Image-based measurement of periodic SPM trajectories

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Abstract— In this paper, measurement of periodic nano-scale scanning probe microscope (SPM) trajectories is achieved by extracting position information from images of standard SPM calibration samples. Image-based approaches have been applied to the measurement of low-speed effects and for the measurement and control of high-speed sinusoidal trajectories. The main contribution of this paper is the application of image-based methods to measure general periodic trajectories that can be represented by a truncated Fourier series. The image-based trajectory measurement approach is discussed in the context of a scanning tunneling microscope (STM) example and simulation results are presented that show the validity of the developed method.

I. INTRODUCTION

In this paper, the measurement of general periodic nano-scale scanning probe microscope (SPM) trajectories is achieved by extracting position information from images of standard SPM calibration samples. SPM devices are critical to the advancement of a broad range of nanotechnologies [1], but an inability to accurately measure the SPM probe trajectory precludes the use of standard control methodologies to improve speed and precision during nano and sub-nano scale operations. The main contribution of this paper is the application of image-based methods, previously used to measure sinusoidal SPM trajectories, to measure periodic trajectories that can be represented by a truncated Fourier series. This method is discussed in the context of a scanning tunneling microscope (STM) example and simulation results are presented that show the validity of the developed method.

Image-based approaches to measure SPM nanopositioning trajectories are advantageous in three cases: (i) when, both, high (angstrom scale) resolution and high operating speed are needed; (ii) when sensor integration is difficult; and (iii) for sensor calibration. First, the resolution of conventional sensors is limited during wide-bandwidth (high-speed) operations. For example, while the theoretical resolution of non-contact capacitive sensors is only limited by quantum noise, the effective noise factor is around $0.02nm/\sqrt{Hz}$ at room temperature. Thus, the resolution for a $1000Hz$ bandwidth is about $2nm$, which precludes the measurement of angstrom-scale SPM motion. In contrast, image-based methods exploit the existing, high-resolution, vertical sensor (probe-sample interaction) to achieve high-resolution estimates of the lateral position. Second, even when angstrom-scale resolution is not necessary, position measurements may be unavailable due to sensor integration issues, especially in highly-parallel SPMs (with parallel SPM probes) being developed to increase the throughput of SPM-based nanotechnologies [2]-[5]. In such highly-parallel SPMs, image-based approaches can be automated, thereby enabling improved control of each SPM probe. Third, even when sensors are available (such as embedded sensors for highly-parallel SPMs [1]), an image-based approach enables the independent calibration of the sensor to account for issues such as sensor misalignment, failure, and cross coupling [6]. Therefore, it is desirable to develop image-based methods to measure SPM-nanopositioning trajectories.

Image-based methods for SPM have primarily focused on the correction of relatively low-speed effects such as DC-gain [7], drift [8], and hysteresis [9]. More recently, image-based methods have been developed to model and correct for errors caused by dynamic effects at high-speeds [10]-[12]. This method uses distortions in high-speed SPM images of standard calibration samples to determine the trajectory followed by the SPM probe while the image was being acquired – the distortions are caused by an inability to track the desired trajectory during high speed operation. In Ref. [11], the use of this method, allowed for a 60 fold increase in operating speed, when compared to standard SPM imaging techniques.

The image-based approach used to measure SPM nanopositioning trajectories has, until this paper, only been applied to the measurement of sinusoidal trajectories [1]. The extension of this method to more complex trajectories has been hampered due to difficulties in the calculation of trajectory properties needed to guarantee accurate trajectory measurement [12]. This process is further complicated by uncertainty associated with the SPM output – i.e. the SPM output is not known until it is measured. Thus, the trajectory properties must be measured for a range of possible trajectories. In this paper, we develop techniques to calculate these necessary trajectory quantities, thus enabling the extension of the image-based method to the measurement of general periodic trajectories.

