STM Simulator Documentation - 10/28/2017

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1. INTRODUCTION TO SCANNING TUNNELING MICROSCOPY

A Scanning Tunneling Microscope (STM) can image the surface of a sample of an electrically conductive material such as metals or semi-conductors at atomic resolution. First a sharp metal tip is brought near to the surface of the sample and a bias voltage is applied between the tip and the sample to cause a current of tunneling electrons. This current is strongly dependent on the distance between the tip and the surface of the sample, the bias voltage, the density of states for electrons or holes in the tip and sample, and other parameters such as the resistance of the sample. It is generally necessary to prepare the sample by chemical cleaning or cleaving to have a well-defined surface, and the STM is often operated in vacuum or controlled atmospheres. Vibration isolation and temperature control are also required.

The tip-sample distance is less than 1 nanometer in quantum tunneling, and this distance must be carefully controlled to prevent “tip-crash” or the cessation of tunneling. Images are obtained by scanning the tip over the surface of the sample. Typically, the tip is mounted on a piezoelectric actuator (PA) to control its position in three-dimensions to accomplish both control of the tunneling current and lateral scanning over the surface. The voltage applied to the PA generates relatively small displacements and a digital stepper motor is generally used to provide greater dynamic range in the motion.
The tip is scanned over the surface of the sample in one of two modes. In the ‘Constant Height’ mode, the voltage to the PA is constant and the measured variation in the tunneling current during a scan is used to determine the local topology of the sample. In the ‘Constant Current’ mode, the voltage to the PA is varied by feedback control to maintain a chosen value of the tunneling current and the measured variation in the voltage to the PA that is required to maintain this current is used to determine the local topology of the sample.

The NewPath Research STM Simulator presented herein, implements the Constant Current mode along with a variety of control algorithms to establish and maintain a specified “setpoint” value for the tunneling current. The Constant Height mode is also implemented, but this mode is only appropriate for samples with relatively flat surfaces or when imaging small areas that are relatively flat, and it will frequently cause loss of tunneling or “tip-crash”. The various control algorithms that are implemented have different effects which the user will see when they are selected, such as changing the response time and the stability of the tunneling current.

2. TYPICAL GRAPHS OF THE OUTPUT FROM THE STM SIMULATOR

The following graphs contain information on the various measurements and controls used to operate the STM simulator. Each graph is plotted against the simulated time. In the STM simulator, the simulated time is calculated such that it takes 1ms for each feedback voltage correction applied, and 10 ms for every step using the stepper motor. Depending on the sophistication of the simulation procedure it may take longer to simulate the creation of the image than to actually do it with a physical instrument based on the same algorithm.

Tunneling Current vs. Time (Short Term)

This graph shows the tunneling current as a function of simulated time. The tunneling current is a measure of the rate that electrons tunnel to or from the tip. The average value of the tunneling current increases as the tip-sample distance is reduced which includes the effects of the simulated slow drift due to temperature changes and vibration. The instantaneous value of the current shows the additional effects of the simulated noise.
The ‘Data Points’ slider adjusts the number of the most recently measured tunneling currents that are displayed on the graph. Fewer data points allow a closer look at the short time-scale changes whereas a larger number of data points lets one see more of the history of the tunneling current.

Tunneling Current (Long Term)

This graph displays the entire record of the tunneling current during the present session. The plot is updated at regular time intervals and can be set by the user in the ‘Sample Interval’ field. The plot also updates when a new maximum tunneling current is observed.
Piezo Voltage vs. Time (Short Term)

This graph plots the applied voltage on the piezoelectric actuator (PA) as a function of time. In constant current mode, this voltage is adjusted to attain a tunneling current that fluctuates about the set-point current. The voltage change as a function of time plotted for the sequence of steps in a scan indicates the change in the local topology of the sample. In an actual STM this graph could also be used to determine the effects of resonance in the PA.
Fractional Tunneling Current Error

This graph displays the normalized difference (in percent) between the measured tunneling current and the set-point current relative to the set-point current as a function of time. Quantizing this error is required to tune the control algorithms.

