Feedback oscillations in STM imaging

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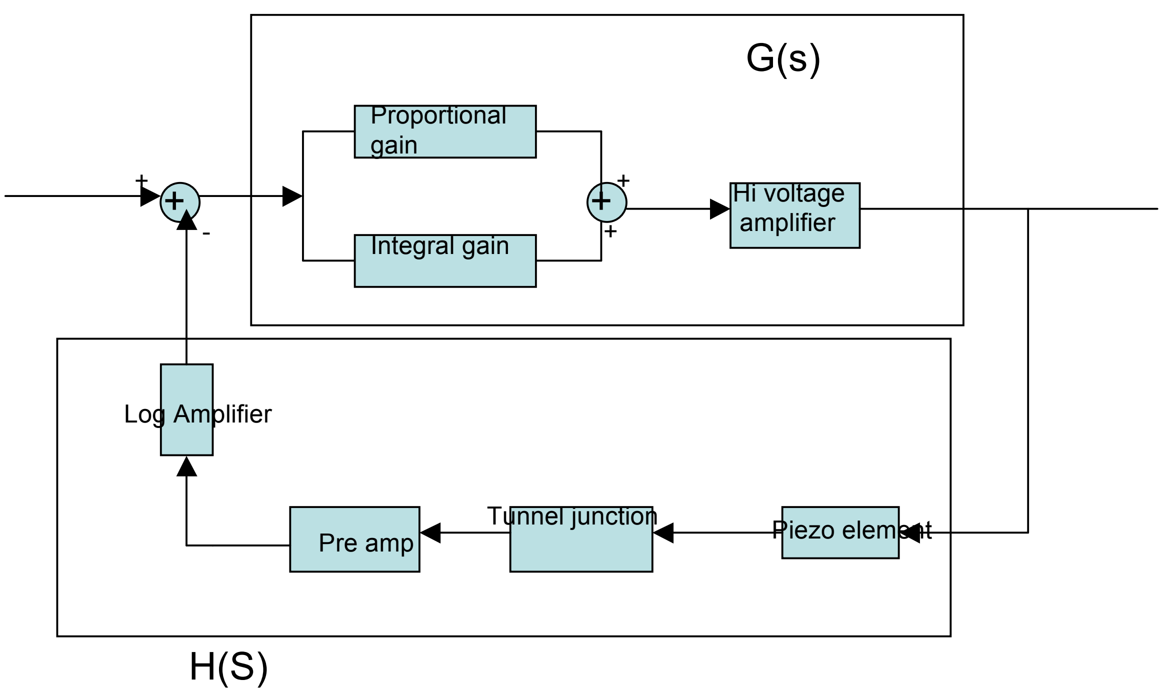
The working principle of STM is relatively simple. It is based on fundamental quantum mechanical principle postulated in 1920's by Gamow and Born and the experimental design of STM was awarded with 1986 Nobel Prize in physics to realize atomic-scale resolutions. STM complexity requires fast feedback electronic design, mechanical vibrations and noise insulation to implement control of bringing STM tip within one atom's diameter from the surface. Therefore, STM system must be fully characterized and very well tested, otherwise the images rendered by computer software could possibly be misinterpreted.



In order to image ligand-stabilized nanoparticles, STM feedback parameters must be set to perfectly trace non-planar surfaces. This can be done experimentally however simple theoretical considerations of the STM feedback system can give very useful insight in the possible effects that basic feedback control can interact with morphological features (nanoparticles) to result in feedback instabilities that manifest as nanoscale features. This short document will demonstrate that surface features Stellacci and coworkers describe in Nature Materials 2004 paper are direct consequence of feedback oscillations set by improper gain settings.

By using the block diagram from the above, the overall transfer function of the system is given by the following expression:

$$F(s) = \frac{G(s)H(s)}{1 + G(s)H(s)} \tag{4.1}$$

where $G(s)$ is overall transfer function of voltage amplifier (assume ideal amplifier) and piezo element. $H(s)$ is feedback control transfer function. To analyze only impact of integral gain on feedback stability, a simple expression can be used for H(s):

$$H(s) = \frac{A}{s} \tag{4.2}$$

where A is feedback gain. However, the transfer function for the STM mechanical system is not obvious. Piezo-response in control theory is typically modeled by a second-order response [1]. This means that the transfer function will have two poles which will result in oscillatory transient behavior. Typical piezoelectric actuator may have transfer function:

$$G(s) = k_p \omega^2 \frac{\alpha s + 1}{s^2 + \omega s / Q + \omega^2} \tag{4.3}$$

where k_p is the DC response of the piezoelectric (angstroms/volt), ω is the lowest resonance frequency , Q is the quality factor, and alpha determines the phase output. Therefore, the sole goal of the feedback control is to minimize the error function (actual minus reference reading) and this can be achieved only if the feedback system is stable (poles are on the left-hand side of the s-plane) and transient response must be appropriate for experimental requirements (oscillations must quickly exponentially decay) before scanner proceeds to the next scan point.

Coefficients in equation 4.3 can be obtained by applying a unit step reference signal to the piezo-actuator and reading the output on an oscilloscope. The Fourier transform of such measured response will contain several resonance peaks and each can be fit in the following form:

$$f(t) = Ae^{-Bt} Sin(Ct + D) \tag{4.4}$$

Any of them can be used to adequately model the system response. Laplace transform into s-space of Eq. 4.4 is compared to estimate unknown parameters in Eq. 4.3.