II. IMAGE-BASED SPM TRAJECTORY MEASUREMENT

A. SPM Imaging

To acquire an image, the SPM-probe is typically scanned above a surface, as in Fig. 1(a), using a periodic probe-position trajectory in the $x$ direction and an increasing probe-position trajectory in the $y$ direction, resulting in a raster scan pattern. During this scanning process, tip-surface interactions can be measured and plotted to create an image. For example, in the STM, variations in the tunneling current between the probe-tip and sample surface (related to the distance between the sample and the probe-tip, as well as the sample’s electronic properties [13]) can be measured and plotted with
respect to the desired probe position \((x_d, y_d)\) to produce an image as shown in Fig. 1(b).

Positioning errors lead to distortions in SPM-images. For example, if there is substantial difference between the desired SPM-probe position \((x_d, y_d)\) and actual position trajectories \((x, y)\), then the resulting images (plotted using \(x_d, y_d\)) will be distorted as shown in Fig. 1(c). Note that poor sensor resolution during wide-bandwidth (high-speed) SPM operation limits the ability to measure the SPM position trajectory and thus limits the ability to plot the sensor data against the actual \(x\) and \(y\) positions to obtain an undistorted image.

**B. Image-based trajectory measurement**

The position \(x\) of the SPM probe cannot be directly measured in high (angstrom scale) resolution SPM-positioning applications. Therefore, to enable measurement of these trajectories, an image-based approach is used to estimate the position trajectory \(x\). Note that, in the following, control of the \(y\) axis trajectory is not considered, because errors in the \(y\) axis tend to be considerably smaller than those in the \(x\) axis due to lower frequency content.

1) **Data points on position trajectory from image**: To determine data points on the SPM-position trajectory \(x\) from an image \(I\), points of interest (POI) in the image \(I\) are compared with POI in a statically-calibrated reference image \(I_{ref}\) acquired at a low scan frequency, e.g. see Fig. 1(b). The POI depend on the calibration surface, for example POI can include centers of carbon atoms in highly oriented pyrolytic graphite (HOPG) samples.

To illustrate this approach, consider the example in Fig. 2. A POI \(P\) from the image \(I\) (Fig. 2(b)) is acquired at time \(t_i\). The image \(I\) can be compared to the reference image \(I_{ref}\) (Fig. 2(a)) to find the corresponding POI \(P_{ref}\) in the reference image, \(I_{ref}\) — \(P\) and \(P_{ref}\) are the same point on the sample surface, they just appear at different locations in the two images due to positioning errors. Since the POI position does not change with the operating speed of the SPM, the location of the reference image \(P_{ref}\) can be used to infer the position of the POI \(P\) acquired at time \(t_i\), yielding a data point \(\{t_i, x(t_i)\}\) on the position trajectory \(x(t)\), as shown in Fig. 2(c). Similarly, other POI in the images can be used to obtain a set of data points

\[ X = \{t_i, x(t_i)\}_{i=1}^{N_t} \quad (1) \]

on the position trajectory \(x(t)\). Implementation details, such as image-processing to find the POI and mapping of the POI to the reference image, are discussed in [10], [11].

2) **Periodic trajectories**: If the same probe-position trajectory is followed for each scan line (as is the case in SPM imaging), then the position trajectory \(x(t)\) is periodic with time period \(T_p\). Therefore, the position trajectory \(x(t)\) only needs to be evaluated over the time interval \(T = [0, T_p]\). The data points at time instants \(t_k\) outside this time interval \(T\) can be mapped into time points \(t_k\) in the time interval \(T\) where

\[ t_k = \tilde{t}_k + N_k T_p \quad (2) \]

for some integer \(N_k\). This set of new data points \(X = \{t_k, x(t_k)\}\) can now be used to determine the position \(x(t)\).
3) Reconstruction of position $x(t)$ from points $X$: In the following, the trajectory reconstruction problem is defined and an image-based reconstruction theorem is presented.

a) Reconstruction problem definition: For a position trajectory $x(t)$ that is band limited to $f_{bw}$ Hz (i.e., frequency content is zero above $f_{bw}$) and a specific calibration sample (i.e., a defined POI pattern), the problem is to reconstruct the position trajectory $x(t)$ from the set of data points $X$ obtained from the image-based approach in Sec. II-B.1.

b) Reconstruction Conditions: The position signal $x(t)$ can be reconstructed from a set of data points provided the image-based approach results in a sufficient number of well-spaced data points in $X$, as shown in the following theorem [12].

