel (*Ch*)	Acquires data from output or input channels of the software
GetFeedPara(*v*)	Gets the value of the feedback parameter *v* and stores it in the variable c
GetScanPara(p)	Get the parameters of the scan parameter window
Goto *marke*	Jumps to the position *marke* defined as Label
GoXY(x,y)	Moves tip to a position inside the current scan range
if .. then	Condition
Move(dir,dist)	Uses the current coarse positioning settings to move sample/ tip
MLockin	Controls the Multi-Lockin Window
ScanPara(p,*v*)	Sets the parameter p in the ScanParameter window to the value *v*
ScanImage	Starts to acquire an image

ScanLine(*Nr*)	Scan *Nr* lines
SetChannel(*Ch, v*)	Sets an output channel number *Ch* to a value *v*
SetHardChannel(a, v)	Writes to Address a the value v
SetLaser( )	Switches the laser On or Off
SpectPara(n,v)	Sets parameter n for the spectrum acquisition to the value v
SpectStart	Starts to acquire and save a spectrum with current settings.
TipCond(type, val)	Tip Conditioning
VPulse()	Voltage Pulse
Wait(t)	Waits for a time t in seconds
Writeln('text',..)	Displays text in the Memo

Commands (alphabetical)

Beep

Example: Beep**;**

ClrSrc

deletes all visible data on the memo.
Example: **ClrSrc;**

CCDScan

takes a spectrum with the attached spectrometer with the current spectrometer settings
Example:
GoXY(0.5,0.5); // Moves to middle of the scan range
CCDScan; // Takes a spectrum

DNCPara (n, value) command

Set the n-th parameter of the DNC window to the value
Parameters: **n:** number of the parameter (1 … 8)
or "AUTOSAVE", INPUTGAIN
value: real
Assigment:

n <-->	**Meaning**
1	Start Frequency
2	Stop Frequency
3	Use Frequency
4	Drive Amplitude
5	Bandwidth Button (On = 1 /off = 0)
6 & 7	TimeConst., RollOff used if Bandwidth button is ON
8	Thermal Noise Button (On = 1 /off = 0)

Example:
DNCPara(3,100); → sets the used frequency to 100
DNCPara('INPUTGAIN', 10);

Attention: The values are overtaken in the currently selected physical unit. If the unit of frequency is set to "kHz", then **DNCPara(3,10);**results in 10.000,00 Hz. If the unit is set to "Hz", then **DNCPara(3,10);** results in 10,00 Hz.

Execute (scriptfilename)

Calls and executes another script file.

Parameters: **scriptfilename:** string

Example:

Execute('Ref-HOPG'); → calls the script " *./scipts/Ref-HOPG.scr* ".

FeedPara ('type', value)

Sets parameters for the feedback system.

Parameters: **type:** string from list
allowed values: Ref, Ki, Kp, Bias, Flyheight ,
enable, preamp, ref2, ki2, kp2, mode, Ratio, BiasDiv
and zOffset, zOffsetSlew, enable from the zControl Window
value: real

Example:

FeedPara('Ki',100); → sets Ki in the parameter window to 100

FileName (YourFileName)

defines a file name for the log file, which collects all data during one script run.
If no file name is defined in the script, the system writes its messages into a file *NoName.txt*. With each run of the script, old data in NoName.txt are deleted.
If a file name is defined, the file name given by the user is extended automatically by the system with a number representing current date and time (date-time-string), so that the log file is *YourName_DateTime.txt*. Thus, the user does not need to rename its file in the script for every run.

Parameters: **YourFileName :** string → file is *./data/YourFileName_DateTime.txt*

Example: **FileName('t3');** → the data are written to *./data/t3_xxxxxxxx.txt*

for start counter to stop counter do begin command(s) end;

Loop definition based on an integer counter. The commands **do begin** and **end** are always required, even if there is one program line in between, only.

Example (measures 20 points along a line in x-direction):

```
X:=100;
for i:=1 to 20 do begin
  Move('CX',X);
end;
```

GetFeedPara ('type')

Gets parameters from the feedback system.

