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Open Source Scanning Probe Microscopy Control Software Package Gxsm

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(Dated: October 13, 2009)

Gxsm is a full featured and modern scanning probe microscopy (SPM) software. It can be used for powerful multidimensional image/data processing, analysis, and visualization. Connected to an instrument, it is operating many different flavors of SPM, e.g., scanning tunneling microscopy (STM) and atomic force microscopy (AFM) or in general two-dimensional multi channel data acquisition instruments. The Gxsm core can handle different data types, e.g., integer and floating point numbers. An easily extendable plug-in architecture provides many image analysis and manipulation functions. A digital signal processor (DSP) subsystem runs the feedback loop, generates the scanning signals and acquires the data during SPM measurements. The programmable Gxsm vector probe engine performs virtually any thinkable spectroscopy and manipulation task, such as scanning tunneling spectroscopy (STS) or tip formation.

The Gxsm software is released under the GNU general public license (GPL) and can be obtained via the Internet.

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I. INTRODUCTION AND OVERVIEW

The development of the scanning tunneling microscope (STM) [1, 2] provided scientists with a versatile tool to image, spectroscopically analyze and manipulate atoms and molecules on surfaces at length scales from ∼100 μm down to the atomic scale. Due to the tremendous potential of scanning probe microscopy (SPM) many different SPM techniques and instruments like the STM and the atomic force microscope (AFM) were developed in the last 30 years[3, 4]. Nowadays, SPM is widely used and belongs to the standard experimental techniques in many different research fields, starting from basic surface science where it is originated, surface chemistry to biology. Especially the potential of local spectroscopic measurements and manipulations on atomic scale was and is still discovered by many research groups. There is a very broad range of different types of spectroscopy and manipulation methods existing and only a few commercial SPM control and software solutions are addressing these needs in a universal way and all of them are build on top of special instruments and hardware solutions. Furthermore, for most systems the source code is not available as open source. Therefore, the extension of these software packages by their users to special dedicated tasks is very limited if not impossible.

Previous publications on various special and universal SPM control hardware cover computer controlled analog or digital feedback loops[5–8] and are demonstrative, but less available (mostly home made hardware) to the scientist as they are not maintained nor supported like Gxsm is.

This paper presents the major updates and new developments of the Gxsm software project and will focus on the new data acquisition and control design and new features since the first publication[9].

In 2003 support for a commercially available completely new digital signal processor (DSP) platform "SignalRanger" [10] (SR) with USB interface was started. At this point a new fully modular Hardware Interface plug-in (HwI) was designed and the HwI for the new platform was created. A fourth generation of DSP code design was put into place. This new design of a low level real time and multitask capable data processing DSP code allows simultaneous scanning, probing (spectroscopy, etc.) or changing of almost every parameter at any time.

Later the invention of the generic Vector-Probe (VP)

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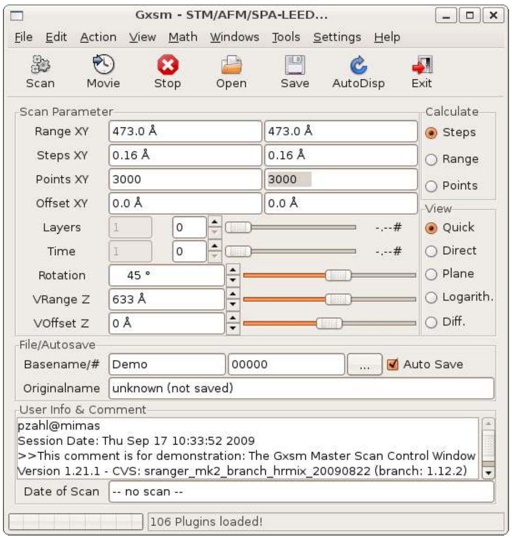

FIG. 1: Screenshot of the Gxsm main control window, only one of many available control windows. Check the Gxsm Home page for more screen shots of "Gxsm in action"[13].

engine took place, a novel approach to spectroscopic measurements and manipulations. This engine allows to perform almost every imaginable spectroscopic measurement or manipulation in real time without the need for low level programming.

Also the vector scan generator and data acquisition engine and data transfer was redesigned for maximum of efficiency and universality. The DSP is now running a full frame scan in real time with zero time loss in between lines for any data transfers, as data is continuously streamed via a FIFO (First In First Out) background task. Also all user interactions with the DSP and scan generator are instant, no delays, no waits for finishing lines, scan start/stop is possible at any time, instantly.

Most recently in 2009, the next generation DSP "SignalRanger-Mark2 (SR-MK2)" with a specifically for SPM and in particular for this project optimized digital to analog and analog to digital interface "SR2-A810" became reality[10, 11] and will be discussed in this paper.

It takes over all the exact same well established DSP software and HwI design to a new hardware providing all known features but delivers over three times of the old SR[12] performance combined with a high precision data conversion and up to 150 kHz sampling rate and USB-2.0 interface – compared to 22 kHz of the old SR with USB-1.0.

This new highly for SPM optimized and very affordable DSP based SPM control and data acquisition hardware solution is suitable for basically all home-made SPM, especially new prototypes intended to invent new modes of operation, where the development of a complete new software system from scratch would be too expensive and time consuming. But it also can replace several commercial systems if there is a need for extended flexibility or functionality.

