Electronics and Software for Scanning Tunneling Microscope

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Introduction

A Scanning Tunneling Microscope (STM) is a device for imaging conducting surfaces at very high magnifications down to the scale of individual atoms. The STM does this by mechanically scanning a sharp tungsten tip over the surface (sample to be scanned). Piezoelectric elements can provide the necessary small translations of the tip. A bias voltage is applied between the tip and the sample. When the tip is brought within about 10Å (1nm) of the sample, electrons from the sample begin to "tunnel" through the 10Å gap into the tip or vice versa, depending upon the polarity of the bias voltage. The resulting tunneling current varies with tip-to-sample spacing, both the sample and the tip must be conductors or semiconductors. The tunneling current is an exponential function of distance. Based on quantum mechanics, the tunneling current (**I_t**) is,

$$I_t = \exp(-kd)$$

where d is the distance between tip and sample surface. This result turns out to be the key to STM. If an atomically sharp tip is used, the tunneling current from the first atom of the tip will be exponentially larger than that of the tip atoms which are slightly behind it. If the separation between the tip and the sample changes by 10% (on the order of 1Å), the tunneling current changes by an order of magnitude. This exponential dependence gives STMs their remarkable sensitivity. STMs can image the surface of the sample with sub-angstrom precision vertically, and atomic resolution laterally. The Scanning Tunneling Microscope (STM) is the ancestor of all scanning probe microscopes. It was invented in 1981 by Gred Binnig and Heinrich Rocher at IBM Zurich. Five years later they were awarded the Nobel Prize in Physics for its invention. The STM was the first instrument to generate real-space images of surface with, so called, atomic resolution (atomic lattice resolution to be precise).

As the concept is relatively simple. Just place a sharp tungsten or platinum-irradium tip close to a conducting surface, so close that the wave functions of the closest tip atom and surface atoms overlap. Apply a potential difference between tip and surface and a tunneling current flows. But there are real challenges to control the distance between tip and sample at few angstrom without crashing the tip to the surface. The feedback circuit, tip approach mechanism, and other electronic modules should be very robust. The overall noise level of the system should be < mV.

The overall scheme of the scanning tunneling microscope (STM) is shown in figure 1. It outlines the data acquisition ,control circuit logic and the feedback loop for the STM.

Block Diagram Representation of STM Electronics Modules:

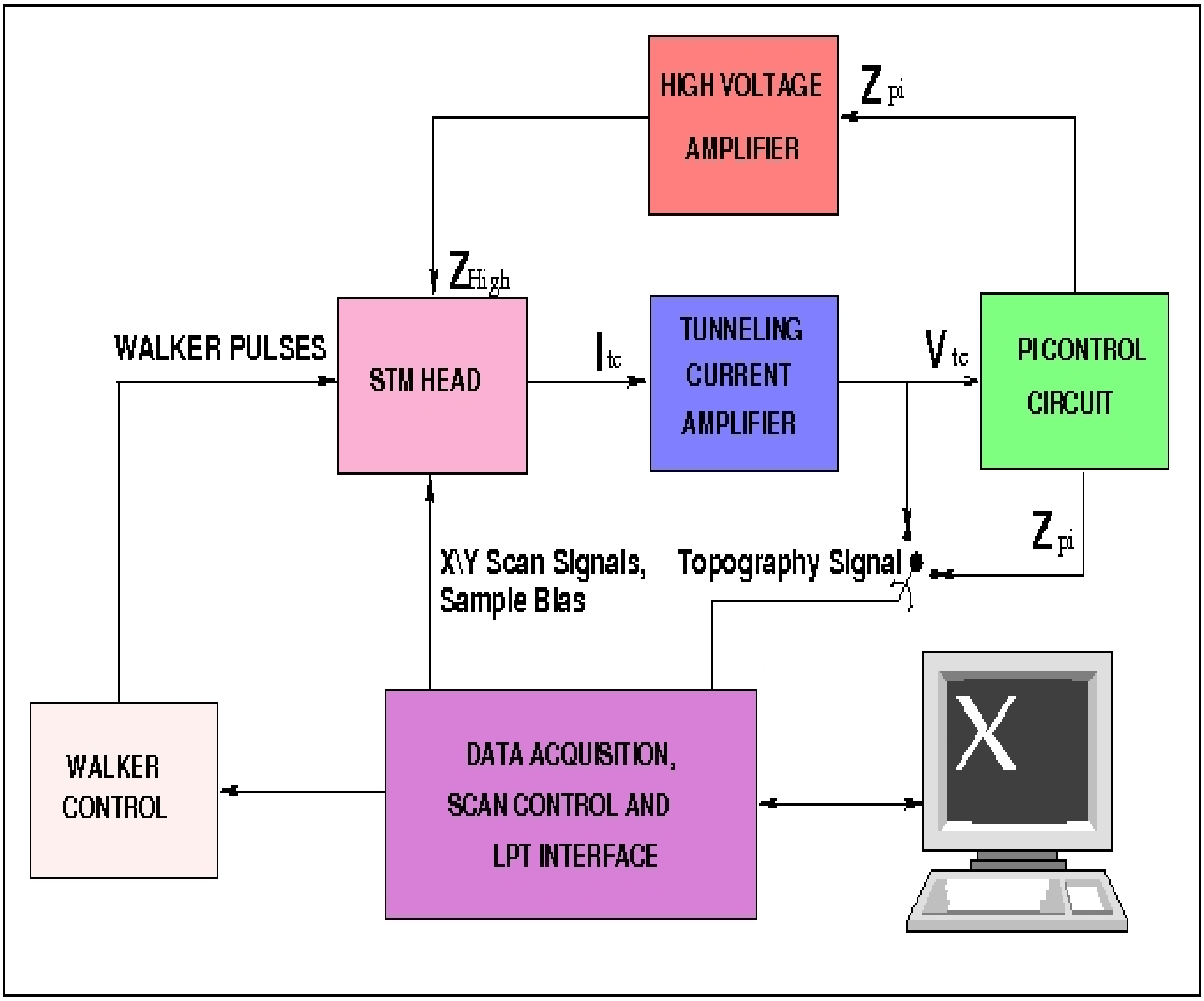


Figure 1: Data acquisition and control circuit logic for the STM. The overall scheme and the feedback control circuit is outlined here.

An Overview of Electronic Modules

The STM electronics comprises of the following modules, performing the following functions :

1. Power Supply

The driving source for all the modules of the STM. Supply voltages needed here are Two +5Vdc, +/- 15Vdc, +/-110Vdc and 110Vac.

2. Tunneling Current Amplifier

Amplifies the Tunneling Current (as it is in the range of pA- nA).

3. PI Feedback Control Circuit

Integrate the error between the tunneling current being observed against a constant value (here termed as Set-Point) of tunneling current that is to be maintained which means that the tip and the sample are always kept at a fixed separation (this error voltage is used to control the z-direction movement of the tip).

4. Slope Compensation and High Voltage Amplifier

The Z-output (integrated error for z-direction movement) from the PI is slope compensated for slope along X and Y axis. It is than level shifted by a High voltage and fed back to the STM Head to keep the tip-alignment steady. Scan voltages X+, X-, Y+ and Y- are amplified to ±100V range using high voltage amplifiers.

5. Piezotube Walker Control Circuit

It controls the coarse approach mechanism for the scanning tunneling microscope. It provides the necessary control signals to the mechanism which is needed to bring the tip and sample surface within the range of scanner piezo (< 1µm), starting from a separation of about a few millimeters.