Parameters: **type:** string from list of values: Ref, Ki, Kp, Bias, Flyheight
result: real number

Example:

c:=GetFeedPara('Ki'); Writeln(c);
→ writes the value of Ki on the screen

GetChannel (Address)

Acquires the data of one A/D input channel or, if negative, the content of the Mirror Memory for the corresponding DAC

Parameters: **Address:** integer

for the A/D-Channels, the Address can found in /Options/Scale/ADC as Port. Here, "32" stands for the 1st ADC-channel (e.g. "T-B" for AFM). To get data from the D/A-channels, one chooses negative channel numbers. E.g, "0" equals the channel "Z" and "-1" the channel "Bias".

Example: **c:=GetChannel(32);**→ reads the input data of the channel AD1
c:=GetChannel(-1);→ reads the bias output provided at DAC 1

GetScanPara('para')

Returns the currently set scan parameters.

Parameters: **para:** string from list of values: Range, Speed, Pixel, X, Y, Angle, SlopeX, SlopeY, LineNr, 1D, AspectRatio, PixelDensity, DriftX, DriftY, Scan, Autosave

result: real number

Example: **c:=GetScanPara('scan'); → returns status of scan, 0 = scan off, 1 = scan on**
Writeln(c); → writes status to screen

Goto marke

Allows to jump to a *marke*. It requires:

- the definition of a label with a **LABEL** statement
- a **Goto** command followed by the labels name
- the label followed by a colon

Labels always start with a character..

Example:

```
LABEL foo, exit;
begin
foo:
 GetChannel(32);
 if c > 1000 then Goto foo;
exit: writeln('Done.');
end.
```

GoXY (x_rel, y_rel)

Moves the tip to the relative positions “x-rel” and “y_rel” inside the currently given scan range. The upper left corner of the image equals (0,0), while the lower right corner is (1,1).

Parameters: **x_rel, y_rel**: real numbers between 0 and 1

Example: **GoXY(0.5,0.5);**→ moves the tip to image center
GoXY(0.1,0.1);→ moves tip to a point close to the upper left corner

if condition then command

Evaluation of conditions. ELSE is not supported. Implementation is not fully Pascal compliant.

Example:

```
if c < -160 then writeln('Channel X =', c);
```

Note: Starting from version 28.8, **begin** and **end** are supported in order to apply several commands after the condition.

Move ('direction', distance)

Allows to operate the coarse positioning system, to set the center position for whole images and to address the functions behind the approach button and retract button in the parameter window. Latter are addressed by their number in the item list, that appears with the right mouse button.

Parameters: **direction** : string from list:
allowed string values: cx, cy, cz, x, y, retract, approach
distance : real → value in physical units or steps

Examples: **Move('CX',10);** → moves the stepper 10 steps in x-direction

Move('Y',-1.5); → sets the center position to -1.5 µm
Move('Approach',2); → starts automated appraoch
Move('Retract',0); → retracts the piezo, only

MLockin ('type',value)   SW.Ver. > 28.7

Control the Multi Channel Lockin Window.
Parameters: **type** : Component Name as string

Examples: **MLockin ('Edit1', 1000);** → Lia1 Frequency = 1000

Note: Visualization of components names is given on page **Error! Bookmark not defined.**.

ScanPara ('type',value)

allows to set scan parameters in the window "Parameter". With the type 'Autosave', the knob 'Autosave' for the image acquisition is toggled.
Parameters: **type** : string from list:
allowed string: range, speed, pixel, x,y, angle, linenr, autosave, aspectratio, pixeldensity, slope, slopex, slopey, 1D, scan, driftx, drifty or the component Name
value : real → value in physical units
→ or index for Combo-Boxes start with counting at 0
Examples: **ScanPara('Speed', 1.5);** → line speed set to 1.5 lines/s
ScanPara('X', -0.5); → image center X set to -0.5 µm
ScanPara('Autosave', 1); → switches automated save on
ScanPara('Pixel', 2); → 3th entry in drop down list => 128
ScanPara('Edit24', 12);→ Ki for Ampl.-Feedback to 12

Note: More parameters can be called by their component names as described on page **Error! Bookmark not defined.Error! Bookmark not defined.**.