Typical values for a piezo actuator are used from reference [1] and they can be used to qualitatively describe feedback response:

$$\omega = 7 \times 10^3 \, rad / \mathrm{sec}$$
$$Q = 20$$
$$\alpha = 2.6 \times 10^{-5} \, \mathrm{sec}$$

The stability of feedback loop can be directly verified by plotting the poles in the complex plane as a function of the feedback parameter A. Such plot can be used to determine the maximum value of A for imaging stability. However, much more sophisticated models have been developed to analyze STM feedback [2] that are beyond the scope of this document and unnecessary to invoke as the imaging problem can be explained more elegantly by the second-order linear response model.

Figure 4.1 illustrates the step response to a unit step excitation for three different values of integral gain. It can be noticed that increasing integral gain will improve response but will also lead system into oscillations.

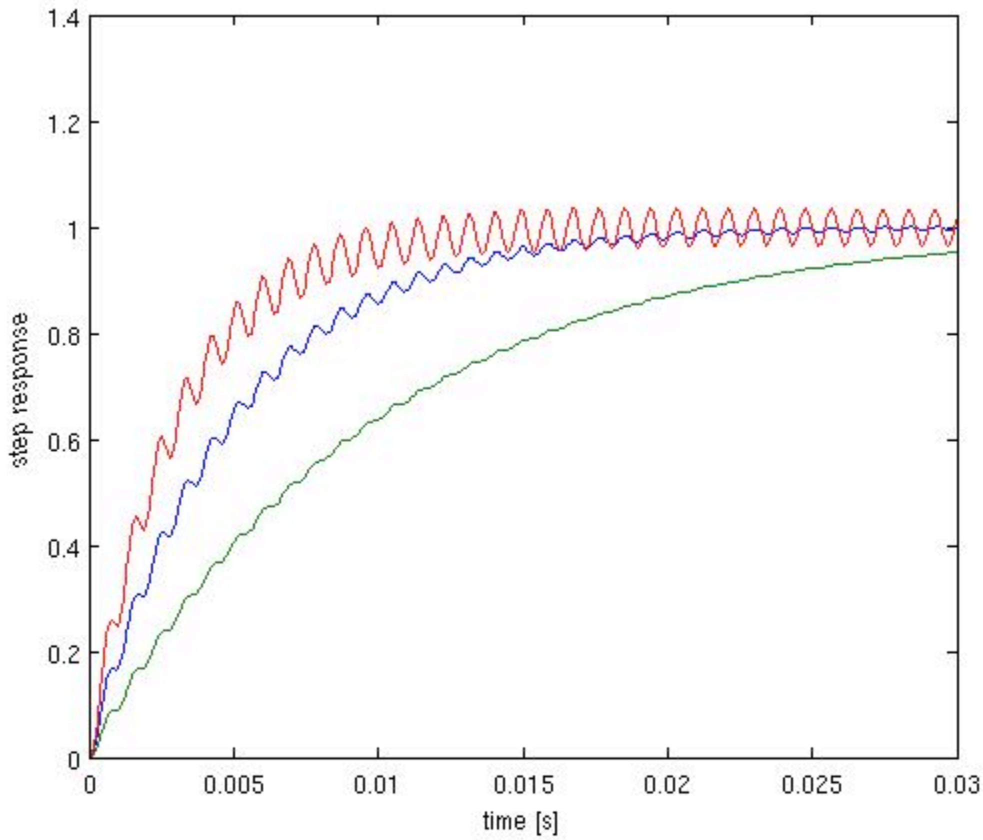


Figure 0-1. Step response for three different feedback parameters. Purple line corresponds to maximum allowable feedback parameter, all values beyond this one will produce exponentially increasing feedback oscillations.

Figure 4.1 also indicates that second-order system response system will equilibrate after about 20 ms. Images of nanoparticles are collected in 512x512 mode at scanning frequencies of 2 Hz (or higher) thus yielding a serious requirement of 0.5 ms for feedback to respond. Increasing the gain of integral controller will improve the rise time by just few milliseconds (Figure 4.2) but so it will increase the oscillatory behavior thus finally leading toward unstable state or feedback oscillations. (Figure 4.3)

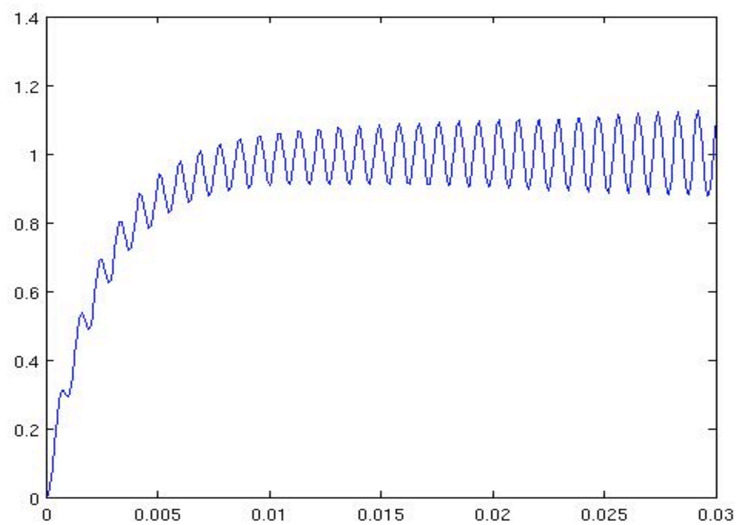


Figure 0-2. Feedback oscillations. Integral gain is set beyond the critical value.