**Theorem:** [Image-based reconstruction] The reconstruction problem ($X \rightarrow x(t)$ in Sec. II-B.3.a) can be solved if the minimal range $\delta$ of the position trajectory over all time intervals of length $T_{ny}$/2 (example range over an interval is shown in Fig. 3(a)) is greater than the maximal spacing $\Delta_x$ between adjacent POI along the scan trajectory $x(t)$, shown in Fig. 3(b), i.e.

$$\delta > \Delta_x, \quad (3)$$

where $T_{ny}$ is the Nyquist period, $T_{ny} = 1/(2f_{bw})$.

Furthermore, when the position trajectory is periodic (with period $T_p$), let the POI in the scan area be projected onto the $x$ axis and let the maximal spacing between adjacent projected POI along the $x$ axis be $\Delta_{x,p}$ as shown in Fig. 3(b). Then, the reconstruction problem can be solved provided

$$\delta > \Delta_{x,p}. \quad (4)$$

III. CALIBRATION SURFACE AND DESIRED TRAJECTORY CHOICE

As shown in the above theorem, properties of the calibration surface and the probe-trajectory, the maximal distance between adjacent POI $\Delta_{x,p}$ and the minimal range $\delta$, respectively, must be chosen to satisfy the condition in Eq. 4. In the following, these properties are discussed.

A. Calibration sample properties

The effects of calibration sample properties on the maximal spacing $\Delta_{x,p}$ between adjacent, projected POI along the $x$ axis (see Eq. 4) were investigated in Ref. [12]. Two important results regarding calibration surfaces with hexagonally organized surface features are repeated here as they are pertinent to the present discussion. Note that the following results are presented in terms of properties of the calibration sample, the distance between features $l$ and the rotation of the sample $\phi$, as shown in Fig. 1(b)

1) Worst-case sample orientation: Over all orientations $\phi$, the worst-case, maximal distance between adjacent projected POI occurs when the orientation is $\phi = \pi/6$ and is given by

$$\Delta_{x,p} = l \cos(\pi/6). \quad (5)$$

At this worst-case orientation, many POI project on the same point on the $x$ axis as shown in Fig. 3(b).

2) Optimizing surface orientation: For the maximal distance between projected POI $\Delta_{x,p}$ to be small, the number of POI should be large and, ideally, equally spaced in the $x$ direction, see Fig. 3(c). This occurs at the optimal deviation $\Psi^*$ (from orientation $\phi = \pi/6$), which was found as

$$\Psi^* = \tan^{-1} \left( \frac{\sqrt{3}}{4N_s + 1} \right), \quad (6)$$

where $N_s = \lfloor A/l \rfloor$ is the number of features that are directly above the center feature in the worst case orientation. Note that $\lfloor \cdot \rfloor$ denotes the floor function and $A$ is the probe trajectory amplitude. The corresponding smallest maximal distance between projected POI is

$$\Delta_{x,p} = l \sin(\Psi^*) = l \sin \left[ \tan^{-1} \left( \frac{\sqrt{3}}{4N_s + 1} \right) \right]. \quad (7)$$
B. Probe trajectory properties

The effects of trajectory properties on the minimum range \( \delta \) (see Eq. 4) are investigated in the following. Consider the general periodic trajectory

\[
x_d = \sum_{n=1}^{N} a_n \cos(2\pi fn t + \phi_n).
\]  

(8)

where \( a_n \) and \( \phi_n \) are the coefficients and phase shifts of the \( n \)th harmonic, and \( f \) is the frequency. This expression is valid for any periodic trajectory, such as cosinusoidal or triangular, and \( a_n \) and \( \phi_n \) can be calculated from measured trajectory data or through root-finding techniques such as the MATLAB function roots.

The minimum range of this trajectory must be found over all intervals of length \( l_T = \frac{T_p}{2} = \frac{1}{2N} \) T. In the following, without loss of generality, the frequency will be set to unity \( f = 1 \), thus \( l_T = \frac{1}{2N} \).