ScanImage

Starts the acquisition of an image. When two or more images need to be acquired, this command has to be repeated.
Example: **ScanImage;** → starts to acquire a whole image

ScanLine (Number)

Starts the scan of Number lines with the current settings. If the scan mode is "2D", it starts to scan a number of lines in an image at the current scan position. If the scan mode is "1D" and "cont. on restart" is off, it scans the 1st line of an image. In "1D" with "cont. on restart" off, it scans the same line (number) times at the current position.
Example: **StartLine(10);** → starts to acquire 10 lines with the current settings

SetLaser(value)

Switches the laser on or off.
Example: **SetLaser(0); Wait(1); SetLaser(1);**
→ switches the laser off for 1 second

SetChannel(channelnumber, value)

Sets the output of an I/O channel to the value given as "v".

Parameters: **channelnumber:** integer
value: real

SetChannel is possible for D/A-channels only. In order to set a value of a D/A-channel, one chooses a (positive) channel number in contrast to GetChannel. E.g, "0" equals the channel "Z" and "1" the channel "Bias".

Example: **c:=GetChannel(0);**→ reads the position of z
SetChannel(0,c+0.1);→ set the position of z 0.1 nm higher
SetChannel(1,-0.6);→ set the Bias at DAC1 to -0.6 V

Note: Physical unit and Scaling are set in /Options/Scale/DAC

SpectPara (Parameter, value)

allows to set parameter in the window "spectroscopy". With *Parameter as* 'Autosave', the knob 'Autosave' in the spectroscopy window can be set. When data are saved automatically, they are saved numbered in the directory ./data/.. In order to find out which data equal which setting, the complete path of the saved file is written into the log file (*NoName.txt* or *YourName_DateTime.txt*).

Parameters: Parameter: number or string
number=0 type of spectrum from the drop down list
number>0 Number of the Edit Box
Strings 'AUTOSAVE', 'POINTS', 'REPEAT'

Examples: **SpectPara(0,0);**→ sets the type to 1st index → "X(z)"
SpectPara(5,50); → sets the distance dz to 50
SpectPara('autosave', 0); → AutoSave off
SpectPara('autosave', 1); → AutoSave on

SpectStart

Starts a spectroscopy data acquisition with the current settings.

Example: **SpectStart;** → starts a spectrum with current settings

TipCond(type, val)

Type: BIAS, TIME, DIVE MODE DO

Example: **TipCond('Bias', 10);**
TipCond('Do', 0); → start

Vpulse (PulseTime, Bias);

Change the Bias-Voltage for "Time" to "Bias"

Example: **VPulse(1.0, 2);**

Note: **Physical unit is set in /Options/Scale/DAC**

Wait (time)

Allows to pause the operation a time given in seconds.

Parameters: **time** : real

Example: **Wait(1.5);** → waits for 1.5 seconds

Writeln ('text1', variable, 'text2', variable2 ...)

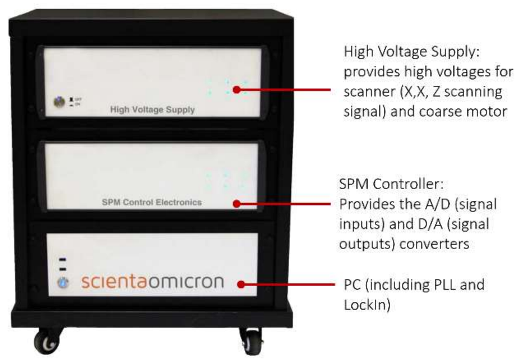
Allows to write additional information in the memo and to the log file (*NoName.txt* or

YourName_DateTime.txt) simultaneously. In the brackets, a series of strings, variables and numbers can be written, which are separated by commas. Strings should be enclosed in **' '**.