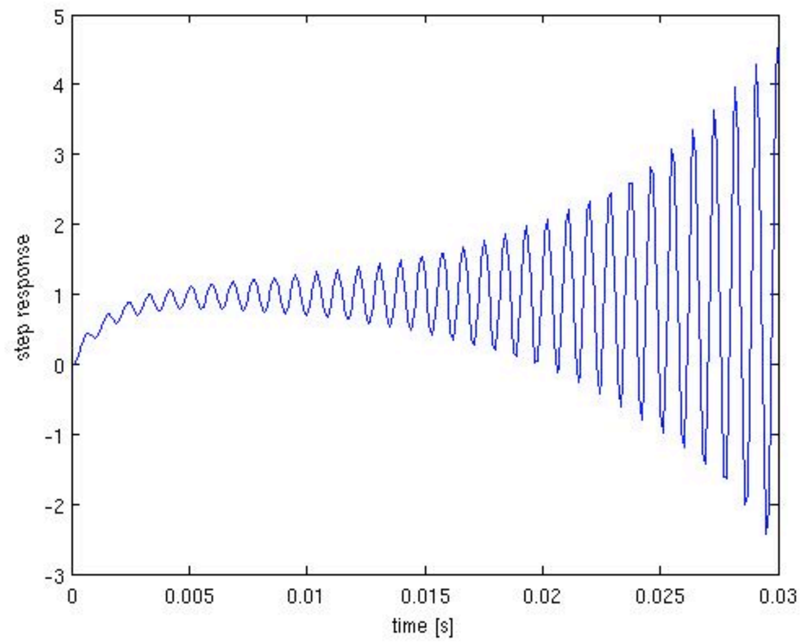


Figure 0-3. Obvious exponential increasing of amplitude of oscillations. Feedback parameter was set high. Such oscillations may occur in STM systems and are usually terminated when STM ends up tip in the substrate.

In order to obtain faster dynamic response, the derivative controller must be introduced. The derivative feedback signal responds to rates of change of error signal instead of the error value. Since derivative signals don't measure the sign of the error they must be combined with integral gain to allow ideal response. Derivative gain can be modeled as:

$$G(s) = A\omega_c \frac{s}{s+\omega_c}$$

where ω_c is the cutoff frequency preventing amplifying high frequency noise in the system. By introducing this gain, response time changes to a few milliseconds (Figure 4-4).

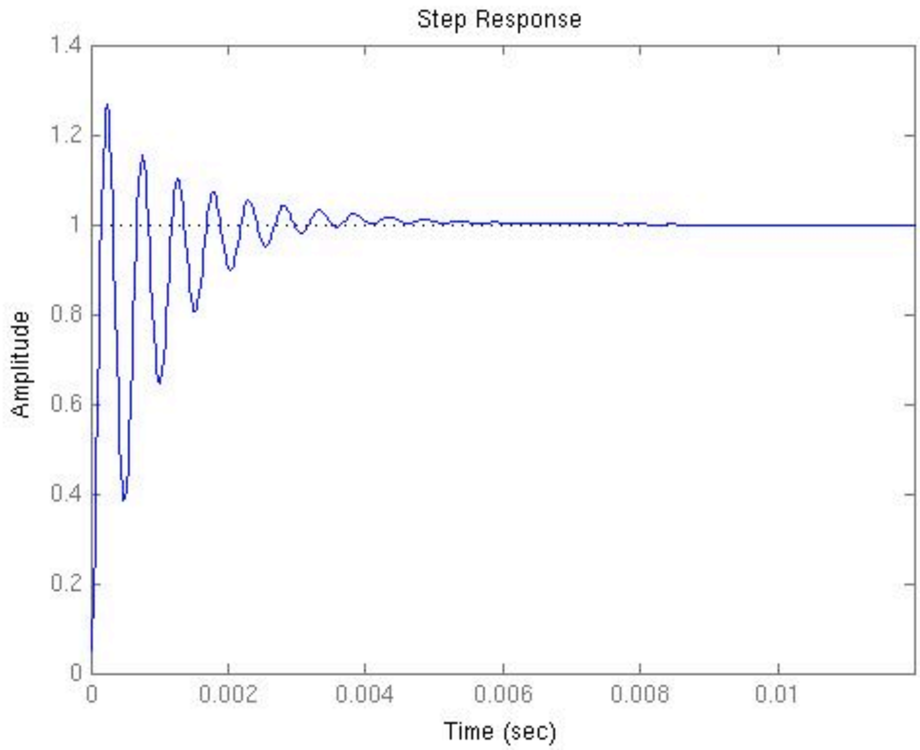


Figure 0-4. Step response improved to about 3 ms by using both differential and integral gain(which is set 10 times the maximum allowable if only integral controller was implemented)

Therefore, combination of integral and proportional gain provides faster response but control theory indicates the potential for instabilities. For most applications integral or integral and proportional gains will satisfy the requirements, however in the case of imaging nanoparticle samples with large curvature, a full proportional-integral-differential (PID) control system is necessary to provide fast response.

Step inputs are generally used to set the standard of controllers in terms of requirements such as overshoot amplitude and rise time. In order to qualitatively illustrate the response of STM feedback controls on realistic inputs such as hemispherical particles on a flat substrate, Matlab provides powerful toolbox for analysis.