XY-Error

This graph displays the error in the X-Y position measured by the difference in the desired and current position at each movement. As the tip scans across the sample, peaks in the X-Y error plot will appear as the desired position shifts ahead to each new position. The aim in tuning the X-Y position controls is to reduce the space between the peaks without much overshoot. The fine resolution in this figure is determined by the choice of parameters that
were used in this simulation. For this image an ideal situation is assumed where the voltage step size is 150 μV with a piezo gain of 24 nm/V such that the step size for the piezoelectric actuator would be $3.6 \times 10^{-12}$ meters.

**Distance based on Piezo Voltage**

This graph plots the piezo spatial displacement distance based on the applied PA voltage and the piezo gain (m/V). There are two plots displayed on this graph: the calculated distance based on the piezo voltage (black), and the averaged distance based on the piezo voltage (blue).

When the tip reaches and settles at each chosen X-Y position, a given number of samples (set by “Samples to Average”) are recorded and averaged. That average is assigned as a Z-value to that pixel. With the Z constraint enabled, measurements are not made unless the tip
position is settled on the Z-axis as well. As the tip settles at a specific position, the calculated height is not included in the average unless the measured current is within a given tolerance of the set-point current. Black lines on the graph indicate samples that have been included in taking the average. On this graph, when a scan is in progress, you should expect to see a profile of the surface that is being scanned. When scanning is disabled, or when a scan is finished, you should expect to see a fairly constant line through the middle. Because the graph is auto scaled the plotted distance will appear the same as the scan profile.

**Scan Image**

This topographic image shows the distance based on the piezo voltage. The topology (meters) of the sample is mapped to a color gradient. This is only a relative distance so the minimum and maximum values must be adjusted. The extremes of the color gradient can be either manually adjusted by changing the ‘Scale Maximum’ and Scale ‘Minimum’ input fields or automatically adjusted by setting the ‘Auto Scale’ field to ON. When auto scale is enabled, both extremes are set to the most recent measured value for the height. As long as it is enabled, auto scale expands the maximum and minimum extremes according the highest and lowest values that are encountered.

A cursor feature allows the user to perform separation measurements on the scanned image. To initiate this feature click ‘Show’ underneath the ‘Cursors’ field. Two cursors can be positioned by the user to arbitrary points on the image. From the cursor positions on the image, the difference in the X, Y, Z coordinates between cursors are calculated as well as the separation between cursors in the XY plane.

At the top of the image scan there are four buttons to help manage and save the collected data. The Reset Image button will clear the image and allow for a new scan to begin again. The Save Image button will open a dialog box where you can choose the file location; the image will be saved in the portable network graphics (png) format. The Export Data button will open a temporary file in Excel populated with a 2D array of values. At this point the user can rename the temporary file and save it to a location of their choosing. The Generate 3D Plot button is discussed in the next section.
3D Plot

When at least one line of a scan has been completed, you can click “Generate 3D Plot,” and a window will open where a 3D plot will be displayed. In order to rotate the 3D image, click and drag on the plot. In order to zoom in and out, hold down the shift key while you click and drag your mouse up or down. Other settings can be accessed when you right click on the plot and go to “3D Plot Properties.”
3. Z CONTROL ALGORITHMS

Control algorithms are needed to properly implement constant current mode such that the measured tunneling current fluctuates about a nominal set point current. The algorithms listed below implement the feedback using various methods and can be explained in more detail by clicking on their respective help button. For each algorithm, a voltage correction to the piezo adjusts the tip position. Since a digital control is used, the voltage applied is coerced to a discrete value that is set by the voltage resolution of the digital to analog converter (DAC).

Unmodified PI

The ‘Unmodified PI’ control algorithm is based upon the general proportion, integral, and derivative (PID) control:

\[ V_C(t) = K_P e(t) + K_I \int_0^t e(t')dt' + K_D \frac{de(t)}{dt} \]
Here $e(t)$ is the error value represented by the residual between the tunneling current and the set-point current, $e(t) = I_T(t) - I_{SP}$, and $K_P$, $K_I$, and $K_D$ are coefficients that determine the contribution of the proportional, integral, and derivative terms, respectively. Due to high-frequency noise the derivative coefficient is generally ignored with an STM so that $K_D = 0$. When simulating the operation of an STM, the time is discretized such that $t \rightarrow t_i$. Thus, the integral is transformed to a summation over $n$ time steps. Additionally, the residual term can be rewritten as a normalized fractional error by dividing by the difference between the measured tunneling current and the set-point current by the set-point current, $e_N(t) = (I_T(t) - I_{SP})/I_{SP}$. This lets the control algorithm handle both positive and negative bias voltages. The resulting voltage correction is then written as