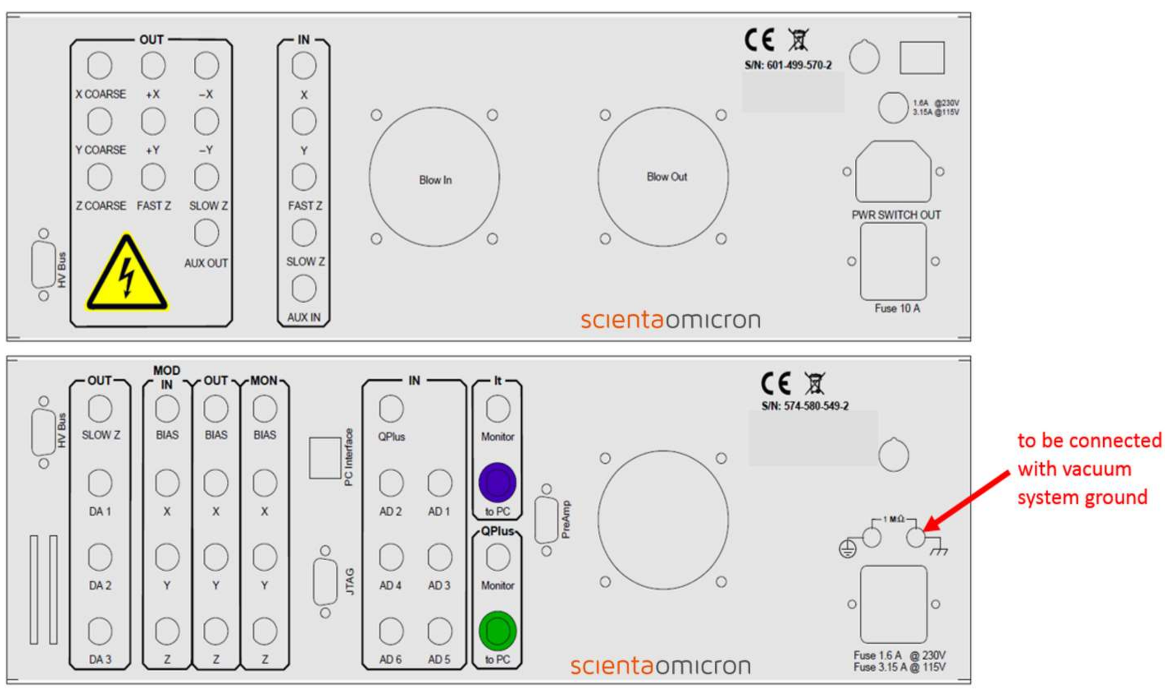
Parameters:	**text1, text2 :** string; **variable1, variable2** : real
Example:	**a := 5 ;** → sets the value of the variable *a* to 5
	writeln('a=', a); → writes “a = 5” in the Memo

The Hardware Electronics

The hardware of the SXM controller consists of 3 main building blocks, i) the PC with software and Lockin/PLL module, ii) the SPM controller and iii) the high voltage amplifiers.



Apart from the coarse signals where high voltage BNC connectors are used, all other signals are easily accessible via BNC connectors.