Equation 4.1 represents the overall transfer function for STM feedback and is used in all Matlab simulations. Initially, only integral gain is considered. The duration of the input signal is 60 ms and the integral gain is set to track surface as faithfully as possible:

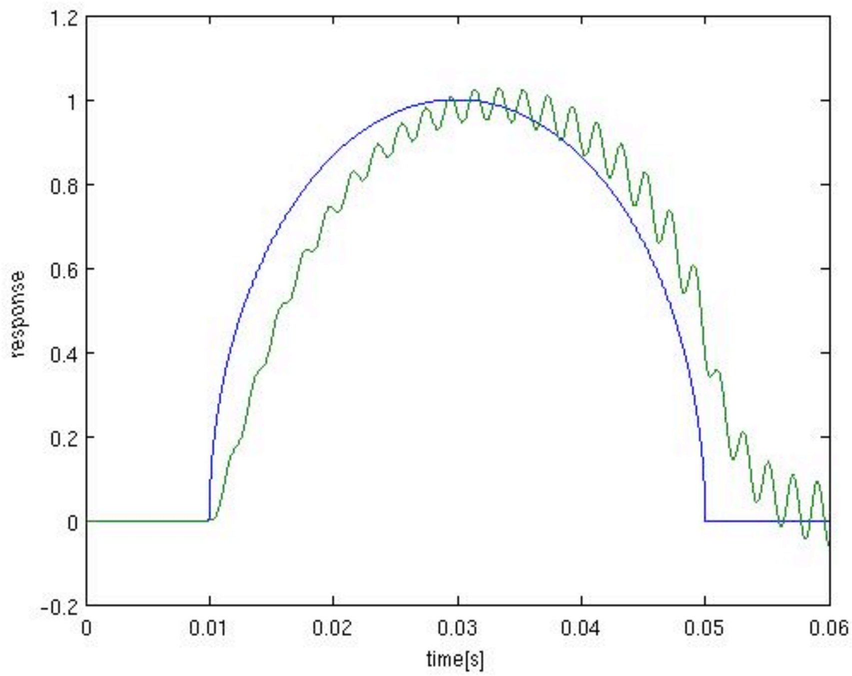


Figure 0-5. Feedback response to reference signal that resemble nanoparticle surface. Only integral gain is utilized. Signal length is simulated to be 60ms and feedback parameters are extracted from [18].

Figure 4-5 shows that high integral gain will overall follow the curvature but with oscillatory behavior. In order to simulate STM scanning and predict images that could be obtained by improper feedback settings, scanning is now allowed in two dimensions. Figure 4.5 shows the result of 2D simulation in which fringes that follow the curvature become apparent. In general, when scanning starts over curved surface, due to feedback oscillations fringes will follow the curvature and converge to two points on the image (Figures 4-6 and 4-7).

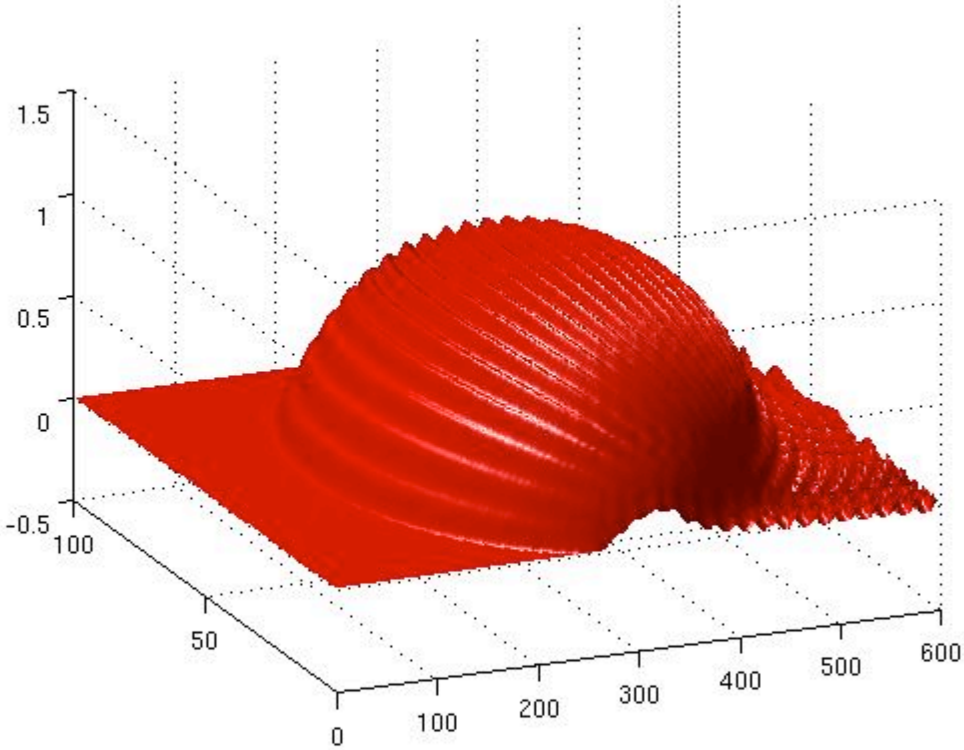


Figure 0-6. 3D rendering of scanning. Feedback oscillations produce fringes that converge to two poles.