$$V_C(t_i) = K_P e_N(t_i) + K_I \sum_{k=0}^{n-1} e_N(t_{i-k}) \Delta t$$

Others have shown how differential equations may be used to model PID control, and in general there are specific rules to “tune” such a system. We have characterized our STM simulator by comparing the stability of tunneling using different values for the Proportional Coefficient and the Integral Coefficient. In the following figure, the region providing stable initial establishment of tunneling (Green) is shown with some of the points defining the outer limits for that region.
The stability was also determined for two other criteria: providing stable tunneling during scanning after tunneling is established. The regions corresponding to these two criteria are progressively larger. That is, it is easiest to maintain tunneling while not scanning. For each of these three criteria, the response is too slow so there is tip crash below or to the left of the stable region (too small a value for the Proportional Coefficient or the Integral Coefficient). Large oscillations occur in the tunneling current above or to the right of the stable region. This may be understood because when the Proportional Coefficient is too large—consider a pendulum as a feedback system having only proportional control. Also, when the Integral Coefficient is too large, each time the set-point Current is crossed the time is increased for the integral to be brought to zero and then reverse its sign.

**Modified Proportion**

The modified proportion algorithm implements the feedback control of the tip position using a voltage correction that is based on only a proportional term multiplied by the normalized fractional error of the tunneling current and set-point such that,

$$ V_C(t_i) = K_p e_N(t_i). $$
However, in the modified proportion algorithm the value of the coefficient is variable and dependent on a condition set by previous values of the normalized fractional error. Specifically, if the sign of the normalized fractional error is constant over the two most recent measurements of the tunneling current, or alternatively $sgn(e_N(t_1)) + sgn(e_N(t_{l-1})) \neq 0$, an additional multiplier is included in the value of the proportional coefficient:

$$K_{P_2} = K_P(1 + M_A).$$

In the opposite case where the sign of the normalized fractional error changed between the last two measurements, such that $sgn(e_N(t_1)) + sgn(e_N(t_{l-1})) = 0$, the coefficient is then,

$$K_{P_2} = K_P.$$

The two terms $K_P$ and $M_A$ are set and optimized by the user. The general idea with this algorithm is that if the sign of the normalized fractional error is constant over successive measurements an additional factor, $M_A + 1$, is included in the voltage correction. In the case where the sign changes between measurements of the tunneling current, meaning that the tunneling current has gone over or under the set-point current, a smaller proportional term is used.

**Digitally Adaptive Steps (DAS)**

The DAS algorithm switches the piezoelectric actuator step sizes between coarse and fine voltage steps when the measured tunneling current crosses a user-defined threshold. The threshold is set by a multiplicative factor (RMS Multiplier) of the non-tunneling current noise. In the simulator, this is determined by the value of the ‘RMS Meter Noise’ parameter given in the Settings tab. In a real world application, the RMS noise can be determined by measuring current fluctuations when the tip-sample distance is large since the current fluctuations should only be due to the precision of the experimental measurement apparatus and extraneous environmental influences. For tip movement in the vertical direction, coarse steps are initially used to quickly approach the sample. Once the tip-sample distance is small enough that the
measured tunneling current is greater than the RMS multiplier times the RMS noise value the
algorithm switches to use a finer step size. At each current measurement, the tunneling
current is compared to the set point current and the voltage step is applied such that the
tunneling current approximates the set-point.

The user is able to logically set three parameters: RMS Multiplier, Coarse Voltage Step
(V), and Fine Step (V). In the simulator it is suggested to use RMS Multiplier values between 1.0
and 10. The value for the Fine Step is defaulted to the smallest value possible as determined by
the voltage resolution of the DAC. This is a natural choice in the case that the RMS noise is
smaller than or on the order of the voltage resolution. However, if the RMS noise is much larger
than the voltage resolution larger fine step sizes are needed.