1) Minimum range for a general trajectory: In general, the minimum range of the trajectory \( x_d \) in Eq. 8 can be calculated as

\[
\delta = \min_{t \in [0,T_p]} \{ \max_{t' \in T} \{ x_d(t') \} - \min_{t' \in T} \{ x_d(t') \} \},
\]  

(9)

where the interval \( T = (t - \frac{1}{8N}, t + \frac{1}{8N}) \) has length \( l_T = \frac{1}{2N} \) and \( T_p \) is the period of \( x_d \). The calculation of minimum range \( \delta \) was studied for sinusoidal trajectories in [12] and for general trajectories with \( \phi_n = 0 \) \( \forall n \) in [14].

2) Minimum range \( \hat{\delta} \) approximation: For the general trajectory \( x_d \) in Eq. 8, the minimum range \( \hat{\delta} \) is approximated as follows. In a general interval \( (t_0 - \frac{1}{8N}, t_0 + \frac{1}{8N}) \), the trajectory can be approximated using a Taylor series expansion as

\[
x_d = \sum_{n=1}^{N} a_n \sum_{m=0}^{M} \frac{\partial^m}{\partial t^m} \cos(2\pi nt_0 + \phi_n)(t - t_0)^m + R_M(t),
\]  

(10)

where \( t_0 \) is the center of the interval and the Lagrange form of the remainder \( R_M(t) \) can be written as

\[
R_M(t) = \frac{\partial^{M+1}}{\partial t^{M+1}} \cos(2\pi n t + \phi_n)(t - t_0)^{M+1} + \frac{(M - 1)2\pi n t^{M+1}}{(M + 1)!},
\]  

(11)

where \( \epsilon \) is between \( t \) and \( t_0 \). Note that by changing the number of terms in the Taylor expansion \( M \), the accuracy of the trajectory approximation in Eq. 10 can be changed.

The Taylor series approximation of the trajectory in Eq. 10 yields a polynomial in \( (t - t_0) \), thus, the minimum and maximum of the trajectory \( x_d \) necessary to calculate the range (the inner portion of Eq. 9, can be found using standard polynomial root finding techniques such as the MATLAB command roots. This process can then be repeated for varying times \( t_0 \in [0,T_p] \), and the minimum range over all these points can be found, as in Eq. 9.

As an example of calculating the minimum range \( \hat{\delta} \), consider the approximate triangular trajectory shown in Fig. 4 and given by the truncated Fourier series

\[
x_d = \sum_{n=1,3,5} k \frac{A}{n^2 \pi^2} \cos(2\pi nt),
\]  

(12)

where \( A \) is the trajectory magnitude and \( k = \frac{A}{\sum_{n=1,3,5} \frac{1}{n^2 \pi^2}} \) is a multiplication factor that scales the trajectory \( x_d \) so that it has an amplitude \( A \).

Using the Taylor series approximation method described above, the minimum range was calculated as \( \hat{\delta} = 0.345A \). This can be verified by inspecting the trajectory \( x_d \) in Fig. 4. The minimum range occurs at the turning point (i.e. \( t = \frac{T}{2} \)). Thus, the minimum range can be found as \( \hat{\delta} = x_d(\frac{T}{2}) - x_d(\frac{T}{2} + \frac{1}{8N}) = 0.345A \), which confirms the approximation.

3) Errors in the trajectory: The above method allows for the approximation of the minimum range, however, this is only possible provided the trajectory \( x_d \) is known a priori. In general, this is not the case due to positioning errors caused by the dynamics of the SPM positioner. For example, an inverse input can be developed using a model of the SPM dynamics \( G \) as follows

\[
u_{inv} = \sum_{n=1}^{N} \frac{a_n}{M(2\pi n)} \cos(2\pi nt + \phi_n - \hat{\theta}(2\pi n)),
\]  