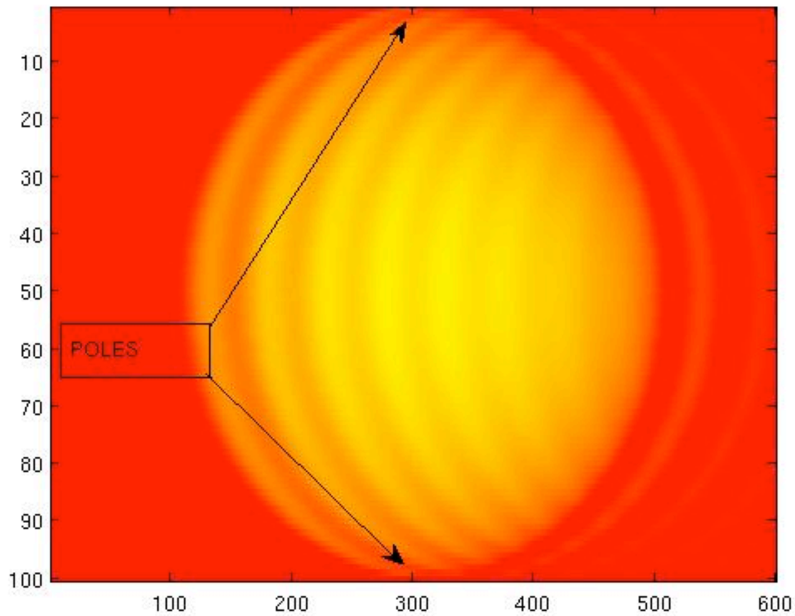


Figure 0-5. Illustration similar to the previous figure but for 6 ms signal input so that number of fringes decreases. Convergence of the fringes at the "poles" is seen.

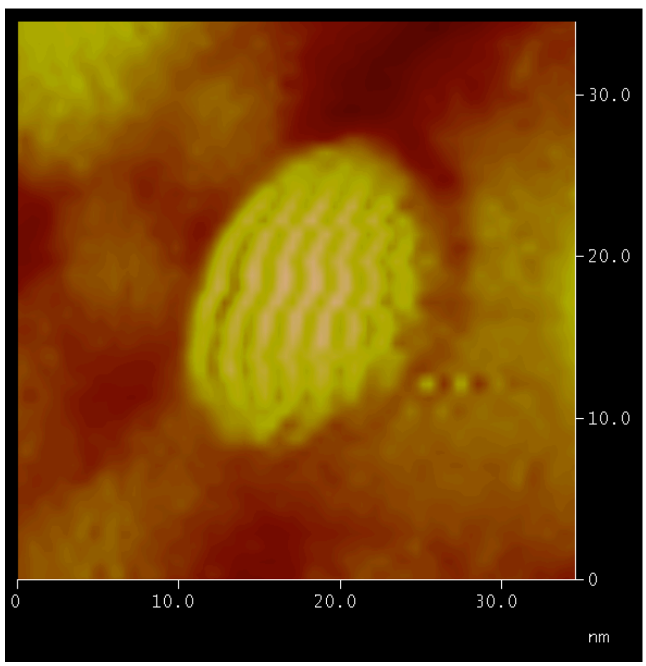


Figure 0-6. Actual STM data. Image of either CdSe nanoparticle conglomerate on gold foil surface or perhaps simply a surface irregularity on a gold foil substrate that indicate the same convergence predicted by second-order linear feedback model.

In order to eliminate surface tracking problem (correct tracking without oscillatory behavior), differential gain is introduced. With the differentiator, tracking becomes good and suppresses exponentially growing integral feedback oscillations. Overall, differential gain shortens the rise time to only a few milliseconds (Figure 4.8)

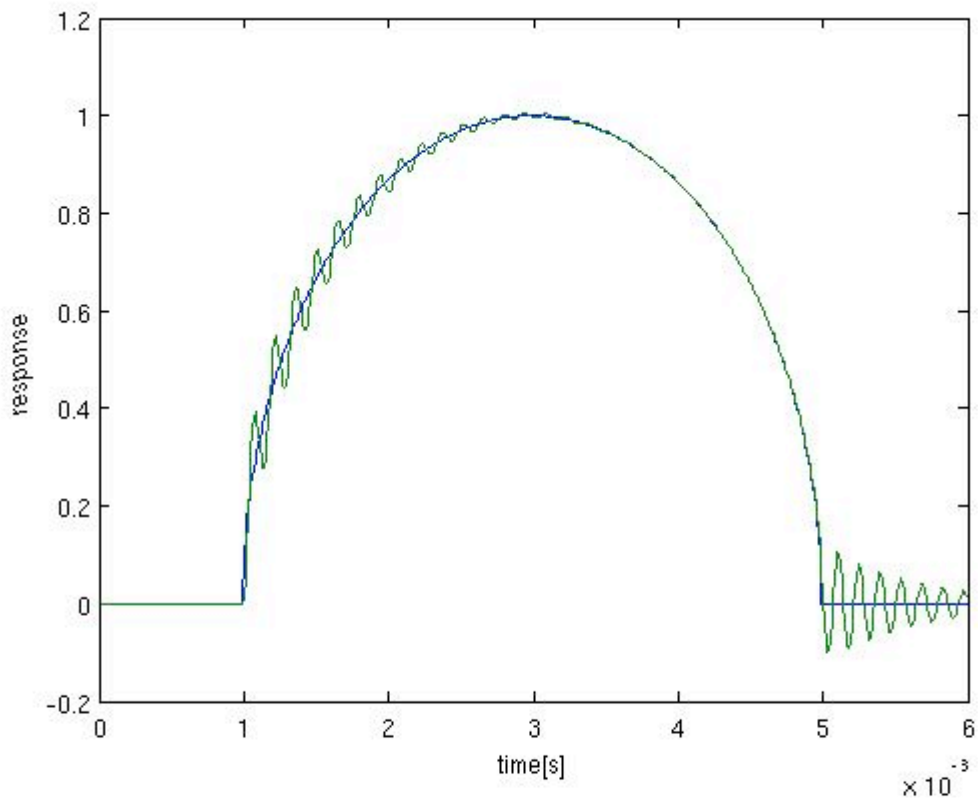


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Figure 0-7. Differential gain is introduced. Surface tracking becomes obviously better as now integral gain can be boosted over the critical point. Differentiator suppresses integral feedback oscillations.