6. Data Acquisition, Control and PC interface Circuit

It co-ordinates between all the electronic modules of the STM. Here the error signal is digitized, containing all the precious information about the surface profile of the sample which is treated cosmetically to present the images on the screen. This board communicates with PC via LPT port. PC ground and the system ground is kept separate to minimize the effect of PC noise.

Tunneling Current Amplifier

The tunneling current between tip and the sample contains all the essential informations. The tunneling current provides the basic topography of the sample surface for the determination of the atomic structute and it gives the tunneling spectroscopy for the electronic structure. Since the magnitude of the tunneling current occurring in STM is very small, typically from 10 pA to 50 nA. It should be amplified by the gain of 10^9 (V/A) to be used in the electronic circuits of STM. Hence the high performance current-to-voltage converter (IVC) is an essential element of an STM.

In our electronics design we have used inverting feedback type IVC, since it is convenient for the detection of a fast and low current signal due to wider bandwidth and lower noise. The inverting feedback IVC can be built easily using commercial ultra-low input bias current and very high input impedence operational amplifiers and a very high-ohm feedback resistor as shown in Fig.2. Ideally the inverting feedback current-to-voltage converter with a large feedback resistance above 1GΩ can provide a proper dynamic range covering the tunneling current (pA-nA) and minimise the noise.

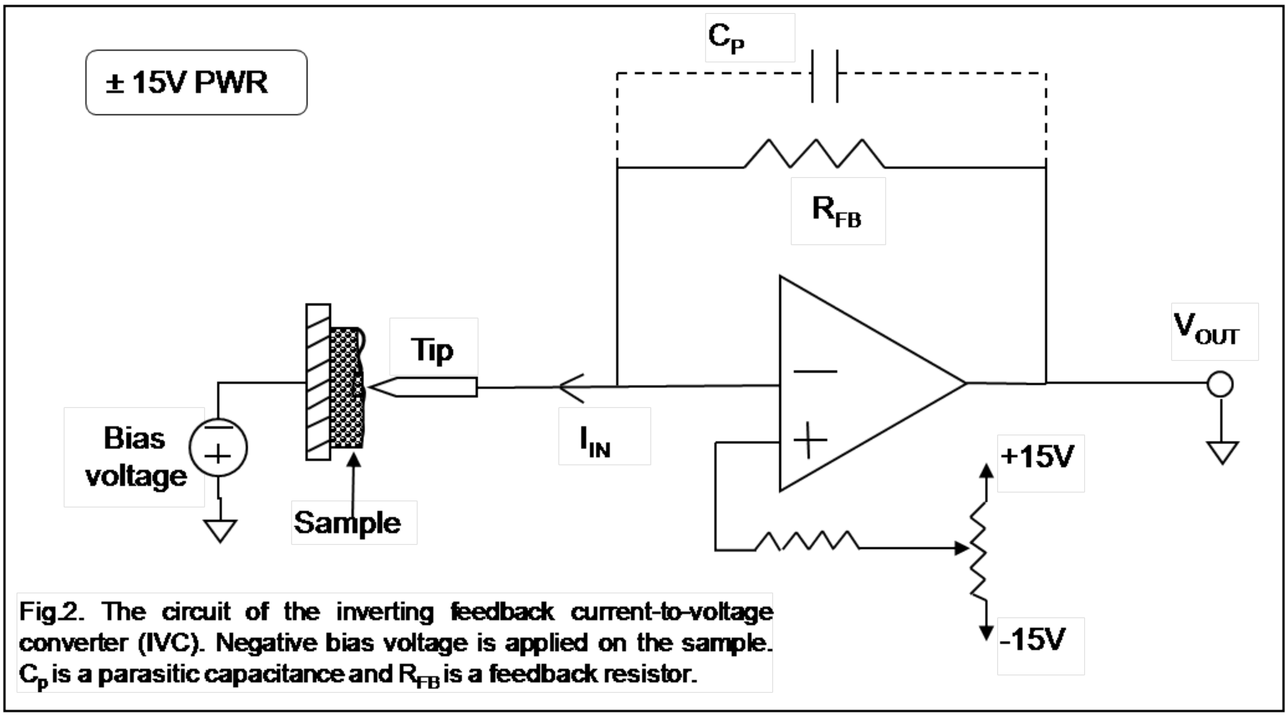


Fig.2. The circuit of the inverting feedback current-to-voltage converter (IVC). Negative bias voltage is applied on the sample. C_p is a parasitic capacitance and R_{FB} is a feedback resistor.

The non-inverting input of the op-amp is grounded, and the voltage at the inverting input should be equal to ground. This implies

$$V_{OUT} = - I_{IN} * R_{FB} \qquad ; R_{FB} \text{ is } 1G\Omega \text{ in our design}$$

In the design we apply negative bias voltage on the sample plate and the direction of current is out of the op-amp. For $R_{FB} = 1G\Omega$, 200 pico ampere of tunneling current results in an output voltage of 200 mV.

Feedback Circuit : P-I control

In scanning tunneling microscopy, a feedback system is used to control the tip-sample spacing in order to maintain a stable tunneling junction. A fixed tip-sample bias voltage is applied and the desired tunneling current is selected by the operator. The feedback control is used to adjust the gap between the tip and the sample until that tunneling current is achieved. The tunneling current picked up is converted into voltage using current-to-voltage converter (IVC) and is compared with a reference voltage, which represents the set point of the tunneling current. The error signal is then sent to the feedback circuit, a robust designed P-I (proportional-integration) amplifier, which sends a voltage signal to the z-piezo. The phase of the collection of all the amplifiers is chosen to constitute a negative feedback i.e. if the tunneling current is larger than the preset current, then the voltage applied to the z-piezo tends to withdraw the tip from the sample surface, and vice versa. Therefore the equilibrium z-position is established through the feedback loop. As the tip scans in the x-direction, the contour height z also changes with time. The function of the feedback circuit is to make the tip accurately follow the constant tunneling current contour at the highest possible speed. A block diagram of the feedback system of an STM is shown in Fig.3.