Today the Gxsm project and design looks back on over 10 years of expertise in using DSPs for SPM control and data handling. It keeps serving the SPM community with a modern and flexible SPM control and data analysis software, which is not limited to SPM data at all.

Since Gxsm is licensed under the GNU general public license (GPL) the full source code is published and everyone is allowed to use and modify the software package for his own needs, not excluding the DSP code. Since over nine years it resides at the Open Source Development Network[13] "sourceforge.net" as "Gxsm" project. Public online help and discussion forums are available. For convenience a Ubuntu based Linux distribution can be downloaded from [14] which includes the Gxsm binaries as well as the source code for further development. The distribution can even run in a live mode without installation on a host PC.

II. THE GXSM ARCHITECTURE

The Gxsm system core provides a highly efficient multidimensional data management module with no software size limits of scans – you can get image sizes up to your hardware (DSP/Analog) capabilities. It allows to store any native scalar numbers (8-bit to 64-bit integers and floating point numbers up to double precision). Natively, two dimensional data are handled as (simple) images, but the core supports up to four dimensions, i.e. stacks of layered images in time. A data access module allows to extract or manipulate data. It can deliver interpolated or averaged data of selected regions, generate cuts in any dimension, copy and rearrange or convert data. Also any number of arbitrary extra data sets, including notes or spectroscopic data, can be attached to any position within this main data set. The universal NetCDF[15] data file format remains the Gxsm native data storage back end and still is compatible with all versions.

Multidimensional data visualization functionality is implemented in the Gxsm core[9]. Further analysis functionality as data filtering, basic math, statistical data extraction and data exchange with other formats is provided via plug-ins. This plug-in interface enables users to write their own plug-ins and thus add functionality they need. We encourage users to share these with the Gxsm user community.

The HwI plug-in provides all hardware specific interfacing and special instrument controls. Thus it decouples the Gxsm core fully from any specific hardware and allows to develop support for other than SR based SPM controls independently.

For example: Recently a Gxsm HwI plug-in was developed by M. Carla (see G. Aloisi et al[16, 17]) to add support their Real-Time Linux Kernel powered "feedback control loop of a scanning probe microscope", which was so far missing a dedicated graphical user interface.

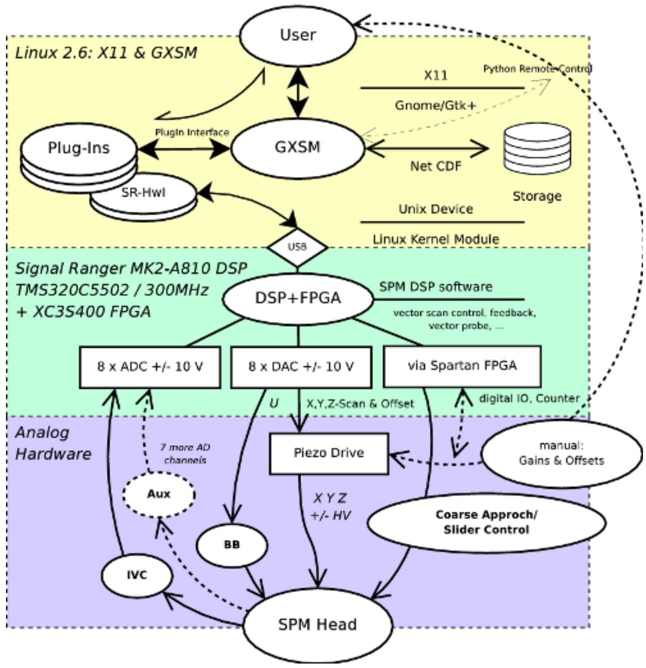

FIG. 2: Schematic diagram of a typical SPM control system using Gxsm and the SignalRanger MK2-A810 DSP: The SPM user interacts with the SPM via the Gxsm software using the X11 window system. A Gxsm HwI plugin sends and receives data via a Unix device, which is managed by a hardware dependent Linux kernel module. This module moves data via the Universal Serial Bus (USB-2.0) to and from the DSP subsystem. This makes Gxsm independent of any hardware, as only the SignalRanger specific HwI plugin talks to the low level hardware and feed data into the Gxsm to manage it further. The MK2-A810 is build around a TMS320C5502 DSP which is interfaced to an XC3S400 FPGA. This FPGA manages digital IO, two 32bit counters and the digital to analog interface which provides 8× high precision Analog Digital Converters (ADC) and 8× Digital Analog Converters (DAC) with each full 16 bits resolution, low drift, low loop delay (in/out) at data conversion rates up to 150 kHz. The bias voltage is passed via a bias buffer/filter (BB) to the SPM. The DSP runs a SPM specialized software. The SPM head/piezo tube(s) are connected to a piezo drive, which provides the needed symmetric $\pm X$, $\pm Y$ and Z voltages at various gains (typically 1×, ..., 20×) to match the needes scan ranges. Analog signal sources (e.g. tunneling current, amplified via a current voltage converter (IVC) and auxiliary (AUX) signals) are connected to the analog input(s). The digital ports are available for a slider control or other optional purposes. Also two independent counter/timer channels are realized.

A. The Gxsm SPM control architecture

Fig. 2 shows all components of a typical SPM configuration using the Gxsm system.

User interacts via the X11 windows system with Gxsm and its plug-ins, both makes use of the Gnome/Gtk+[18] graphical user interface library.