**Proportion + Average**

The “Proportion + Average" control algorithm considers the entire history of the error.
The voltage correction in this case is written as,

\[ V_C(t_i) = K_P e_N(t_i) + w_R K_A e_N(t_i) + (1 - w_R) A(t_i), \]

where

\[ A(t_i) = (1 - w_R) A(t_{i-1}) + K_A e_N(t_{i-1}) w_R \]

\[ A(t_0) = 0. \]

\( K_P \) and \( K_A \) are the coefficients for the weight of the proportion and average
components and \( w_R \) is a ratio that weighs the contribution of previous errors. The weight ratio
may be disabled in which case it defaults to 0.5, where the contributions of current and
previous terms are equally weighted.

**Constant Height Mode (Constant Piezo Voltage)**

The other control algorithms may be used to approach the sample. Then, when
Constant Height mode is enabled, the piezo voltage remains constant as it scans over the
sample. The image is built by plotting the calculated height based on measured current rather
than the piezo voltage. Constant height mode is appropriate for imaging small areas or samples with relatively flat surfaces. This control algorithm is, however, prone to loss of tunneling or tip crash for samples that are not lying perfectly perpendicular to the tip.

**Tests for Software Verification**

Each of the control algorithms presented in the STM simulator are pre-set with default values and subsequently vary in the imaging quality and also the total simulated scan time. The table below demonstrates the approximate simulated time required to reach the first stepper motor step, the set-point value, and to complete an image scan for each of the respective control algorithms using the default parameters.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Simulated Time to 1st Stepper Motor Step (s)</th>
<th>Simulated Time to reach Set-Point (s)</th>
<th>Projected Scan Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unmodified PI</td>
<td>235.2</td>
<td>414.8</td>
<td>390000</td>
</tr>
<tr>
<td>Modified P1</td>
<td>785.4</td>
<td>1299</td>
<td>426000</td>
</tr>
<tr>
<td>Modified P2</td>
<td>912.8</td>
<td>1511</td>
<td>442000</td>
</tr>
<tr>
<td>Modified P3</td>
<td>914.2</td>
<td>1315</td>
<td>407900</td>
</tr>
<tr>
<td>DAS</td>
<td>1315</td>
<td>2205</td>
<td>424000</td>
</tr>
<tr>
<td>Proportion + Average</td>
<td>137</td>
<td>226</td>
<td>393000</td>
</tr>
<tr>
<td>Constant Height</td>
<td>NA</td>
<td>NA</td>
<td>289000</td>
</tr>
</tbody>
</table>

The results presented above will naturally vary due to the injection of noise into the simulation and measurements show that they fluctuate on the order of a 1% for the time taken to reach the first stepper motor step and the set-point but on the order of 10% for the total time needed to scan the image. It is noted that although the time taken to reach the first stepper motor step and set-point vary significantly between control algorithms, the total expected scan times are approximately equivalent. This demonstrates that the time required for the tunneling current to approximate the set-point is highly dependent on the control algorithm. However, once tunneling is established, the choice of control algorithm is not as important in regards to the total scan time.
The nominal set-point used for these measurements is at a value of 500 nA. It is suggested that the user does not exceed this value as it makes each of the control algorithms highly prone to tip-crash. To maintain a higher set-point, the tip must be brought extremely close to the sample. Under these conditions, stepping in the X-Y plane can result in tip crash if the tip is located in a “valley” where the neighboring positions on the surface are higher than the tip position. A possible solution to this is to introduce much finer X-Y steps, however, a fundamental limit in the step size of the X-Y positioner is eventually reached. The alternative is then to reduce the set-point current, such that steps in the XY plane do not crash into the sample.

4. SIMULATION CALCULATIONS

Tunneling Current

The measured tunneling current based on the current separation between the tip and sample is calculated at each time step. The exact expression for the tunneling current is non-trivial and is dependent on source properties such as the lattice geometry, electrical configuration, and spreading resistance as well as experimental properties including the tip size and bias voltage. As a first-order approximation, the tunneling current is calculated as,

\[ I_t = \frac{AV Be^{-B z_d}}{1 + ARe^{-Bz_d}} \]

Where the R is the series (or constant spreading) resistance, A and B are tunneling current coefficients (described in “Settings”), and \( z_d \) refers to the vertical separation between the tip and the sample.