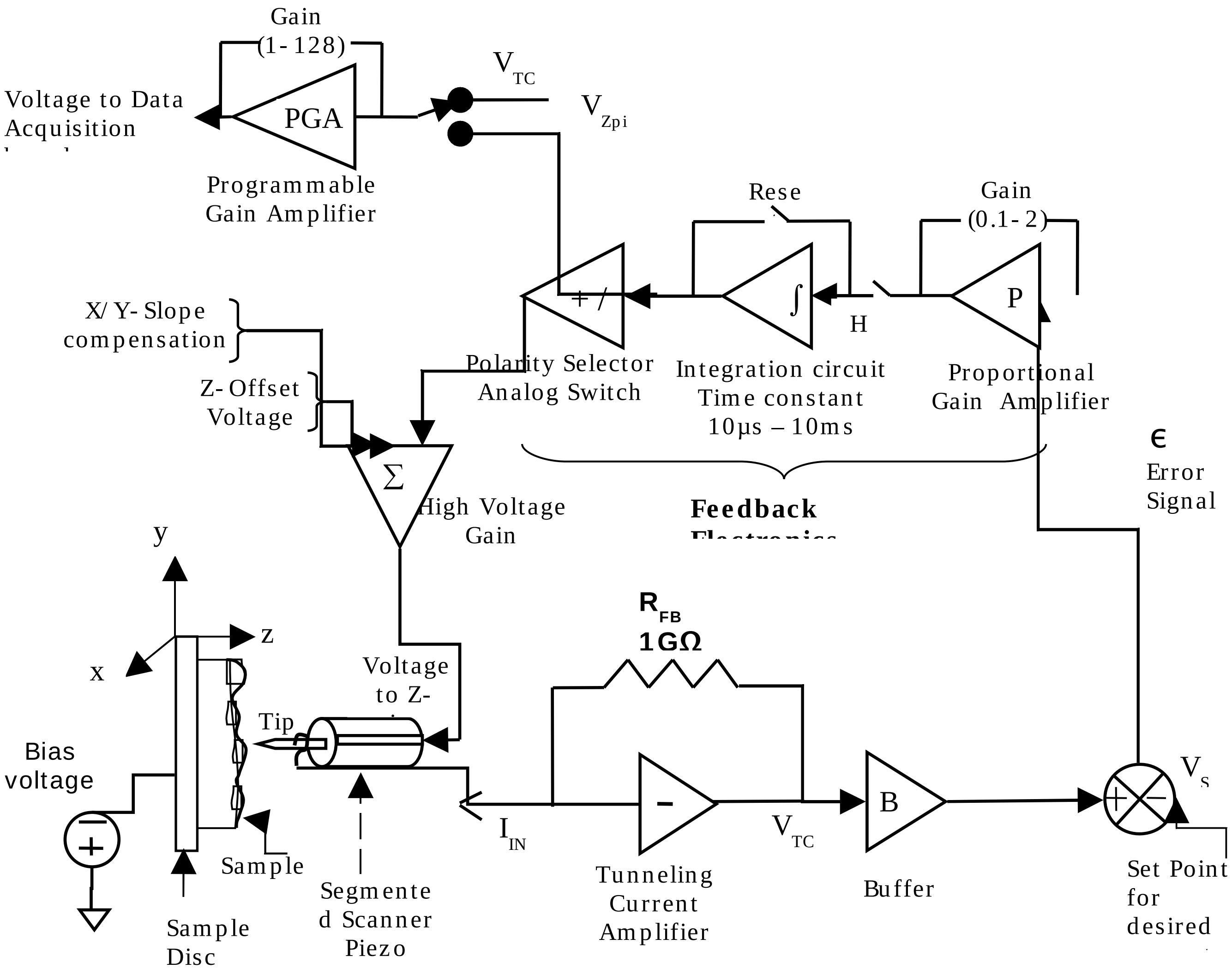


Fig.3. A schematic of the feedback loop in an STM.

Figure.3. illustrates the block diagram for the z-motion, i.e. the motion of the tip perpendicular to the plane of the sample, of the STM. A straight forward analysis of the system may be performedif the system is assumed to be linear. Most of the components behave in a fairly linear fashion except for the tunneling gap. The tunneling gap output is an exponentially varying current for linear variations in the gap distance but it can be treated as linear if the variations in the gap distance are small. By this assumption we can omit the requirement of logarithmic amplifier after current to voltage converter in the design. The goal of the feedback circuit design is to minimize the error signal 'ϵ'. The control block is developed such that the system maintains the desired tunneling current with the necessary accuracy. The constraints put on the electronics design are :

1. The resulting system must be stable, i.e. the error signal 'ϵ' must not increase in an unbounded fashion (when the feedback loop is on) as a function of time.
2. The steady state error of the system must be small.
3. The transient response of the system must be reasonably fast and oscillations should decay quickly.

Keeping in mind the above basic requirements of the system design, the error signal 'ϵ' is processed by the feedback electronics which typically contains a proportional gain amplifier, an integrator circuit and a high voltage gain amplifier. The proportional gain amplifier has a simple proportional control function

$$G_1(s) = k_P \omega_c / (s + \omega_c)$$

Where k_P is the dc-gain and ω_c is the high frequency cutoff at $f_c = \omega_c/2\pi$. Since the steady state error signal 'ϵ' in our design is reference signal divided by the term $1+G(s)$, so if the proportional gain k_P is large then the steady state error signal 'ϵ' is small, but not zero. Practically we have seen that for sufficiently high gain the system becomes unstable. Thus there is a compromise between reducing the steady state error signal and maintaining the system stability with proportional stage. A low pas filter has been included in the proportional gain stage to improve the system stability. The cutoff frequency ω_c is much lower (~ 1.6khz) than the piezoelectric element's resonant frequency (~ 10khz). This low pass filter prevents the proportional gain stage from amplifying the resonance. The dc gain of the propotional gain stage varies from 0.1 to 2.

The finite steady state error has been eliminated by including an integrator in the control block. In fact we can say this feedback control is more like a integration only control system. In the design integration stage follows the proportional gain stage and the resulting transfer function is

$$G_1(s) = k_P \omega_c / (s + \omega_c) * k_I / s$$

Here the first term is the proportional gain with an upper cutoff frequency ω_c, while the second term is an integrator with gain k_I. The integrator causes a small error signal to be integrated in time, producing more and more control action until the error is eliminated. Thus the steady state error of this system is zero for a signal that changes in a step like manner.

The polarity selector switch selects the phase of the signal such that the system constitute negative feedback to maintain a constant current in closed loop. The signal is followed by the high voltage gain amplifier. The high voltage amplifier has a transfer function

$$G_2(s) = k_{hv}\,\omega_{hv} / (s + \omega_{hv})$$

Where k_{hv} is the dc gain and ω_{hv} is the high frequency cutoff of the amplifier.

The integrator circuit provides an integration compensation, typically time constant varies from 10 µs to 10 ms. A high voltage amplifier provides an output of ±100V to drive the z-piezo. The output of the feedback electronics is applied to the z-piezo (tip), to keep the error between the actual tunneling current and the reference current very small. As the tip is scanned across the surface, variations in the sample topography and electronic structure affect the tunneling current. The feedback control circuit must react to bring the current back to the desired value. Ideally, the correction should be made instantaneously and exactly. However, there is always a finite response time of the feedback control system. The voltage applied to the tip (before high voltage amplifier) is digitized with 16-bit resolution analog-to-digital converter (ADC) and recorded as the topographic image.

P-I Control Settings :

Proportional dc Gain:

$$Vp = K_P * (V_T - (1/10)V_S)$$
$$Verror = V_T - Vs$$
$$k_P = (100\Omega + 20k\Omega(\text{variable})) / 10k\Omega$$
$$= 0.1 \text{ to } 2.1$$

P-Gain Dial Pot (10-turns) Settings: 6.5

$$k_P = (100\Omega + (6.5/10)*20k\Omega) / 10k\Omega$$
$$= 13.1k\Omega / 10k\Omega$$
$$= 1.31$$

Integration circuit settings:

$$Zpi = 1/T * \int_t (Vp)\, dt$$

I-Gain Dial Pot (10-turns) Settings: 3.0

$$R_I = 100\Omega + (3.0/10)*100k\Omega = 30.1k\Omega$$
$$C_I = 0.1uF$$

Integral Time Constant:

$$T = 30.1 * 0.1\mu f$$
$$= 3.01 * 10^{-3} s$$
$$= 3.01 \text{ ms}$$

Feedback Bandwidth:

$$f = 1/T$$
$$= 1/\ 3.01 * 10^{-3}\,s$$
$$= 3.33\ kHz$$

Piezoelectric Scanner Tube Theory : X, Y Scan voltages

A piezoelectric tube is a ceramic tube in which the many molecular dipoles, or positive-negative charge separations, are polarized at an elevated temperature by applying a (typically) positive voltage to an outer electrode (inner at ground). The positive outer voltage causes the molecules to partially align themselves with the positive directed outward, resulting in + outer and - inner radial polarization. The ceramic is then cooled to retain this polarization permanently. The resulting ceramic has a net negative charge on the inside surface and net positive charge on the outside surface. When a smaller voltage is then applied with the same polarity as the polarizing voltage, the element experiences a temporary expansion in the polarizing direction (i.e., the tube radius expands) and contraction in the perpendicular direction (i.e., the tube length contracts). It is this contraction that results in the tube bending, thus allowing X-Y scanning.