Efficient and fast handling of multidimensional data is the main task of the Gxsm core. The details about the capability to handle basically unlimited amounts of data in up to four dimensions and powerfull visualisation tools are are not discussed here, but online and within the Gxsm Manual [13, 19].

A special new type of plug-in is the HwI plug-in. There can be multiple HwI plugins existing, but only one (or none) can be loaded at Gxsm startup to connect to a given SPM (or similar) hardware.

The HwI has to provide all essential hardware control functions and feed the data to the Gxsm core. Also all hardware specific user interface modules are implemented at plugin level (see II B).

The hardware, here the Signal Ranger MK2-A810 DSP Board, does all real time work, feedback, scanning, probing, data pre-processing, digital to analog (DAC) and analog to digital (ADC) conversions and also provides a 16 bit wide interface of generic programmable digital inputs/outputs (GPIO) plus digital inputs for two independent high-resolution, hardware (FPGA) gated counter channels of 32 bits each (16 bits on the FPGA, increased to 32 bits on DSP software level, can be increased further to any width in software), both with quadrature input option.

The real time DSP system then connects via analog and optional digital IO to the SPM head. A low noise 5-channel $(\pm X, \pm Y, Z)$ Piezo Voltage Amplifier "Piezo Drive" [20] with analog offset inputs and manual 10-turn offset contol knobs and manual or computer controlled gains is used to drive commonly used PZT type segmented piezo tube scanners. Selectable gains are ranging from 1× to 20× as required for typical PZT scanner piezos (± 200 V). It also provides a selectable bandwidth limiter/low pass filter for all channels (1kHz, 10kHz, 50kHz).

The bias voltage is feed via a buffer/amplifier/filter to ths SPM head.

A current to voltage amplifier[21] is used to pick up the tunneling current if the feedback loop is running on a tunneling junction in STM mode. In this case, the default logarithmic linearization of the input signal is done by the DSP. Otherwise a linear mode can be selected for non tunneling feedback signals as commonly used for AFM.

For coarse motion and automatic tip approach several, modes are supported. Especially XY-piezo inertia driven motions used by "Mover" (Besocke/Beetle)[22] type SPMs are supported. But also digital IO can be used to drive external motor controls. A Python[23] scripting interface allows to implement additional custom approach variants.

B. Hardware Interface plugin for SignalRanger DSP

The Hardware Interface plug-in (HwI) implements the basic set of methods required by the fully abstracted hardware base class defined by Gxsm and thus providing basic SPM control user interfaces and scan functional-

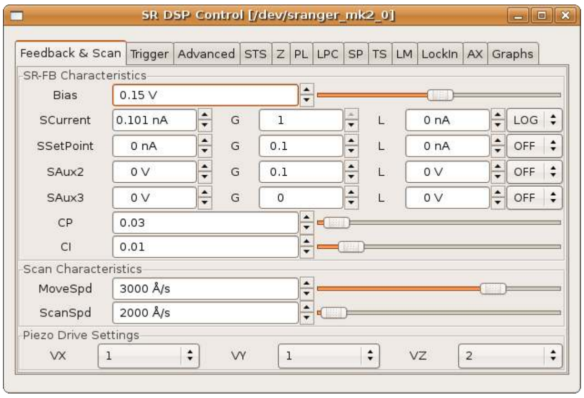

FIG. 3: Screenshot of the Signal Ranger HwI control window, feedback folder selected. The other folders are for "Trigger" (Trigger parameter changes while scanning), "Advanced" (IIR filter configuration, Raster Vector Probe setup and expert scan settings), "STS" (ordinary I/V spectroscopy with option for gap (Z) adjustments, repetitions, multi-position probes, etc.), "Z" (vertical manipulation), "PL" (generate bias/Z pulses for tip forming, etc.), "LPC, SP" (custom user modes), "TS" (Time Spectrum), "LM" (Lateral Manipulation), "LockIn" (DSP LockIn amplifier settings), "AX" (Auxiliary data collection, i.e. from a spectrometer via the counter channel). Via "Graphs" the user defines which data should be collected and how to plot it.

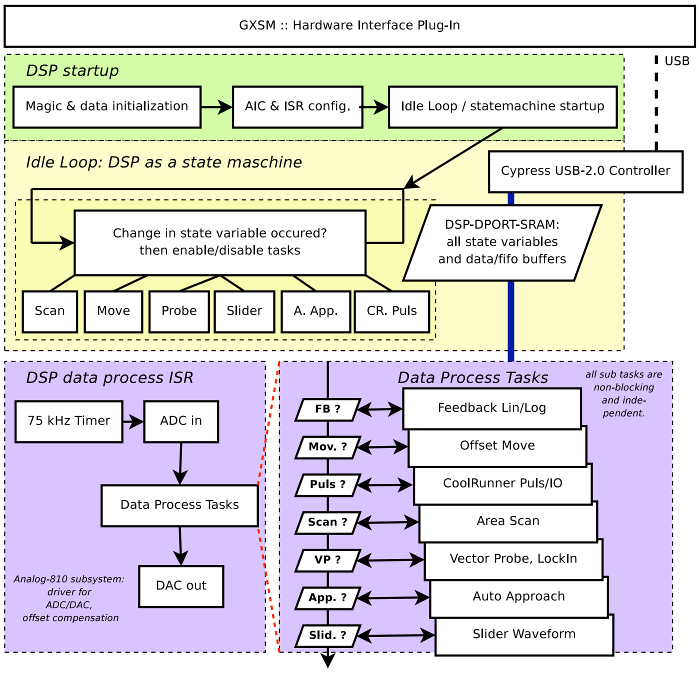

FIG. 4: Schematic diagram of the DSP code topology: Startup section configures the DSP system, sets up timers for data processing interrupt subroutine (ISR) and enters the never ending idle loop, which implements a state machine.

ity to the whole Gxsm system. Any further more specialized task or management of DSP interactions, like feedback controls, scan speed or spectroscopy, has to be implemented by the HwI including the Graphical User Interface (GUI). This allows a maximum of flexibility in supporting any hardware and instrument by just adding a HwI for it. Every HwI plug-in can be set up to automatically store additional parameters into the NetCDF data file at the time of data file saving.