Simulated Surfaces

Each simulated surface is a unit cell in a tessellation pattern. The following images are produced from running the STM simulator on a unit cell from each surface material type. The geometry of the unit cells are based upon various experimental results. In addition to the surfaces shown below a sinusoidal surface is also included as a simple model for testing.
HOPG


Graphene


Silicon and Silicon Reconstructed


P. R. Watson, M. A. Van Hove and K. Hermann, NIST Surface Structure Database - Ver. 5.0 National Institute of Standards and Technology, Gaithersburg, MD (2004). The pictures have been prepared from NIST SSD output and processed with BALSAC by K. Hermann. SSD is the NIST Standard Reference Database no. 42 by P. R. Watson, M. A. Van Hove, and K. Hermann.
Slow drift

Slow drift error takes into account experimental factors such as vibration or thermal effects, or non-linear motion in the piezoelectric actuator or stepper motor, all which can create unwanted low-frequency displacements in the tip-sample distance. The STM simulator approximates this by generating random jumps in the tip-sample distance. At each moment the slow drift is implemented, there is an equal probability of upward, downward, or no shift. The time interval at which each step in the slow drift shift is generated is set by the Slow Drift Average Interval and the Slow Drift Interval Standard Deviation. The magnitude of each step is controlled by Slow Drift Step Amplitude.

Calculated Tunneling Current Coefficient (1/m)

The equation that is currently used to calculate the tunneling current in these simulations is as follows:

\[ I_t = \frac{AV_B e^{-B z_d}}{1 + AR e^{-B z_d}} \]

Where “B” is determined as follows:

\[ B = \frac{2\sqrt{2mq\Phi_{ev}}}{\hbar} \approx 1.025 \times 10^{10} \sqrt{\Phi_{ev}} \text{ mtr}^{-1} \]

Here \( \Phi_{ev} \) is the work function of the tip electrode in electron volts, m and q are the mass and charge of the electron, and \( \hbar \) is Planck’s reduced constant. The modular structure of the software permits adding more accurate methods of analysis used by others.


**Piezo Actuator Range (m)**

The Piezo Actuator Range is the maximum displacement the piezoelectric actuator can reach. It is limited to this range to maintain linear motion.

**Tip-Sample Distance when Current Equals Set Point (m)**

This uses the equation:

\[
Z_d = \frac{\ln \left( \frac{V_B}{I_{SP}} - R \right) + A}{B}
\]

To calculate what the distance should be at the set-point current. \(I_{SP}\) is the set-point current.

**SD of Tip-Sample Distance (m)**

The SD of Tip-Sample Distance is the standard deviation of the noise that is used to simulate the jitter of the stepper motor.

**Minimum Voltage Step Size (V)**

The Minimum Voltage Step Size is the minimum voltage change allowed due to the BITS. This voltage step size is calculated by taking the full rail to rail voltage and dividing by \(2^{BITS}\). In our calculation, voltage instability is neglected.

**Minimum Size of Piezo Actuator Step (m)**
The Minimum Size of Piezoelectric Actuator Step is the corresponding distance to the minimum voltage step size. It is calculated using the gain of the piezoelectric actuator multiplied by the “Minimum Voltage Step Size.”

**Piezo Voltage Required to Induce Tunneling Current (V)**

This value is the estimated piezo voltage needed to move from the surface of the sample to the threshold where tunneling can first be detected. A fraction of this size should be used in adjusting the coarse voltage step size of the D.A.S. control algorithm.

**Piezo Limit Between Steps (V)**

The Piezo Limit Between Steps is the maximum voltage allowed before taking a stepper motor step.
5. SETTINGS

**Surface Type**

The surface type can be changed using this drop down menu. The currently available surfaces are: Silicon (100), Silicon (100) Reconstructed, HOPG (Highly Oriented Pyrolytic Graphite), Graphene and Sinusoidal surfaces.

**Slow Drift Change Average Interval**

The Slow Drift Change Average Interval is the interval at which a shift is applied in either the positive direction, negative direction or not at all.

**Slow Drift Step Amplitude (m)**

The Slow Drift Step Amplitude is the distance shift that is applied at each interval to simulate slow drift, vibration and thermal effects.