The bending of the a piezo tube in X and Y direction (as shown in Fig.4b.) is due to the potential difference over different segments of the scanner piezo. Voltage variations over X+/X- make it deflect right and left whereas over Y+/Y- causes deflection up and down. The four segments are shown in Fig .4a.

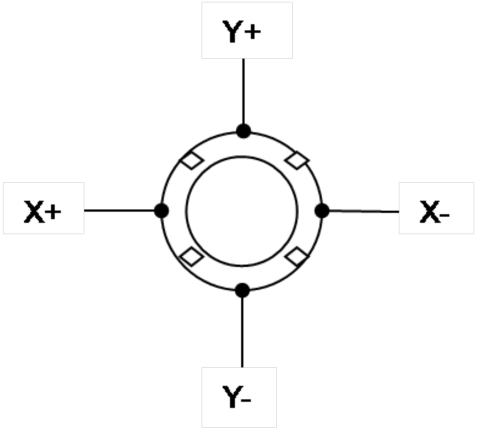


Fig.4a. Outer electrode of scanner piezo are segmented at 90^0.

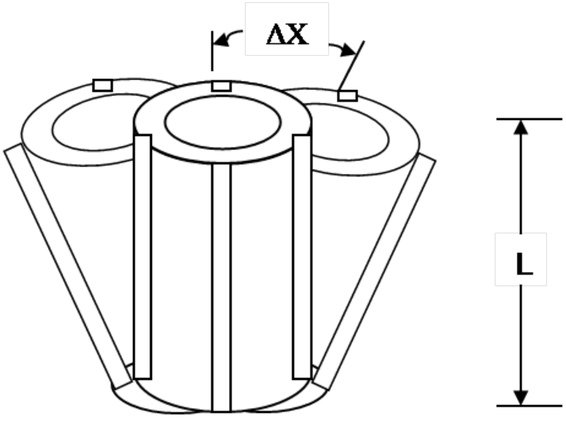


Fig.4b. Deflection of Piezoelectric tube shown in X direction.

Extracting design parameters:

For calculating X and Y movement/volt we assume that equal and opposite voltages are applied on the opposite quadrants. X-Y Flex motion using multi-electrode configuration is given below:

$$\Delta X = 1.8 * d_{31} * V_x * L^2 / [ID * (OD-ID)]$$

where,

ΔX : Deflection produced in the scanner piezo along X-axis
d_{31} : Piezoelectric Charge Coefficient (pC/N)
L : Length of the Scanner Tube
V_x : Applied Voltage
ID : Inner Diameter of the tube
OD : Outer Diameter of the tube

Our Piezo Parameters are:

d31 : -215 pC/N
L : 11.0 mm
V_x : 1V
ID : 5.33 mm
OD : 6.60 mm

Therefore, for V_x = 1V

$$\Delta X = 1.8 * (-215 * 10^{-12}) * 1 * (11 * 10^{-3})^2 / [5.33 * 10^{-3} * (6.60-5.33) * 10^{-3}]$$
$$= 6917.7 * 10^{-12} \text{ m}$$
$$= 6.9177 * 10^{-9} \text{ m}$$
$$= 6.9177 \text{ nm}$$

So, the deflection produced in the piezo tube in X/Y direction = 6.9177 nm/V

Peculiarity of Design:

Since, the voltage applied on the opposite faces of scanner piezo segment are of opposite polarity - the potential difference between these two faces is double of the actual voltage applied. So, when the DAC output on the X/Y segments of the scanner piezo is, say V volts – the deflection produced in the tube corresponds to 2V volts.

Hence, in this case the deflection produced for when X/Y Scan signal is 1V is changed. $\Delta X = 2 * 6.9177$ nm = 13.835 nm/V

The value of deflection produced (in this case) in X/Y direction = 13.835 nm/V

These calculations gave fair idea of the order of X and Y scan voltages required. These X and Y voltages will come from Digital-to-Analog converter's driven by software. Since our DACs are 12-bit resolution with range ± 10V. So the minimum change in X, Y voltages will be 20000 mV/ 4096 steps = 4.88 mV per step in the large area mode of scanning. The maximum scanning area of about 2800 angstroms by 2800 angstroms (280nm x 280nm) is achieved with ±10 volts and 256 steps per line scan, with our scanner tube. In the small area mode(highest resolution), DACs producing X and Y scan voltages are restricted to ±2.5V range over 12-bit resolution, so the minimum change in X, Y voltage is 5000 mV/4096 = 1.22 mV. The minimum scanning area (with highest resolution) of about 43 angstroms by 43 angstroms is achieved with this scan mode. Since a typical atom size is around 3 angstrom in diameter, so with the small area mode we can resolve the atoms e.g. HOPG (Highly Oriented Pyrolytic Graphite) sample.

There is a another set of DACs provided (one each for X and Y) called offset DACs which will position the tip on x-y plane to take highest resolution scans on different locations of the surface. We can position the tip using these offset DACs in x-y plane and generate two equal and opposite sawtooth waves i.e. X+ on one electrode quadrant and X- on opposite electrode quadrant using scan DAC. Many sawtooth waves will be generated during X-scanning (named horizontal scanning) with Y incremented at the end of each x-scan/retrace line. Alternatively, many sawtooth waves will be generated during Y-scanning (named vertical scanning) with X incremented at the end of each y-scan/retrace line.

To further increase the scan area we are using high voltage amplifiers which is amplifying these X+, X-, Y+ and Y- scan voltages. In effective we are increasing the range of surface area scans. These high voltage amplifier can be used in two gain modes either 1X or 10X, which is software controlled. The 1X gain mode is keeping the scan voltages in the +-10V range. Where as 10X gain mode jacks up the scan voltages to ±100V range. Effectively our maximum scan area in the 10X mode is about 2.8 µm by 2.8 µm.

Z - Motion of scanner piezo : Driver voltage

The Z-voltage controls the lateral motion of the tip. Z-positioning in the scanning mode, uses a ± voltage range to vary the tip position to keep the tip within an angstrom or two of the sample surface, via feedback maintenance of a constant tunneling current. The major component of Z-voltage comes from the feedback circuit, which tries to maintain a constant current set by the feedback. The lateral movement of the scanning tube is calculated by formulae

$$\Delta L = 2 * d_{31} * V_Z * L / [OD-ID]$$

where,

ΔL : Change in length in the scanner piezo along Z-axis

d_{31} : Piezoelectric Charge Coefficient (pC/N)