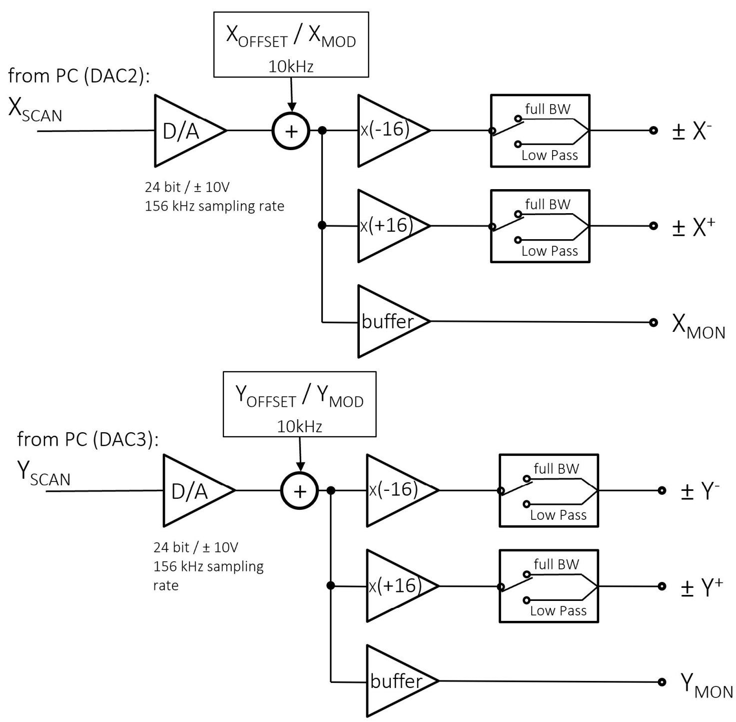


Block diagram: Outputs

High Voltage Signals for STM

The low voltage signals from the outputs of the SPM controller (24bit, +/- 10V) and added offset/modulation (if used) are linked via BNC cables to the input of the high voltage amplifier. The high voltage amplifiers with a gain of +/- 16 amplifies the scanning signals to maximum +/- 160 Volts. The high voltage amplifier is equipped with a low pass filter to reduce the noise for high resolution qPlus imaging. The low pass filter can be activated by the SXM software (options\scanner\power ➔ chose "active" for full bandwidth or "low BW" for reduced bandwidth).

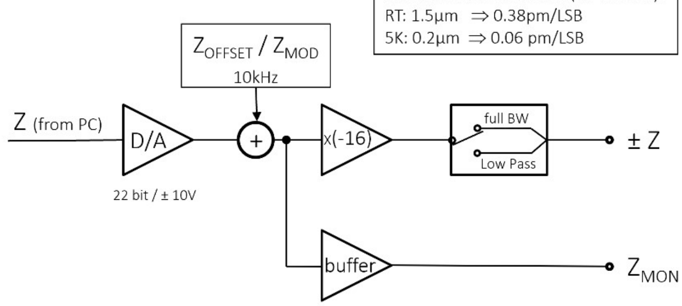
X- and Y- signal for scanning:



Resolution for Scan (for TRIBUS):
RT: 10µm x 10µm ⇒ 0.59 pm/LSB
5K: 1.8µm x 1.8µm ⇒ 0.107 pm/LSB

Z-signal for scanning:

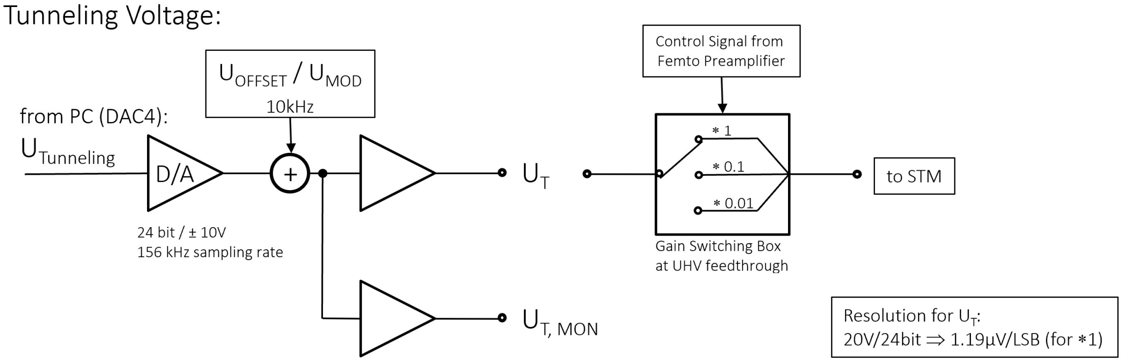
Bit-Resolution for Z-Scan (for TRIBUS):
RT: 1.5µm ⇒ 0.38pm/LSB
5K: 0.2µm ⇒ 0.06 pm/LSB