The Signal Ranger HwI implements the methods to interact with the Signal Ranger DSP subsystem. It is responsible for setting all parameters and data streaming. For the users the controls are presented within one control window as shown in Fig. 3, ordered by tasks and separated into folders for feedback and scan control (as shown here).

In addition to standard SPM functions such as setting the bias voltage and I/V-spectroscopy, the HwI plug-in also provides several advanced functions. For instance, Gxsm is able to perform automatic spectroscopic measurements during scanning (raster vector probe) and scan parameters can be changed automatically when passing given positions during scans (trigger function). For sample and tip manipulation, Gxsm supports modes for lateral and vertical manipulation of atoms or molecules as well as voltage pulses that can also be used for tip forming. A full description of available features can be found in the Gxsm manual and on the web site[13].

Its open design allows users to add their own custom designed "probe" or "manipulation" tasks simply by adding a new tab to enter the desired boundary conditions from which the DSP vector probe table is generated to set up the custom mode (refer to section III B).

III. DSP SOFTWARE DESIGN FOR SIGNAL RANGER

The design of the DSP program is similar to a state machine. The state engine is implemented as "idle loop" as shown in Fig. 4. The interrupt subroutine (ISR) "data process" is a real time job running at the fixed data conversion rate of 75kHz. Every time the ISR is executed a new set of 16bit data samples from all 8 ADCs is available for processing. Depending on the current state none or several non blocking sub tasks were executed and finally a modified set of 16 bit data for the 8 DACs is ready for conversion at end of this ISR. The full loop delay is 5 samples (2 in and 3 out) or 67 μs.

The major SPM tasks are to run the Z position control feedback loop, generate XY offset and scan motions coordinated with all data acquisition tasks. A full frame real time vector scan generator and multi channel data collecting task, automatic bandwidth adaption to current scan speed via digital data over sampling is implemented, including trigger for sub-grid probe and X scan position sensitive trigger for pre-defined parameter changes.

Further a control module for tip/sample coarse motion usable for typical inertial driven motors for positioning and automatic tip approach is available. For spectroscopy and manipulation the "vector probe engine" was designed and implemented (see section III B). Also a full digital lock-in amplifier with bias modulation providing results for two arbitrary phase settings for 1st and 2nd order signals is implemented. It can be used for dI/dV imaging or spectroscopy. It typically operates at multipes of 586 Hz up to approx. 5 kHz.

Real time multitasking of all above mentioned DSP jobs is realized synchroneous with the data sampling rate, so any actions/reactions of all jobs appear simultaneously, including the gating of both counters, which is synchroneous to the data sampling on hardware level and ensures any counting windows matched to the scanning. All tasks are designed as non blocking and fully finishing their designated job withing every cycle. Job control is realized in two ways: On the one hand jobs get started and canceled via the state machine as reaction to an user request, on the other hand jobs can be triggered in real time by an already running job, can cancel them selfs (if finished) or can be canceled by a different job. The status of any job (running or stopped) can be determined on user request at any time.

The scan and feedback jobs in particular are designed so that control parameters can be adjusted at any time and take effect immediately, a scan can be interrupted even in the middle of a scan line at zero delay.

Further, the whole driver architecture is multitasking capable. This allows to run multiple jobs on user level watching or manipulation DSP parameters and data, as long as this does not interfere the DSP operation itself. (i.e. two request to scan an image from two different jobs will certainly not work), whereby it is possible to have Gxsm scanning and have a different job requesting a vector probe, offset move, watch Z, etc.

A. Vector scan generator

A vector scan generator implemented on the SR platforms runing real time full frame scans, including scan rotation. Scan sizes and number of data points can be set freely to any number not exceeding the DAC resolution limits. The number of acquired data sources (channels) and scan speed is only limited by the effective USB-2.0 bandwidth (including FIFO overhead and transfers protocols) as the effective data stream has to keep up to prevent buffer overruns. All analog inputs, the data of the digital lock-in amplifier and 32-bit precision gated counter (DSP/FPGA based) are available. Data can be taken in forward and/or backward scan direction. Digital bandwidth adjustment according to scan speed of the acquired incoming data is performed.