L : Length of the Scanner Tube

V_Z : Applied Voltage

ID : Inner Diameter of the tube

OD : Outer Diameter of the tube

$$\Delta L = 2 * 215 * 10^{-12} * 1 * 11.0 * 10^{-3} / [6.60-5.33] * 10^{-3}$$

$$= 3724.4 * 10^{-12} \text{ m/V}$$

$$= 37.244 \text{ A}^{o} / \text{V}$$

$$= 3.7 \text{ nm} / \text{V}$$

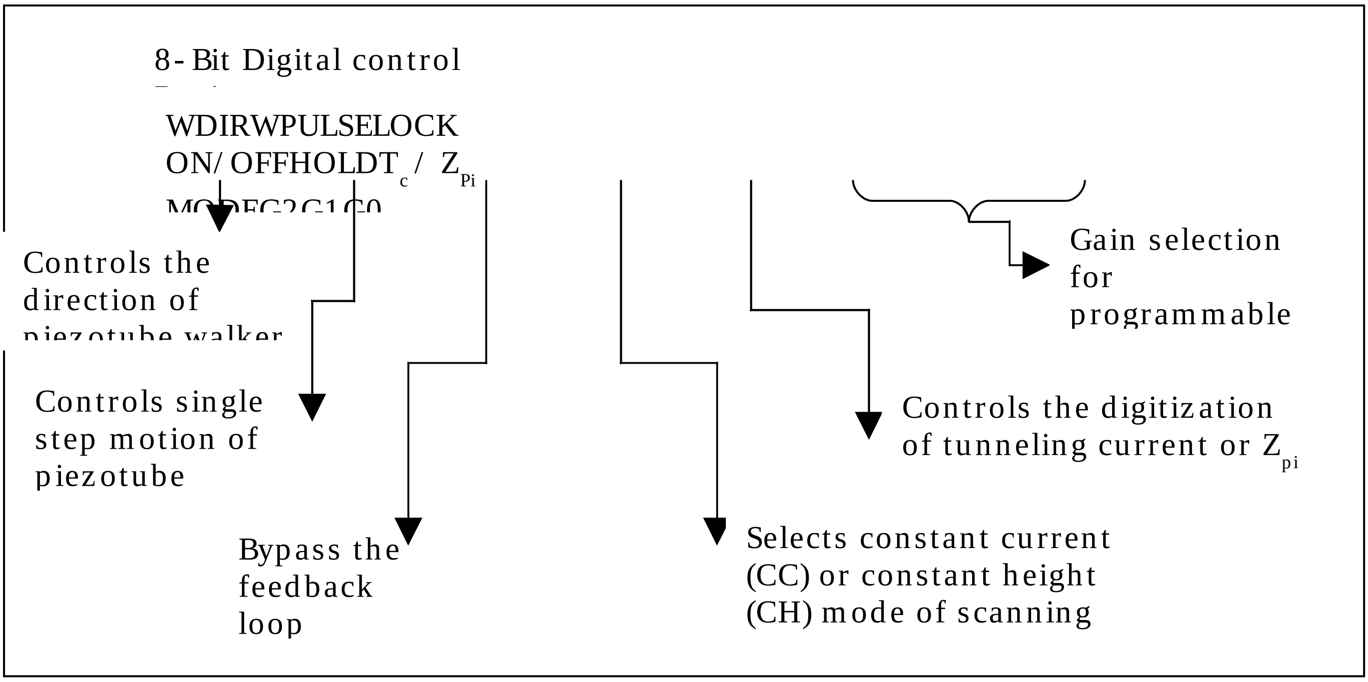
In our scanner piezo this value comes out to be 3.7nm/V. There are other components which are added at the high voltage stage i.e. Z-offset voltage (12-bit DAC), ranges ±10V, and X/Y slop compensation. Since in the topographic image we are interested in smaller variations of the feedback voltage. The Z-offset component corrects the dc-offset introduced by the feedback circuit in the Z-voltage. The slop compensation component is effective while scanning and eliminates any slop between the tip and sample surface. The final Z-voltage after high voltage amplifier is,

$$Z_{hi} = \text{HVA-Gain} * (Z_{pi} + Z_{offset} + \text{X/Y-Slope Components})$$

$$\text{HVA-Gain} = 10$$

Data Acquisition and PC Interface :

All the control voltages required in the design are generated in the data-acquisition and interface board. Data acquisition is accomplished using 16-bit analog-to-digital converter (ADC). Each display point sampled would contain the analog Z position, so we have used at a minimum a single 16-bit analog-to-digital convertor (ADC). Control is done by 12-bit digital-to-analog convertors (DACs). Eight channels of DACs are used in the design. In addition to these fine analog control signals, 8-digital control signals are provided. All these signals are software driven through LPT port. To minimize the PC noise to the STM electronics, optical isolation has been provided between the PC ground and the system ground. High speed optical isolators (10Mbit/s) are used.



The ADC digitizes the Z_{Pi} signal when the loop is on and digitizes the tunneling voltage V_{TC} signal irrespective of the loop on/off. This feature is implemented since while coarse approach we want to check the tunneling voltage with feedback loop on. It makes the coarse approach automatic as soon as tip and sample are within tunneling range the coarse approach mechanism stops and feedback loop takes the control of tip movement. The programmable gain amplifier (PGA) provides the gain, 1 to 128 ($2^0 – 2^{7)}$, selection before the signal fed to the ADC. ADC has input range ±10V with 16-bit accuracy and 1MHz conversion clock. As soon as ADC converts the data, it is read by the PC via parallel port.

Piezotube walker control signals WDIR, walker direction (forward or backward) and WPULSE, (interrupt signal to the micro-controller in walker circuit.) are software driven. These two signals control the walker motion and set the direction as farward during coarse approach. If we want to extract the tip we set the direction backward and provide walker pulses, it will move the walker in backward direction and tip comes out of tunneling.

Power Supply and Piezotube Walker control circuit :

Power supply design :

Since the noise level of the system needs to be kept < 1mV. The power supply design is a very crucial. The power consumption of the system is about 20W. Since optical isolation has been provided to keep the noise level under control at the cost of additional +5V dc, 500mA power supply requirement. Digital +5V dc, 500mA, power supply will power the digital circuit of the system. Both of these +5V dc supplies are linear regulated designs. The analog portion of the system is powered with ±15V dc , 200mA linear regulated power supply. For high voltage section of the system ±110V dc supply is required. It is a linear regulated design with 40mA current output. All the power supply grounds are isolated and joined at the appropriate points on the electronics boards, e.g. analog ground and digital grounds are combined at ADC to avoid the ground loop problems in the design.

Piezotube walker : compact coarse approach mechanism

The coarse approach mechanism of tip, called a piezotube walker, controls the Z-direction movement of the piezotube walker. This mechanism is needed to bring the tip and the sample surface within the range of the scanner piezo (< 1 um), starting from a separation of about a few millimeters. The walker control circuit is implemented using a microcontroller and six triacs synchronized with main control board. The direction of motion i.e. forward or backward is controlled from the main board. Basically microcontroller fires the six triacs one by one as soon as it gets a walker pulse signal from the main control board. This sequence generates six synchronized voltage outputs one each for six sections of the walker tube. This step voltage (± 150V AC), as shown in Figure .5, is applied to each section one by one, moving them along the same direction. Then the voltage on each section is slowly brought down to zero at the same time. This constitute one step of the piezotube walker.