(13)

where \( \hat{M}(2\pi n) = |\hat{G}(2\pi n)| \) is the magnification and \( \hat{\theta}(2\pi n) = \angle G(2\pi n) \) is the phase shift of the model \( G \). Provided the model \( \hat{G} \) is accurate, this input will result in a perfectly tracked trajectory (after transients have died out) and the minimum range \( \hat{\delta} \) of the output will be as calculated above. However, if modeling error exists, i.e., the actual magnification and phase shift \( M(2\pi n) \) and \( \theta(2\pi n) \) differ from the model, i.e., \( M(2\pi n) = \hat{M}(2\pi n) \Delta M_n \) and \( \theta(2\pi n) = \hat{\theta}(2\pi n) + \Delta \theta_n \), then the output trajectory will be

\[
x = \sum_{n=1}^{N} a_n \Delta M_n \cos(2\pi nt + \phi_n + \Delta \theta_n)
\]  

(14)

and will have error

\[
e = x_d - x = \sum_{n=1}^{N} a_n C_n \cos(2\pi nt + \phi_n + \beta_n)
\]  

(15)

, where \( C_n = \sqrt{1 + \Delta M_n^2 - 2 \Delta M_n \cos(\Delta \theta_n)} \) and \( \beta_n = \tan^{-1}\left( \frac{-\Delta M_n \sin(\Delta \theta_n)}{1 - \Delta M_n \cos(\Delta \theta_n)} \right) \). This error \( e \) presents a problem because, in general, modeling errors \( \Delta M_n \) and \( \Delta \theta_n \) are not known, making the output trajectory \( x \) unknown, so the minimum range \( \hat{\delta} \) cannot be easily calculated.
4) Calculation of minimum range for given modeling error: In order to find the minimum range of the probe trajectory in the presence of modeling error, the minimum range for a range of trajectories with varying amplitudes $a_n \Delta M_n$ and phases $\phi_n + \Delta \theta_n$, from Eq. 14, must be calculated. To do this, a minimum range calculation algorithm – approximate amplitude-linearity phase scanning (AALPS) – will be used. AALPS uses the approximately linear dependence of the of the minimum range $\delta$ on the amplitude terms $a_n \Delta M_n$ to reduce the search space for the minimum range $\delta$. To show this approximately linear dependence the minimum range $\delta$ can be rewritten assuming the time for the maximum of $x$ is $t$ and the time for the minimum is $\bar{t}$ as

$$\delta = \sum_{i=1,3,5} (a_n \Delta M_n \cos(2\pi n t_0 + \phi_n + \Delta \theta_n) - a_n \Delta M_n \sin(2\pi n t_0 + \phi_n + \Delta \theta_n)) - \cos(2\pi \bar{t}) \sin(2\pi \bar{t})].$$

(16)

The variation of the maximum and minimum times $t$ and $\bar{t}$ is bounded, thus the terms in square brackets are approximately constant, showing an approximately linear dependence on the amplitude terms $a_n \Delta M_n$. Given this almost-linear dependence on $a_n \Delta M_n$, the number of calculations for each phase $\phi_n + \Delta \theta_n$ combination is dramatically reduced.

5) Choosing ranges for the modeling error: Given a modeling error range, the AALPS algorithm can determine the minimum range $\delta$ for all possible probe trajectories $x$ – the probe trajectories will change based on the modeling error $\Delta M_n$ and $\Delta \theta_n$. This modeling error corresponds to trajectory tracking error $e$ as shown in Eq. 15.

Limits on this error come from the POI mapping algorithm being used. For example, for a proximity-based POI mapping algorithm, the error must be less than half the distance between features, i.e. $e < \frac{\bar{t}}{2}$ [11]. This yields the condition

$$e = \sum_{n=1}^{N} a_n C_n \cos(2\pi n t + \phi_n + \beta_n) < \frac{\bar{t}}{2}.$$

(17)

There are two scenarios that are of use to the SPM user: the modeling error a) increases progressively with frequency or b) is constant for all frequencies.