Any parameter like scan speed (given in Å/s), feedback controls, bias, offset, trigger points, can be changed any time while scanning. The only exception to that is the scan geometry (size and number of points). Any probe can be performed while scanning without interrupting the scan process, i.e. the tip keeps moving – if desired. The position of the probe is recorded and marked within

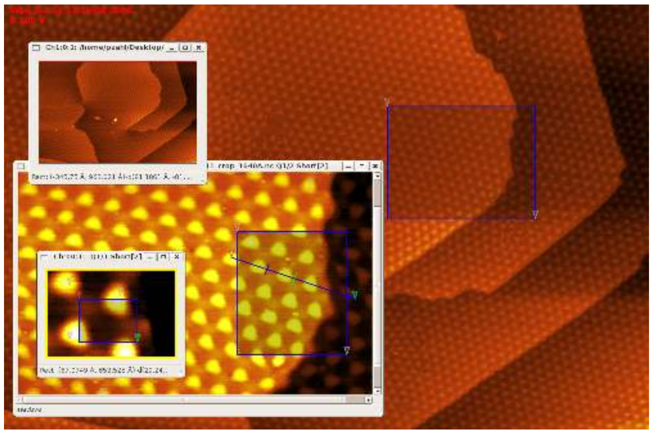

FIG. 5: STM image demonstrating atomic resolution of a epitaxially grown single graphite layer (graphene) on top of an Ruthenium film. Steps and the very dominant Moiré is very well resolved as the consecutive zoom-ins are showing (zoom into the original big data set as shown in full in the small inset of 250 nm × 250 nm (scanned with 10,000×10,000 pixels). (provided by P. Albrecht, CFN)

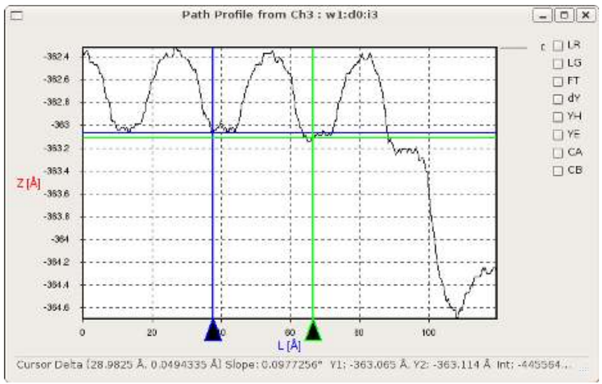

FIG. 6: Profile as extracted from Fig. 5 via the “Showline tool” as marked with a line.

the scan for later review. Gxsm is also keeping track of when and where and how major parameters where changed while scanning, i.e. Bias, Speed and Setpoint changes are recoreded for later review.

Several tools for on-the-fly profile and data extraction/visualisation and back ground corrections are available and can be used any time, even while a scan is in progress. In Fig. 5 a sample STM scan is showing atomic resolution of a epitaxially grown single graphite layer (graphene) on top of an Ruthenium film. Steps and the very dominant Moiré is very well resolved as the consecutive zoom ins are showing. The insets are zooms into the original big data set as shown in full in the small inset of 250 nm × 250 nm which was scanned with 10,000×10,000 pixels resolution. The profile (showline tool) is shown in Fig. 6.

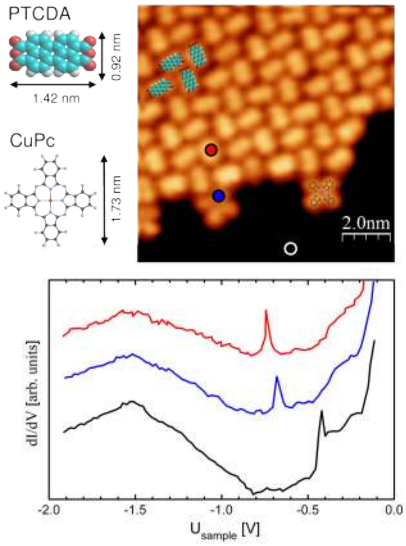

FIG. 7: A LT-STM/STS study performed with Gxsm: the STM scan shows a Cu(111) sample covered with a submonolayer of PTCDA and a small amount of copper phthalocyanine (CuPc) molecules, which are found to be in contact to the PTCDA islands at low temperatures (8K). The spectroscopy data was measured at distinct positions of the molecules as indicated by the coloured dots. As a reference, the dI/dV spectrum of the bare Cu substrate is given (black line). It exhibits the Shockley Surface State at $\sim 0.45\,\text{eV}$ below Fermi Energy. The PTCDA molecules show an interface state (sharp feature at -0.75 eV). Due to molecule-molecule interaction, some benzene rings of adjacent CuPc molecules also show this interface state, in this example shifted by 100meV. (provided by group of R. Möller)

B. Vector probe engine

A powerful feature of scanning probe microscopy is the ability to perform spectroscopic measurements and manipulations on the atomic scale. The most common example for scanning probe spectroscopy are I/V and dI/dV curves taken with STMs where the tunneling current (I) and its derivative (dI/dV) is measured as function of the bias voltage to study the local electronic structure of the sample, see Fig. 7. Countless variations of scanning probe spectroscopy are used by different research groups. However, many SPM control software systems are restricted to the most common spectroscopy modes such as I/V curves. Gxsm features a novel approach to scanning probe spectroscopy and manipulation, the vector probe (VP) engine. Gxsm's universal vector probe allows almost every imaginable spectroscopy or manipulation task to be performed without the need to modify the DSP code. Nevertheless, the VP engine DSP code is small and extremely efficient to reduce the memory footprint and increase performance.

The basic idea behind Gxsm's VP is that every spectroscopic measurement (probe) can be described by the state of the instrument at each measurement point and the data acquired at this point and how to get to the next state. A full generic probe usually can be split into sections s of specific actions like "go from the current state to the initial intended probe state" (i.e. ramp from current bias to the start bias), then "run the probe itself" (ramp from start to end bias) and "finish with a return to the original state" in the last section.