However, Matlab simulation with larger integral gains reveals surface features that match STM experimental data. In general, all STM data contains zigzag features that Stellacci and coworkers attribute to perfectly visible hexagonally packed molecular head groups. However, this is not true as the simulation predicts the same features as results of scanning artifacts (Figure 4-9 and 4-10). These zigzag features are experimentally apparent scanning artifacts as they always belong to scan lines and never change their orientation upon orientation of the substrate. As observed in STM experiments (Figures 4.11 and 4.12), such regions are only a few scan lines wide which match with the results of Matlab simulation in Figure 4-8.

Hexagonal dots in both theoretical an experimental data appear as beats in feedback oscillations thus generating:

1. fringes, if in two consecutive scanning rows peaks are shifted by the same amount which produces visual effect of fringes
2. zigzag features, if two consecutive scanning rows are shifted enough that mismatch produce zigzag visualization effect

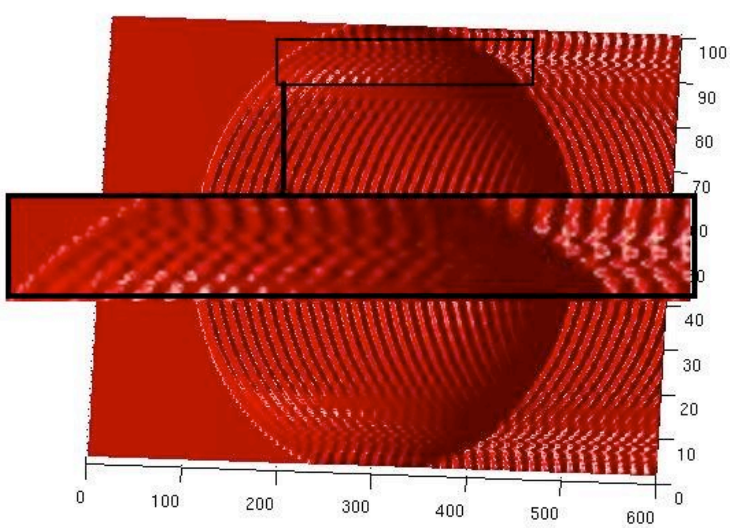

Figure 0-8. Result of Matlab simulation at which integral is set beyond critical point. Hexoganaly packed feedback oscillation appear at the beginning of scanning and transform into fringes.

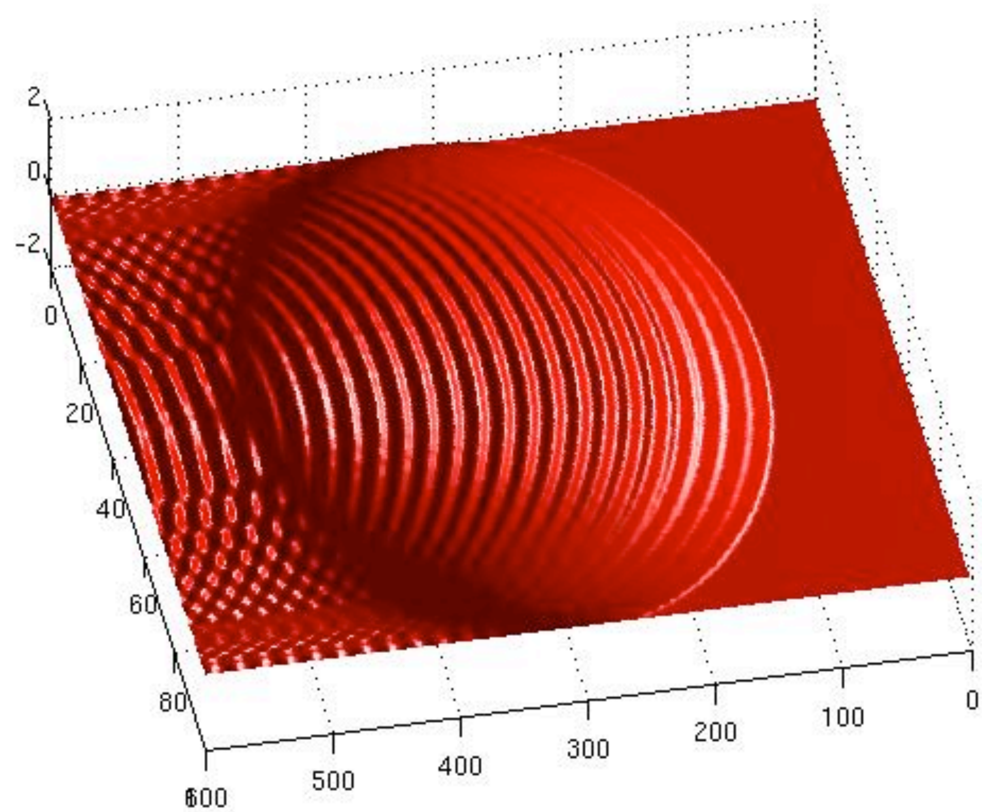

Figure 0-9. Similarly to the previous figure, but now hexagonal packing is more apparent after the tip goes off the surface of nanoparticle, phenomenon noticed constantly in real STM experiments.