a) Progressive modeling error: Assuming that a model of the dynamics is not available, the input must be determined using known information. Typically, the input that was used to obtain the reference image $I_{ref}$ can be sped up to obtain the higher speed image $I$ [10], [11] – doing this uses the known low-frequency model to approximate the unknown higher-frequency model. As the speed of the input is increased (say by $\Delta f$), the frequencies of higher harmonics increase at higher rates – $f n$ is increased to $(f + \Delta f)n$. Thus, the known low frequency model is projected to higher frequencies for the higher harmonics, motivating a progressive modeling error.

b) Constant modeling error: Assuming a base modeling error of $\Delta M$ and $\Delta \theta$, an example choice of modeling error increase would yield an error relationship, from Eq. 17, as follows

$$e < \sqrt{N + (\Delta M)^2} - 2 \Delta M \cos(\Delta \theta).$$

(18)

Here the magnitude modeling error $\Delta M$ increases by power $n$, and the phase shift error $\Delta \theta$ is multiplied by $n$.

6) Choosing the trajectory amplitude $A$: In order to choose a trajectory amplitude $A$ that satisfies the image-based reconstruction theorem in Eq. 4, the effects of amplitude $A$ on the minimum range $\delta$ and the maximal distance between adjacent projected POI $\Delta x,p$ must be considered. For example, Fig. 5 shows both the optimal maximal distance $\Delta x,p$ from Eqs. 18 and 19 for $l = 2.46\text{Å}$ and the minimum range $\delta$ for the truncated triangular trajectory in Eq. 12 plotted versus the trajectory amplitude $A$. Note that the maximal distance between adjacent POI $\delta$ is related to the amplitude $A$ through the optimal rotation angle’s (Eq. 6) dependence on $N_s = \lfloor \frac{A}{T} \rfloor$. The modeling error values $\Delta M$ and $\Delta \theta$ used to find the minimum range $\delta$ are determined from Eqs. 18 and 19 for $l = 2.46\text{Å}$. From this plot, the magnitude $A$ must be chosen greater than approximately $A = 11\text{Å}$ if using a progressive modeling error (case a) or greater than approximately $A = 10\text{Å}$ if using constant modeling error (case b), in order to satisfy the image-based reconstruction theorem in Eq. 4. Note that the sample rotation angle changes with the maximal distance between adjacent POI as shown in Eq. 6.

IV. TRAJECTORY MEASUREMENT SIMULATION

Simulated STM images of HOPG were used to measure the probe position output, which is desired to have the triangular form in Eq. 12.
A. Simulation setup

Using the information in Fig 5, the trajectory magnitude was chosen as \( A = 11 \text{Å} \) (using a progressive modeling error), which corresponds to a sample rotation of \( \phi = 65^\circ \). Using this amplitude, a reference image \( I_{ref} \) and a high-speed image \( I \) with a desired scan area of \( 22 \text{nm} \times 22 \text{nm} \) were simulated and are shown in Fig 6(a) and (b), respectively. The POI in the images were chosen as the centers of the carbon atoms and the POI in the image \( I \) and the reference image \( I_{ref} \) were mapped based on proximity [10] – the POI are shown in the images as black asterisks. Additionally, the reference POI are shown on the high-speed image \( I \) in Fig 6(b) as white asterisks for reference.

B. Simulation results

Using the image-based measurement method, points on the probe trajectory were determined as shown in Fig. 6(c) as asterisks – note that these points are offset by 1 Å to differentiate them from the other data. These points were then used to develop a continuous probe trajectory by using a least squares fit, shown in Fig. 6(c) as a solid line. This resulted in a very accurate measurement of the probe trajectory. The image-based trajectory is almost identical to the simulated trajectory, shown in Fig. 6(c) as a dotted line, offset by 1 Å – this image-based measurement and simulation agreement is also shown by a maximum percent error of approximately 0.325% as shown in Fig. 6(d).

V. CONCLUSIONS

In this paper, measurement of general periodic nano-scale scanning probe microscope (SPM) trajectories is achieved by extracting position information from images of standard SPM calibration samples. The main contribution was the application of image-based methods to measure general period trajectories that can be represented by a truncated Fourier series. This method was discussed in the context of a scanning tunneling microscope (STM) example and simulation results showed the accuracy of the proposed method – the trajectory was measured with approximately 0.325% error.

REFERENCES