The state of the instrument $S_{s,i}$ is defined by all variables controlled by the DSP. For most SPMs, the state vector $\vec{S}_{s,i}$ at point i within a section s is defined by

$$\vec{S}_{s,i} := (v, x, y, z, FB),$$

where v denotes the bias voltage, (x, y, z) the three-dimensional tip position, and FB the feedback status (on/off). It should be noted that this definition of $\vec{S}$ is only an example. Gxsm provides enough flexibility for controlling instruments that may require a different set of control parameters.

Assuming a linear state change within every section, the change of the SPM state between two consecutive measurement points i and $i+1$ is described by the step vector $\mathrm{d}S$:

$$\mathrm{d}\vec{S} := (\mathrm{d}v, \mathrm{d}x, \mathrm{d}y, \mathrm{d}z, FB)$$

Each component of the vector simply describes the change of one parameter controlled by the DSP, only the FB flag just tells the feedback to be on or off.

Similar to the state, the data acquired at each measurement point i in a section is selected from the DSP's input channels by the data vector $\vec{D}$:

$$\begin{aligned}\vec{D} \;:=\; &((ADC_0, ADC_1, \ldots, ADC_7),\\ &(Z_{\mathrm{mon}}, L_0, L_{1\mathrm{a}}, L_{1\mathrm{b}}, L_{2\mathrm{a}}, L_{2\mathrm{b}}))\end{aligned}$$

Here, ADC_n is a analog input channel with $n = 0\ldots7$, Z_{mon} is the current z value given by the feedback loop, and L_x denotes data generated by the build-in digital lock-in amplifier. The components of the data vector are flags which are set to 1 when data is to be acquired and to 0 if no data is taken (to optimize data transfer bandwidth only requested data is transferred to and recorded by Gxsm).

A section of a vector probe event is then described by the change of the systems state $\mathrm{d}\vec{S}$ between the individual data points and the data sources $\vec{D}$ to be acquired at each data point:

$$\vec{p}_s := (\mathrm{d}\vec{S}, \vec{D}, n, \nu),$$

where n is the number of times to apply $\mathrm{d}\vec{S}$ and also the number of data points in this VP segment and ν is the rate in vectors per second, which defines the duration (n/ν) of every probe segment.

A complete VP is defined by a list of probe vectors $\vec{p}_s$ that are executed consecutively. A null vector is used as program end mark for the VP engine.

For example a simple delay is done by just setting all components of $d\vec{S}$ to zero and the FB flag as desired and then use n and ν to define the total duration n/ν of this segment. A simple bias ramp can be achieved by setting just the value for dv, the total bias change will be defined as $n \cdot dv$ and the duration again by n/ν.

This description is simplified, as the real implementation includes digital oversampling, data averaging and has additional vector components. Our vector probe engine also has dedicated vector program control parameters to allow simple and nested loop constructs in addition to consecutive vector execution.

As the generation of a set of probe vectors for a specific task is not complicated but also not user friendly, the Gxsm HwI implements a vector generator for several SPM typical probe tasks as described in II B. It derives the needed vector set for the desired task and downloads it to the DSP for execution. The design of this vector generator including the GUI is kept simple and is user extendable.

C. Gridded Probe

Gxsm allows to set up an automated gridded probe while scanning. The vector scan engine can trigger any probe action every n-th data point. We are assuming a scan speed slow compared to the probe time (i.e. the time inbetween triggering single probes must be at least larger than the probe duration itself). This probe action is performed fully simultaneous to the scaning, meaning the tip keeps – very slowly – moving. The advantage of this is that the scan image stays undisturbed by any means of piezo non-linearities, like creep. The first trigger within every line is shifted by an computed number of pixels (offset from left) to get an optimized coverage of the whole scan with data points. By using this linewise variation of the offset, the probe data are not only acquired on a fixed grid (e.g. every n-th point in every m-th line) but in every line. While maintaining a constant raster speed of the tip, the number of datapoints can be increased so that an implemented filter algorithmen can be used to interpolate between the two-dimensional distributed probe points to restore a multidimensional, hence multi-layered probe image with the full pixel resolution of the topography image.

D. Roadmap and latest developments for the MK2-A810 SPM Control

As experimental code release a high resolution (HR) mode for the DAC converts is implemented. This will allow to increase the bit resolution of selected output channels by 1...3 bits. This is possible on DSP software level now running sampling and data processing at full 150 kHz but limiting all other DSP tasks like scan and feedback to a reasonable fraction of this. For all input channels an automatic scan speed depending bandwidth adjustment (simple averaging) is used as before, but now the gained resolution due to statistics is not any longer thrown away (rounded off to integer), but the full 32 bit accumulated value and normalization count is kept and transferred. A normalization to the original 16 bit magnitude, but now as floating point number, is done by the HwI as data post processing. For performance reasons and future expansions the FIFO data stream consisting of a set of 32 bit signals is now compressed using first order linear predictor and custom encoded byte packed.