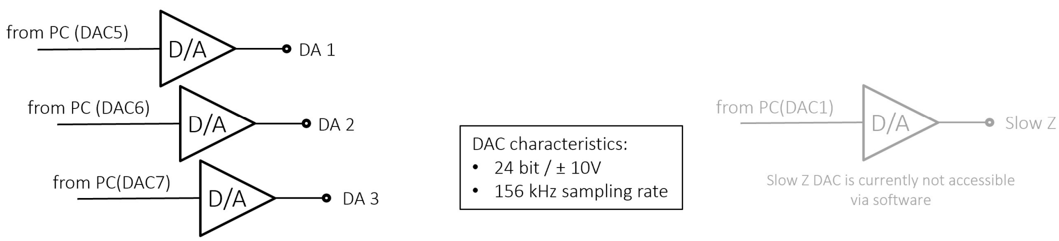
Low Voltage Signals for STM:

The bias voltage is provided by a 24bit D/A converter. The maximum voltages are +/- 10 Volts. To improve the signal to noise ratio for tunneling spectroscopy a voltage divider is placed directly at the BNV feedthrough of the instrument. The voltage divider offers in total 3 voltage ranges: i) +/- 10V, +/- 1V and +/- 100mV that can be set in the SXM measurement software.

Tunneling Voltage:



3 further DACs for free use (plus Slow Z):



Wiring

Wiring of STM (STREAM, INFINITY or POLAR)

The SXM controller needs to be connected to the SPM. The controller provides all signals for SPM operation. For the measurement regulation of the SPM temperature, a temperature controller (Lakeshore, typ. LS325) needs to be connected to the corresponding feedthrough at the SPM base flange.

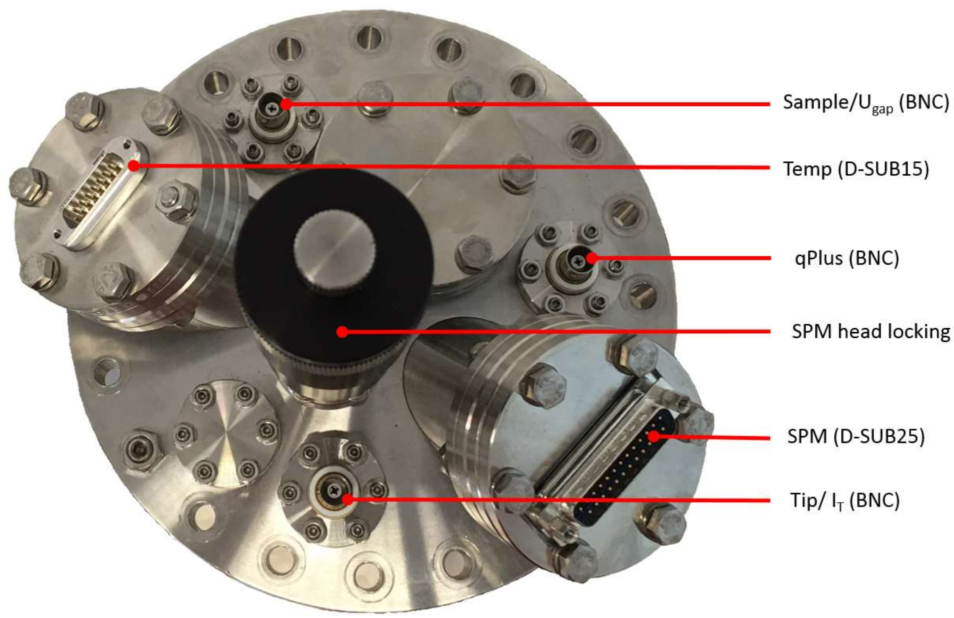


Figure: As an example, the above picture shows a birds eye view of the INFINITY SPM base flange. Apart from the wobble stick, all interactions with the instrument take place on the top of the instrument (e.g. head clamping, cable connections)

Please follow the next steps to connect the cables to the instrument:

- Remove at first the short circuit plugs (grounding plugs) from the feedthroughs.