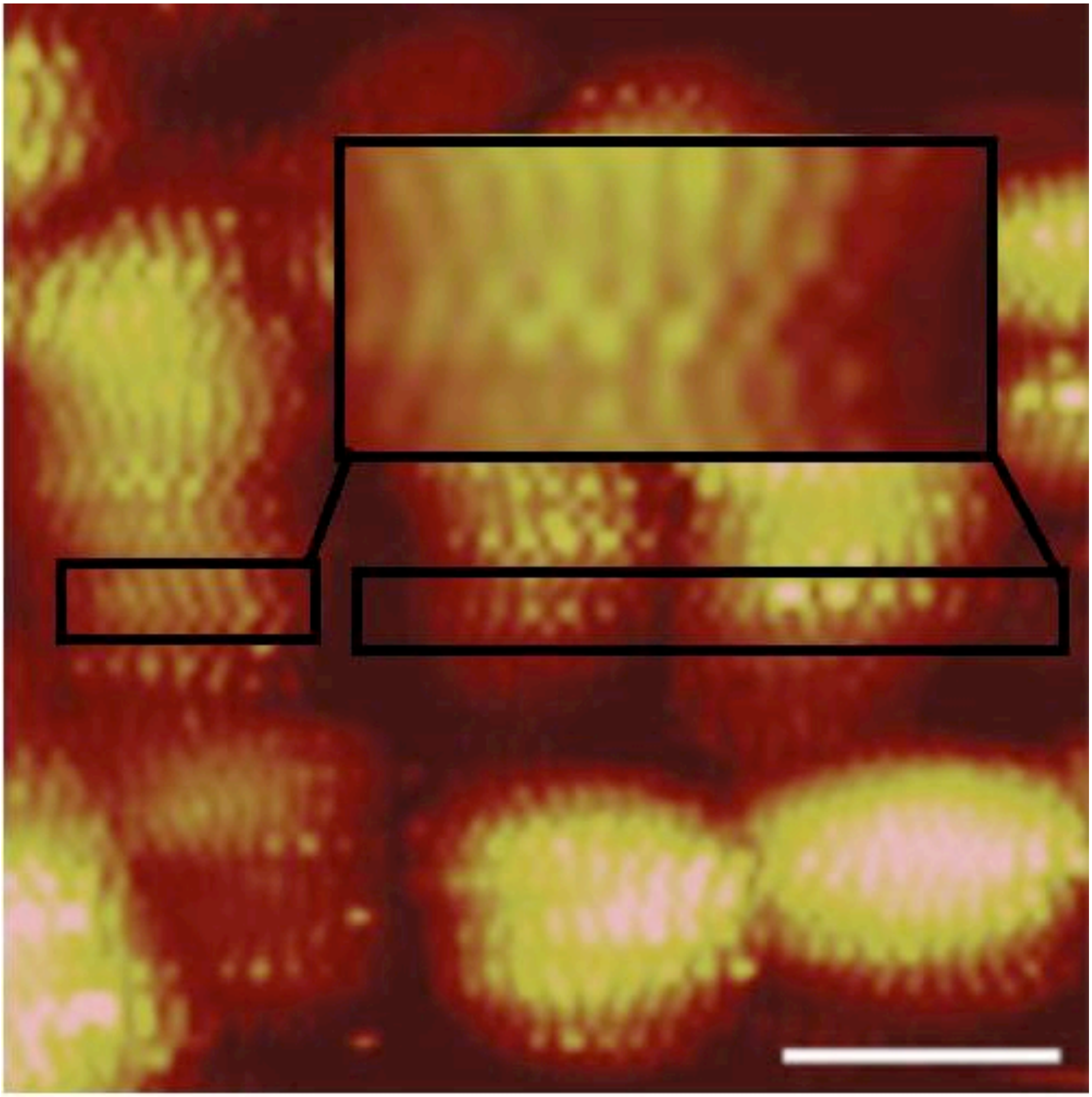

Figure 0-10, Real STM image of gold nanoparticles. Size bar is 10nm. Image directly extracted from [16] indicating the same type of feedback artifacts illustrated in the previous figures. Notice that hexagonal dots run directly along scan lines, on and off nanoparticle surface, in the same form as in theoretical simulation.