In particular the signal to noise ratio of small or noisy signals will increase automatically with lowering the scan speed (given here in pixels/s). All available input channels ADC_i are managed in this automatic scan speed

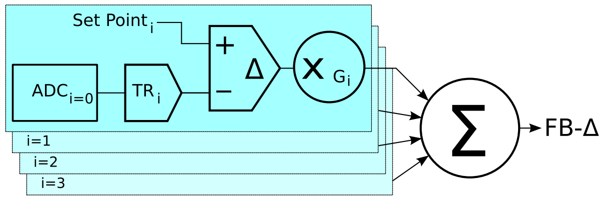

FIG. 8: Schematic diagram of the new DSP feedback with four signal source mixer. The input signals are transformed as requested (TR_i: linear/logarithmic/fuzzy) and the error signal Δ_i is computed for every channel i using individual set points. The sum of previously with gain G_i scaled delta signals is computed and feed into the feedback algorithm FB as Δ.

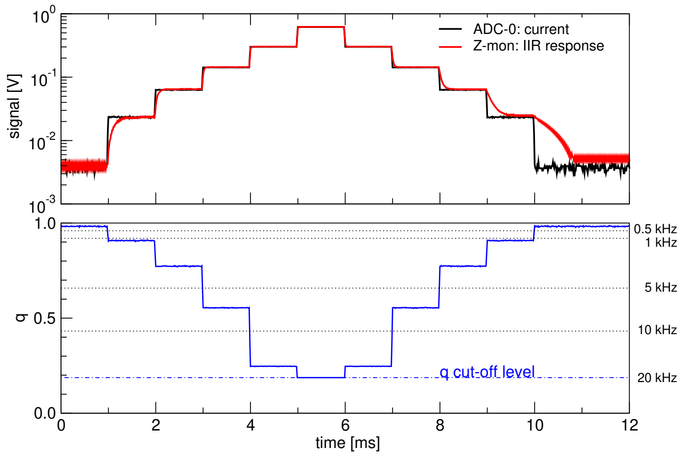

FIG. 9: Life IIR performance demonstration in Gxsm self-test[24] configuration. A stair case like current input signal starting at 3.6 pA noise level assuming 1 V/nA (or a $\times 10^9$ gain) with logarithmic steps starting at 20 pA and scaled by $\times 2$ for the following steps (ADC-0 (black)) is generated using the Gxsm "PL"-Vector Probe mode. At the same time the IIR-response (via Z-mon (red)) and the real-time q (blue) is recorded. IIR settings used: $f_{\min} = 50$ Hz, $f_{\max} = 20$ kHz, $I_c = 500$ pA.

matching bandwidth mode:

$$V = \frac{1}{N}\sum_{n=0}^{N-1} \mathrm{ADC}_i(n), \quad N = \frac{75000\,\mathrm{Hz}}{\mathrm{Pixel/s}}$$

or in signal noise gain (S_N) terms

$$S_N = 20\log\left(\frac{1}{\sqrt{N}}\right)$$

is the gain in signal to noise ratio – assuming statistical noise – on top of the available 16 bits (1 bit RMS) of the SR2-A810[11].

Further the latest experimental release revises the feedback loop configuration and allows up to four signals (provided on ADC0. . .3) to be user configurable as feedback sources using linear or logarithmic signal transformations and even can be mixed and weighted in different ways via the gains G_i as illustrated in Fig. 8. It also includes a special "FUZZY" mix mode for signal level depended enabling of a particular chanqnel only if its signal is beyond a given level; only the "amount beyond" is used for Δ_i computation.

This multi channel feedback mode allows for example contineous transitions between STM and AFM or Dynamic Force Microscope (DFM) operation modes. The "FUZZY" mode can be used in many ways, one may be a kind of "tip guard" mechanism watching for special conditions, i.e. watching the power dissipation signal commonly available from Phase Locked Loop (PLL) controllers used for DFM.

For channel ADC_0 a real time self adaptive Infinite Respose (IIR) filter which adjusts its frequency as function of the signal magnitude is implemented – assuming to be used for sampling the tunnel current in STM mode. The user selects a crossover current I_c and cut-off lower limit frequency f_{min}, also the upper bandwidth can be limited to f_{max}. This will then in real time limit the ADC_0 input bandwidth in dependence of the signal magnitude $|\mathrm{I}_n|$ according to:

$$f_0(q) = -75000\,\mathrm{Hz}\frac{\ln(q)}{2\pi}, \quad q(\mathrm{I}_n) = 1 - \frac{\frac{f_{\mathrm{min}}}{f_{\mathrm{max}}}\mathrm{I}_c + |\mathrm{I}_n|}{\mathrm{I}_c + |\mathrm{I}_n|}$$

This real time computed q is limited to a q_{min} matching the given f_{max} before the bandwidth limited (IIR filter) current signal $\tilde{\mathrm{I}}_n$ which is recursively computed on the DSP according to:

$$\tilde{\mathrm{I}}_n = q\tilde{\mathrm{I}}_{n-1} + (1-q)\mathrm{I}_n$$

Fig. 9 illustrates the IIR filter response to a logarithmic steepening stair case test input signal. This is a live IIR performance demonstration utilizing the Gxsm Vector Probe Engine itself and having Gxsm and the MK2-A810 set up in a self-test[24] configuration. The stair case like current input signal is starting at about 3.6 pA noise level assuming 1 V/nA (or a $\times 10^9$ gain). The logarithmic steps start at 20 pA and scale by $\times 2$ for the adjacent steps (ADC-0 (black)). The test signal is generated using the Gxsm "PL"-Vector Probe mode. At the same time the IIR-response (via Z-mon (red)) and the real-time q (blue) is recorded.