**Slow Drift Interval Standard Deviation**

The Slow Drift Interval Standard Deviation is used to give a normal distribution to the slow drift interval.
**Initial Sample-Tip Distance (m)**

The Initial Sample-Tip Distance sets the initial distance between the sample and tip at the start of the program. In a real-world application, this can be approximated using measurement tools, however, in the code the default value is set to 100 nm.

**Tunneling Current Coefficient (Siemens)**

The Tunneling Current Coefficient $A$ is a constant used in the equation to calculate the tunneling current as a function of distance. In the STM simulator here the $A$ coefficient is set to 0.1.

**Tip-Sample Distance SD Coefficient**

The Tip-Sample Distance SD Coefficient includes the effects of higher frequency noise on the tip-sample distance. The noise is generated at each time interval by adding a random number generated using a normal distribution with a standard deviation corresponding to the Tip Sample Distance SD Coefficient.

**Current Meter Noise Coefficient**

The Current Meter Noise Coefficient represents the statistical noise associated with the measurement of the tunneling current. In actual applications this is set by the precision of the current meter used. In the STM simulator, this noise is generated at each time interval using a normal distribution with a standard deviation being the Current Meter Noise Coefficient.

**Additional Distance Adjust (Å)**

The Additional Distance Adjust allows instantaneous shifts in the z-position of the tip. This control may be changed as the simulation is running to test the responses of different control algorithms.
**Spreading Resistance (Ohms)**

The Spreading Resistance sets the value of R in the tunneling current calculation. In the STM simulator, this is assumed as a constant which is generally true for metals, but not for semi-conductors.

**Set-Point Current (Amps)**

The Set-Point Current is the nominal current that is maintained by the feedback algorithms. The recommended value for imaging is 500 nA which is set as the default value. In physical applications, the set-point current can be as low as 1 nA. Increasing the set-point current requires that the tip-sample distance to be reduced and generally this provides better imaging quality. However, by increasing the set-point current, there is a greater possibility for tip-crash. A lower value for the set-point current reduces the quality of the images, but will result in faster scans and lower probability of tip-crash.

**Bias Voltage (Volts)**

The Bias Voltage is the voltage difference applied between the sample and the tip. A greater bias voltage increases the rate of electron tunneling, but may make the STM behave unstably.
DAC Bits

In a real-world application, a digital to analog converter (DAC) is used to translate a digital number to an applied voltage on the piezoelectric actuator. For each control algorithm, the program simulates a digital to analog converter by coercing each change in voltage to a minimum possible step size. For a given number of bits, the minimum step size is determined by:

\[
\frac{V_{pp}}{2^{Bits}}
\]

Where \(V_{pp}\) is the DAC Voltage Range from peak to peak.

DAC Voltage Range (\(V_{pp}\))

This parameter sets the full voltage range capability of the digital to analog converter (DAC) in Volts from peak to peak.

Piezo Tube Gain (m/V)

The Piezo Tube gain parameter sets the given vertical displacement of the piezoelectric actuator for a given voltage input. This parameter is what is used to convert the applied voltage into a distance in order to map out the surface of the material.

Stepper Step Size (m)

The Stepper Step Size controls the size of a stepper motor step. The total number of steps taken can be viewed to the bottom right of the Long Term Tunneling Graph.

Tip Electrode Work Function (eV)

The Tip Electrode Work Function is used when calculating the distance as a function of tunneling current.
X-Y Position Standard Deviation (m)

The X-Y Position Standard Deviation sets the error distribution in the x and y axis’ positions. Each step of the program simulates a Gaussian x-y error around the target location. This error, from noise in the piezoelectric actuator, causes “blurring” in the images.

6. ABOUT

This program was developed in National Instruments™ LabVIEW™ and tested on three systems:

System 1
Windows 10 x64
Intel® Core™ i7 CPU 870 @ 2.93GHz
8.00 GB RAM

System 2
Windows 10 x64
Intel® Core™ i5-2400 CPU @ 3.1GHz
4.00 GB RAM

System 3
Windows 7 x64
Intel® Core™ i3 CPU M330 @2.13GHz
4.00 GB RAM

Version 1.1

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