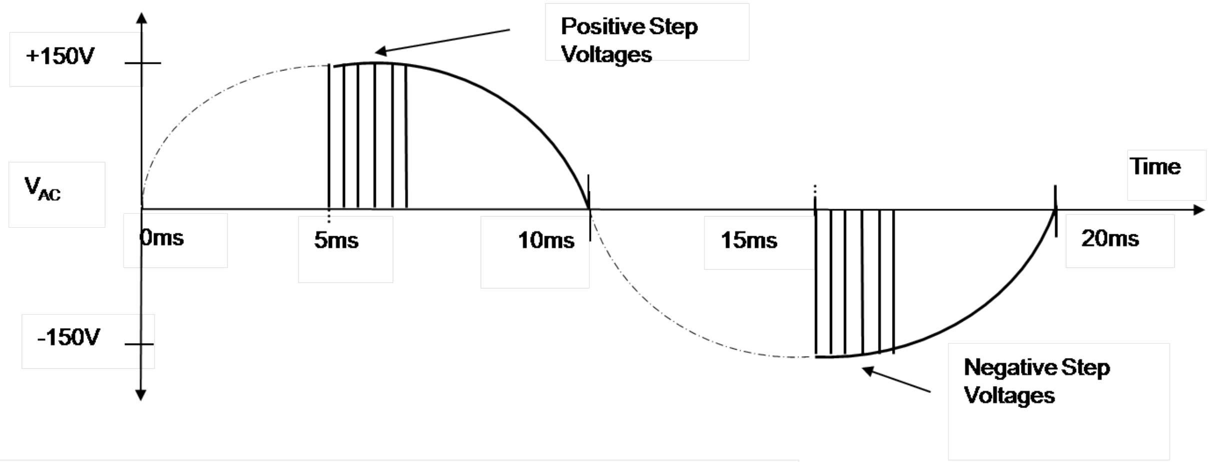


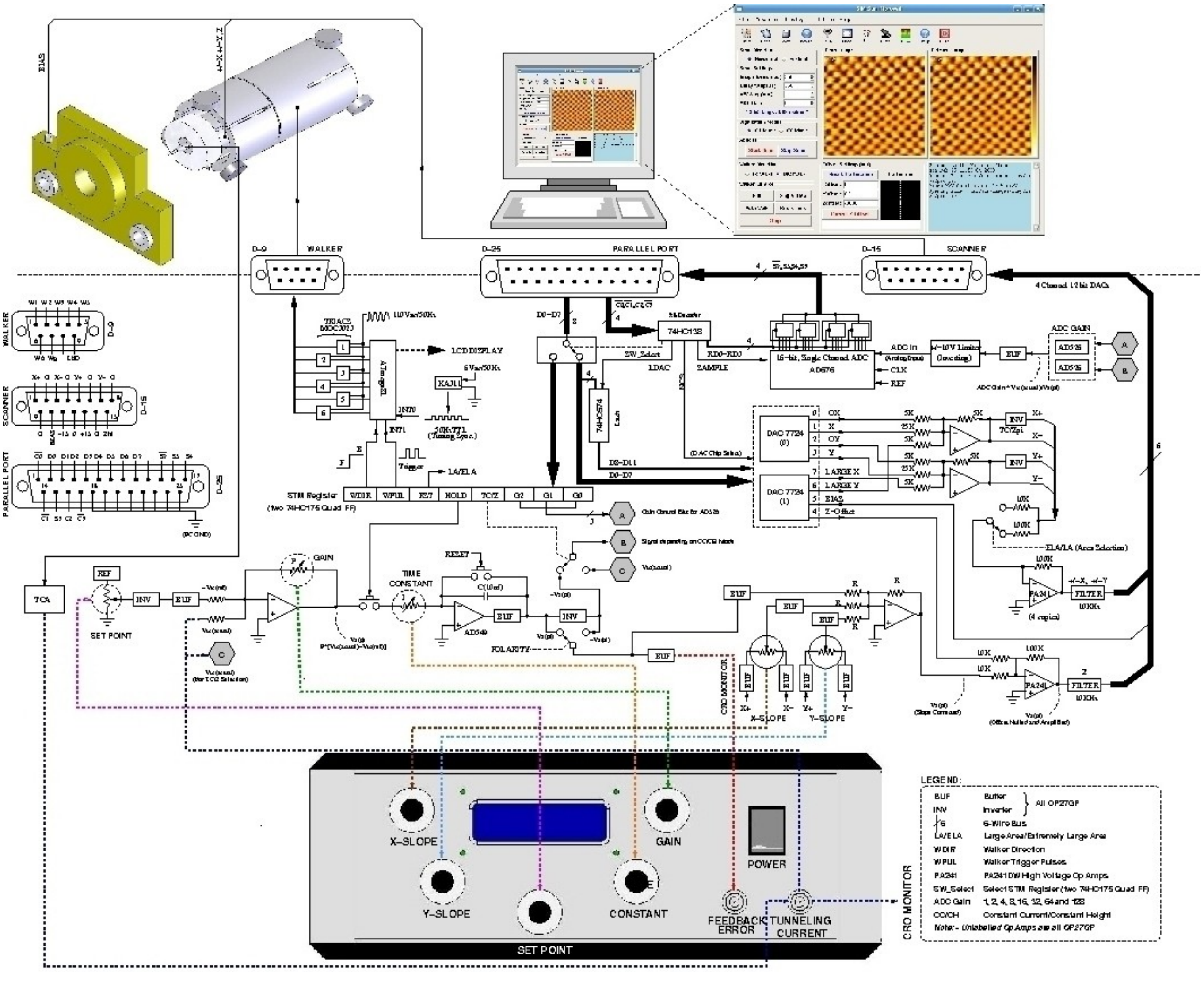
Fig.5. The voltage waveform used for the walker motion(farward or backward) ; six vertical lines show the voltage steps for six sections of the walker tube and the later part of the waveform is same for all the sections.

If the walker assembly takes positive step voltages to make forward motion then the negative step voltages will give backward motion to the walker. These step voltages are extracted from 50 Hz ±150V peak-to-peak AC signal.

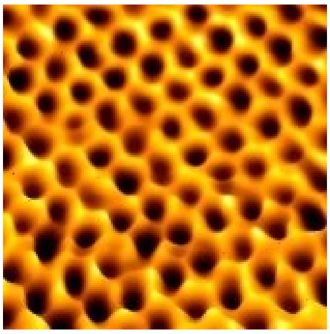
Software:

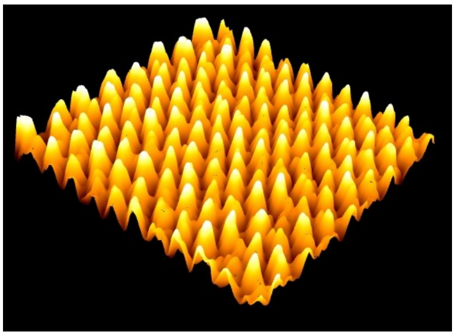
The acquisition and the analysis software for the STM is written with Python scripts and Tkinter for graphical user interface (GUI). A wrapper driver in C is written for the LPT oort and inserted as a kernel module.

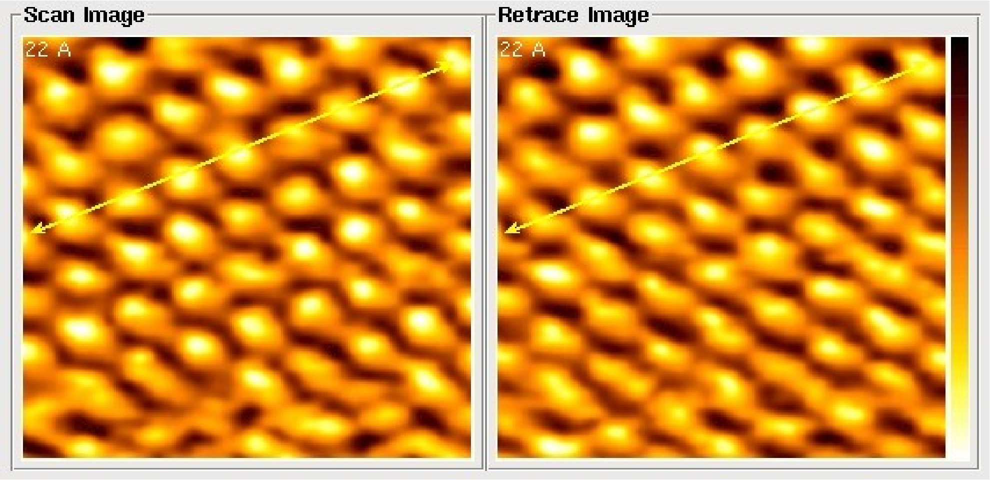
Overall design view of mechanical assembly of scan head piezo, sample holder , graphical user interface (GUI) and the control electronics :