The IIR settings used for this demonstration are: $f_{\mathrm{min}} = 50\,\mathrm{Hz}$, $f_{\mathrm{max}} = 20\,\mathrm{kHz}$, $\mathrm{I}_c = 500\,\mathrm{pA}$.

Looking at the IIR signal (red) the filter effectivity is clearly visible for small signals, also the fast "step-up" response is demonstrated by comparing with the slower "step-down" response. Also note the q cut-off indicated as the q cut-off level at 20 kHz.

For a low signal to noise ratio (given for tunneling currents in the pA regime) the feedback stability can be gained by a combination of IIR filtering and slower scanning. This digital self adapting IIR filter implementation allows full control of the frequency ranges and guarantees a fast tip response to a sudden increase of the tunnel signal (up to full band width) as needed to prevent the tip from crashing into step bunches or other "edges".

E. Conclusion

We present an update on the Open Source Scanning Probe Microscopy control project Gxsm. The Gxsm control software is already a versatile data processing tool for multidimensional data obtained by scanning probe microscopes. In combination with a DSP based hardware it becomes a complete real time SPM control system including a full digital feedback, scan generator, and a flexible spectroscopic/manipulation mode. The project does not only provide the software binaries and its sources to the scanning probe community free of charge but also support by community driven online discussion and help forum[13, 14].

Acknowledgments

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[1] G. Binnig, H. Rohrer, C. Gerber, and E. Weibel, Phys. Rev. Lett. **49**, 57 (1982).

[2] G. Binnig, H. Rohrer, C. Gerber, and E. Weibel, Phys. Rev. Lett. **50**, 120 (1983).

[3] E. Meyer, H. J. Hug, and R. Bennewitz, *Scanning Probe Microscopy: The Lab on a Tip* (Springer, 2003), 1st ed.

[4] B. Bhushan and H. Fuchs, eds., *Applied Scanning Probe Methods II: Scanning Probe Microscopy Techniques*, NanoScience and Technology (v. 2) (Springer, 2006), 1st ed.

[5] A. Boudreau, B. Paillard, and P. Rowntree, Measurement Sci & Technol. **13**, 1599 (2002).

[6] D. Brodbeck, L. Howald, R. Luthi, E. Meyer, and R. Overney, Ultramicroscopy **42-44**, 1580 (1992).

[7] T. M. H. Wong and M. E. Welland, Mesas. Sci. Technol. pp. 270–280 (1993).

[8] C. Barchesi, C. A, R. Generosi, C. Giammichele, M. Luce, and M. Rinaldi, Rev. Sci. Inst. **10**, 3799 (1997).

[9] P. Zahl, M. Bierkandt, S. Schröder, and A. Klust, Rev. Sci. Inst. **74**, 1222 (2003).

[10] SoftdB, manufacturer of all the SignalRanger DSP boards, URL: `http://www.softdb.com`.

[11] MK2-A810: Signal Ranger MK2 with Analog810 module, URL: `http://www.softdb.com/a-dsp_SPM_Controller.html`.

[12] SR-STD, SR-SP2: Signal Ranger Standart, Self-Powered 2.

[13] P. Zahl and A. Klust, gxsm Software Project Homepage: URL: `http://gxsm.sourceforge.net`.

[14] Gxsm Life CD/DVD Ubuntu System can be downloaded here: URL: `http://www.ventiotec.com/linux/GXSM-Linux.iso`, provided via Ventiotec Dolega Wagner GbR, Marler Straße 100-102, 45896 Gelsenkirchen, Germany.

[15] Unidata, NetCDF Homepage: URL: `http://www.unidata.ucar.edu/packages/netcdf`.

[16] G. Aloisi, F. Bacci, M. Carla, D. Dolci, and L. Lanzi, Rev. Sci. Inst. **79** (2008).

[17] Florence Open SPM, see here URL: `http://spm.polosci.unifi.it`.

[18] The GNOME desktop environment: URL: `http://www.gnome.org` Miguel de Icaza.

[19] P. Zahl, A. Klust, and S. Schröder, *The Gxsm Manual*, Institut fr Festkörperphysik, Hannover, Germany; Colorado School of Mines, Golden, CO, USA; University of Washington, Seattle, WA, USA (2002), Online available here: URL: `http://gxsm.sourceforge.net`, section Manual/Help.

[20] Piezodrive by Ing. Büro W. Reimann, Germany. Go to URL: `http://gxsm.sourceforge.net` and look at the section hardware for details.

[21] Femto: model DLPCA-200 Variable-Gain Low-Noise Current Amplifier, or any other current to voltage amplifier with typical gains $10^8, 10^9$.

[22] K. Besocke, Surf. Sci. **181**, 145 (1987).

[23] Python scripting language: `http://www.python.org`.

[24] Gxsm self-test configuration: Bias looped back to Feedback input (current) for current simulation. Using the mixer and feedback settings typical situations can be tested using various vector probe modes. Here, for this IIR performance test, the feedback is configured in linear mode with proportional gain one and integration set to zero. This means the IIR filter output (feedback input signal) can be monitored as Z signal. URL: `http://www.gxsm.sf.nethttps://sourceforge.net/apps/wordpress/gxsm/2009/10/09`.

[25] A complete list of all Gxsm developers can be found at URL: `http://sourceforge.net/projects/gxsm/`, click on "view members".