> ***Attention:***
> ***The grounding plugs must be connected during UHV baking of instrument or if the instrument is cooled down without a connected SXM controller.*** *They are important to ensure that the voltage that is produced by compression/expansion of the piezos due to a change of temperature will be eliminated by grounding the piezos.* Otherwise, the high voltage amplifiers of the SXM electronics can be destroyed.

- Make sure that the SXM controller is switched off

- Connect the cables accordingly to Figure, see below

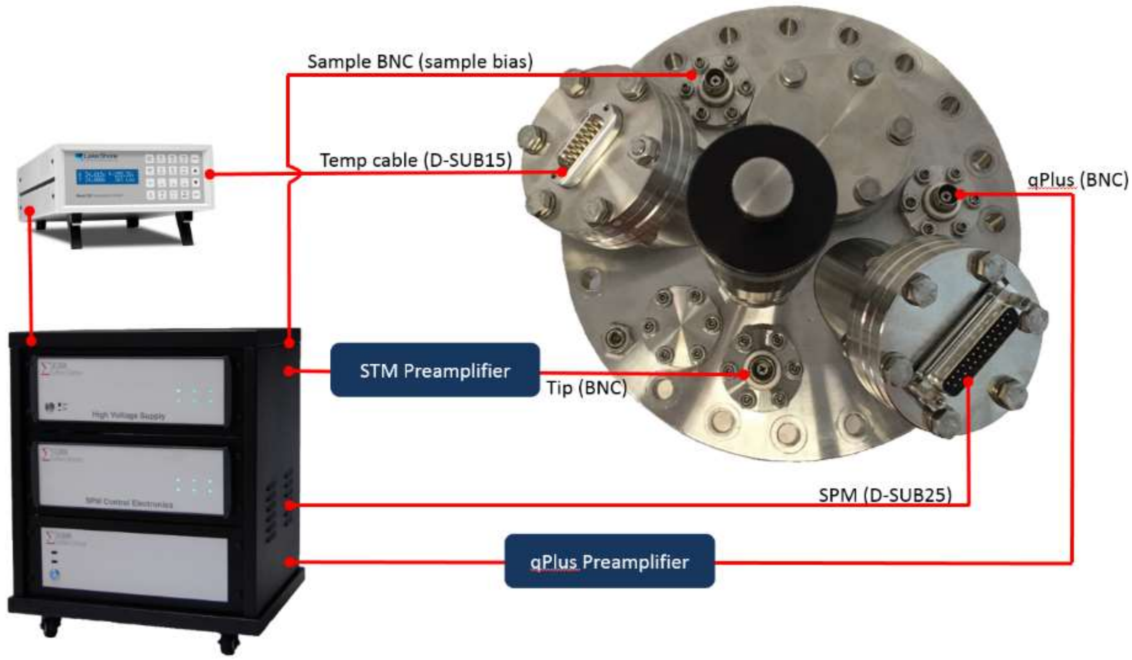


Figure: Schematic wiring of the INFINITY SPM

Wiring for SPM measurement:

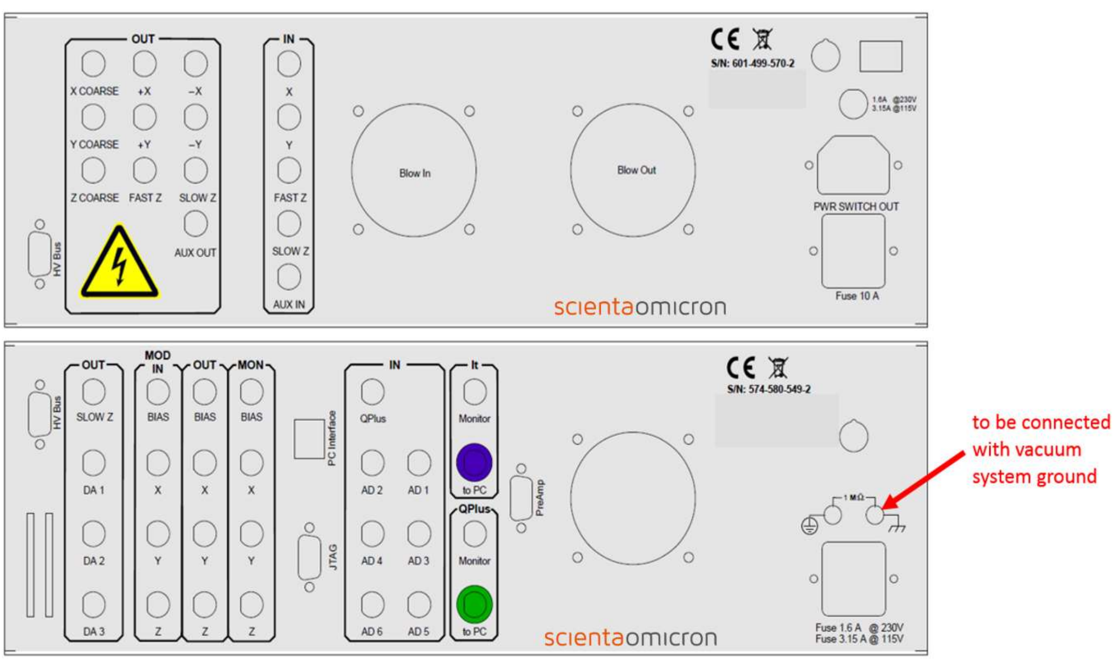
Signal	Connector at the SXM controller	Cable	To be connected to the following feedthrough
Tunneling Voltage	BNC connector “OUT / BIAS”	Single BNC cable (3m)	Floating BNC, sample (or tip)
Tunneling Current	Mixed-D-Sub connector “PreAmp”	STM-preamplifier	Floating BNC, tip (or sample)
Scan Signal X+	BNC connector “OUT / +X”	SPM Cable, pin: X+	“SPM D-SUB25”
Scan Signal X-	BNC connector “OUT / -X”	SPM Cable, pin: X-	“SPM D-SUB25”
Scan Signal Y+	BNC connector “OUT / +Y”	SPM Cable, pin: Y+	“SPM D-SUB25”
Scan Signal Y-	BNC connector “OUT / -Y”	SPM Cable, pin: Y-	“SPM D-SUB25”
Scan Signal Z	BNC connector “OUT / FAST Z”	SPM Cable, pin: Z	“SPM D-SUB25”
Coarse X	High Voltage BNC “OUT / X COARSE”	SPM Cable, pin: Xc	“SPM D-SUB25”
Coarse Y	High Voltage BNC “OUT / Y COARSE”	SPM Cable, pin: Yc	“SPM D-SUB25”
Coarse Z	High Voltage BNC “OUT / Z COARSE”	SPM Cable, pin: Zc	“SPM D-SUB25”
Excitation	Ref. A (red BNC)	SPM Cable, pin: R	“SPM D-SUB25”

Optional Signals:			
qPlus Signal	InA (blue BNC)	qPlus preamplifier	Floating BNC, qPlus
Sample 1-10	e.g. DA1-DA3 or AD1-AD6 of the SXM controller or to be connected to third party equipment	SPM Cable-10, pins: S1-S10	Please ground all contacts that are not in use
The SPM control electronics need to get its power (220V) from the UHV system electronics rack to avoid any ground loops and related 50 Hz noise.			

Wiring for Temperature Measurement:

Signal	Connector at the Temperature Controller, LS 325	Cable	Cable to be connected with the following feedthrough
Si diode 1	Input A	Temp Cable, pins: 1, 2, 9, 10	“Temp D-SUB15”
Si diode 2	Input B	Temp Cable, pins: 3, 4, 11, 12	“Temp D-SUB15”
Pt thermometer	Input A or Input B	Temp Cable, pins: 5, 6, 13, 14	“Temp D-SUB15”
The temperature controller need to get its power (220V) from the SPM electronics rack to avoid any ground loops and related 50Hz noise.			

Figure: Backplane of the SXM electronics: High Voltage Amplifier Unit (top) and SPM Controller with A/D and D/A converters (bottom)



Wiring of STM (VT- or LT STM)