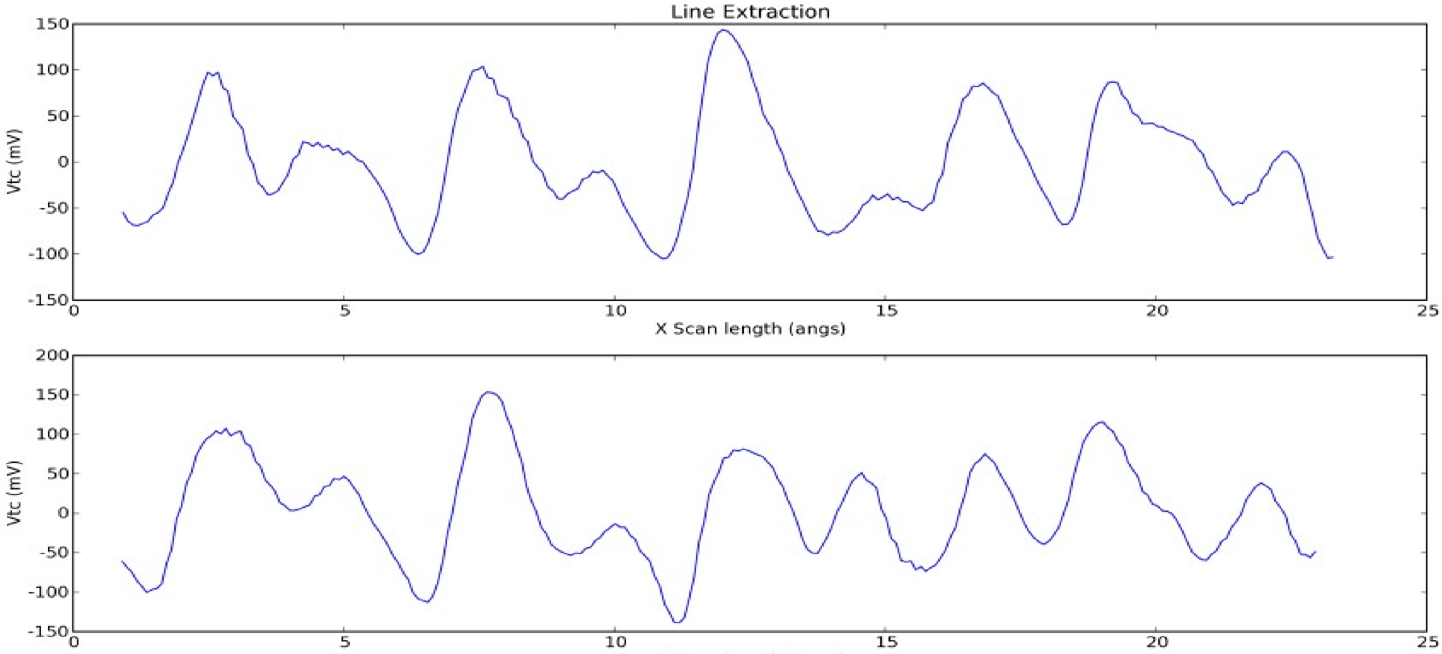


Results: Topographic image of Highly Oriented Pyrolytic Graphite (HOPG)









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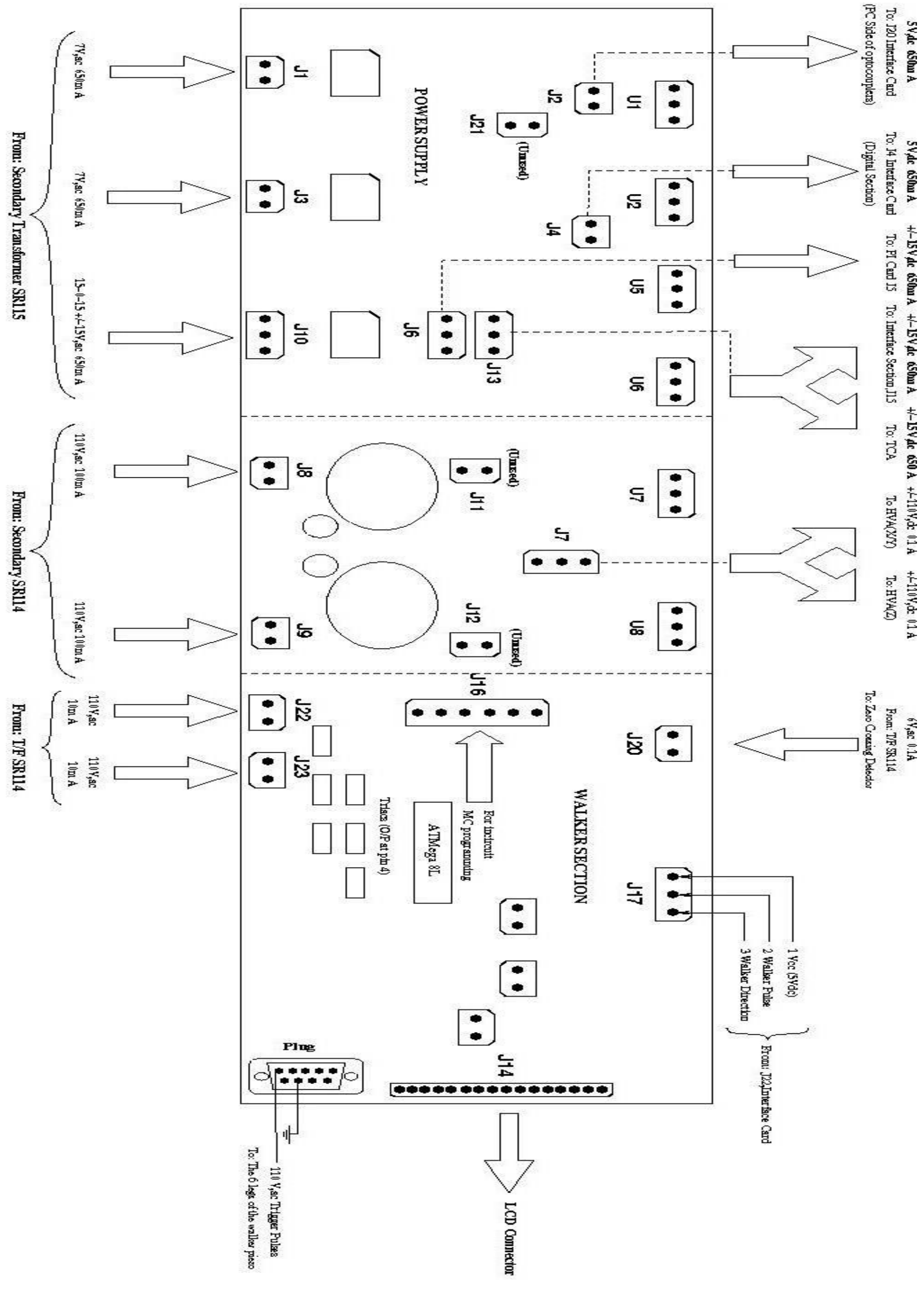
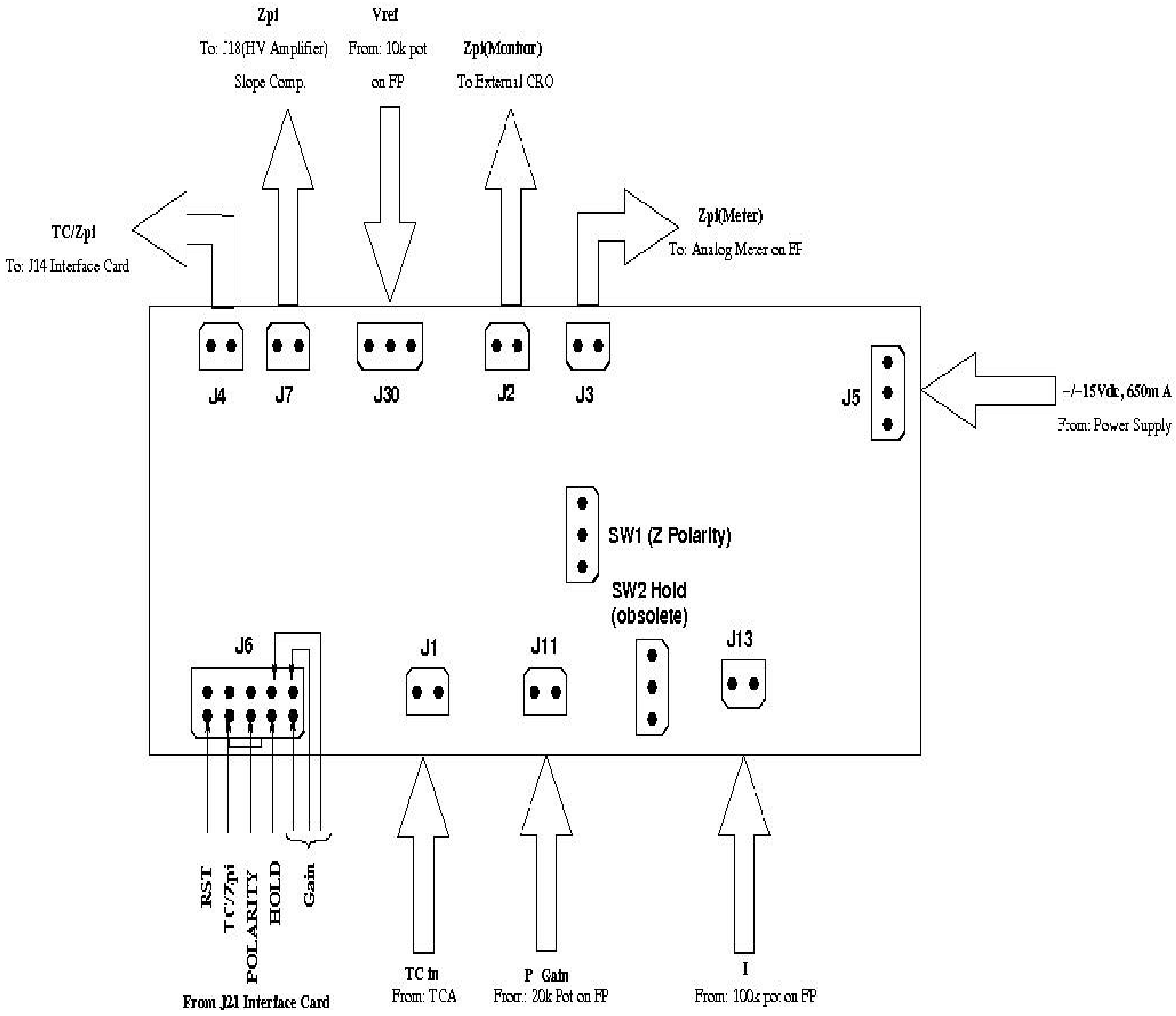
Functional Description of STM Electronic Cards:

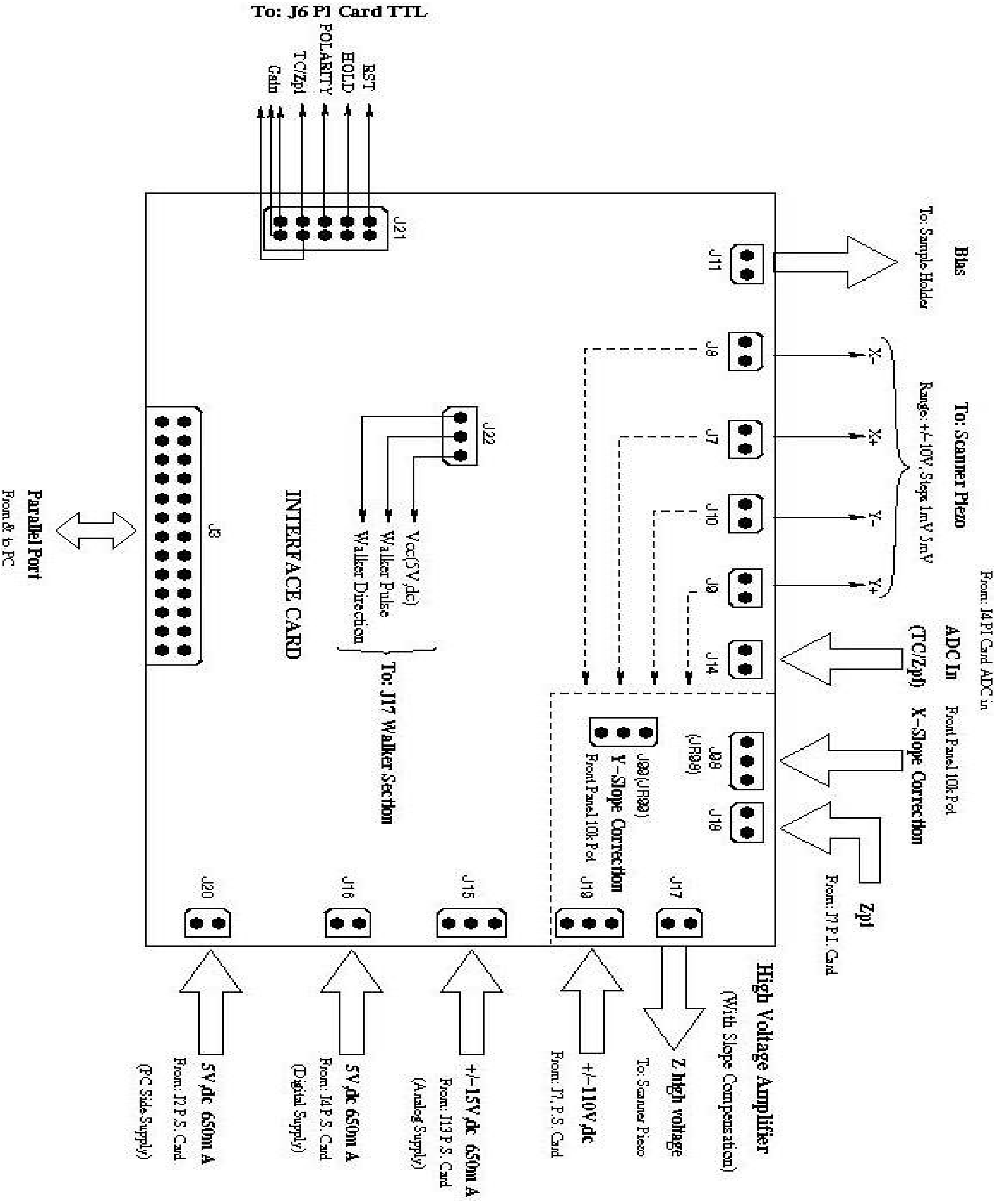
1. POWER SUPPLY AND WALKER CONTROL PCB assembly:



2. FEEDBACK CONTROL PCB assembly:



3. **DATA ACQUISITION and COMPUTER INTERFACE board assembly:**



4. **TUNNELING CURRENT AMPLIFIER PCB assembly:**