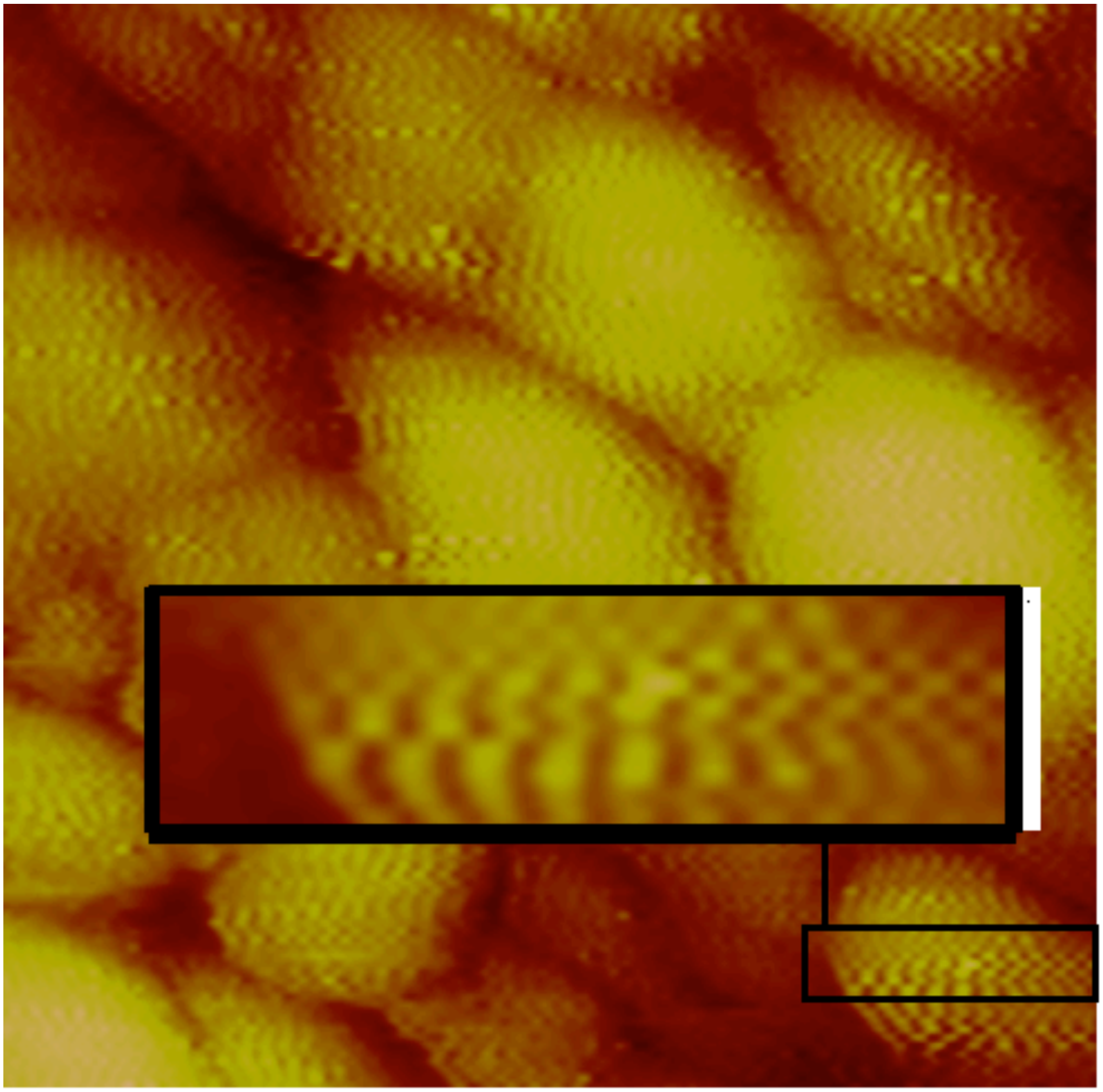

Figure 0-11. STM image of ITO surface without ligands. The same feedback artifact is observed indicating that STM images are not images of molecules on the surface but are images with feedback oscillations that propagate along scan lines.

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A simple Matlab simulation becomes quite enough to qualitatively demonstrate appearance of false surface features upon applying improper gains on curved surfaces. However, if such surface features exist, experimentally:

A. then they will be scan speed independent
B. would not consist of features always belonging to the scan lines (statistically impossible)
C. fringes would rotate with different substrate orientation
D. current error should be minimal (this eliminates feedback artifacts)

Imaging larger areas of nanoparticles experimentally fails on all criteria. Matlab simulations certainly do not and are not intended to reproduce STM data. However, only one parameter (integral gain) simulation of response of second order linear system undoubtedly demonstrates all STM experimental features thus concluding the work of Stellacci et all completely erroneous.

It was argued previously that fully implemented PID controller will enable faster feedback response. In order to reduce the risk of improper surface tracking even more, images with smaller scan sizes (between 50 and 100 nm) must be generated if STM is working in constant-current mode. Scan speed must be set precisely to allow feedback system to accurately achieve set point. Therefore, prior to imaging, feedback loop must be fully characterized to understand the limits of feedback response as function of scan rate/speed. In order to observe molecular features on the nanoparticles surface it also must be reassured that noise level of the voltage preamplifier is acceptable. In general, in constant current mode, feedback oscillations are the most damaging to imaging as it is not always obvious what cause them. The most obvious reason is improperly set gains and this problem can be alleviated by dropping the gains. If feedback oscillations appear as a function of proportional gain, then reducing lower cut off frequency will solve the problem. In case of derivative feedback, reducing the derivative gain will set system into oscillations (due to integral gain instability).

Therefore the whole problem of feedback oscillations is very well known in STM metrology and it may give meaningless results. The best way of securing the system of oscillations is during imaging: to monitor carefully the tunneling current and assure that oscillatory behavior in tunneling current doesn't appear.

[1] Kaiers W and Stroscio J. Scanning tunneling microscopy. Academic Press, San Diego, 1993.

[2] E. Anguiano et al. Optimal conditions for imaging in scanning tunneling microscopy Theory. *Review of Scientific Experiments,* 69:3867-3874, 1998.