Abstract: The Atomic Force Microscope introduced the surface investigation with true atomic resolution. In the dynamic mode of operation both amplitude and frequency modulation methods can be implemented by using Phase-Locked Loops. Here it is shown that Phase-Locked Loops can improve the performance of the Atomic Force Microscope providing the feedback signal to control both the amplitude and the oscillation frequency of the cantilever. It is also presented a method to design stable third-order Phase-Locked Loops.

Keywords: Frequency Modulated Atomic Force Microscopy, Phase-Locked Loop, Nonlinear Dynamics.

1. INTRODUCTION

Atomic Force Microscopy started in 1986 when the Atomic Force Microscope (AFM), Fig. 1, was invented by G. Binnig at Stanford University [1]. Since then, a considerable number of improvements and developments had been made, and many results had been achieved by simple contact measurements. Nevertheless, contact AFM cannot generate true atomic resolution in a stable operation.

In 1995, non-contact AFM achieved true atomic resolution under attractive regime at room temperature [2, 4]. Non-contact AFM operates in static mode or dynamic mode, i.e., static AFM or dynamic AFM, respectively. In static AFM the force \( F_{ts} \) interacting between tip and sample translates into a deflection of the cantilever, and the image is a map \( z(x, y, F_{ts}) \) with \( F_{ts} = \text{constant} \) [4].

On the other hand, in dynamic AFM, the cantilever is deliberately vibrated. The two basic methods are Amplitude Modulation (AM-AFM) and Frequency Modulation (FM-AFM) [4–6].

In AM-AFM the cantilever is vibrated at a fixed amplitude and at a fixed frequency near the cantilever eigenfrequency. The tip-sample interactions cause changes in both amplitude and phase, these changes are measured and are used as the feedback signal.

In FM-AFM the cantilever is also driven to oscillate at a fixed amplitude by an automatic control loop. The control signal is used to generate dissipation images. Another control loop is used to keep constant the cantilever’s oscillation frequency by adjusting the tip-sample distance [5, 7]. The distance control signal is used to generate topographic images. Using FM-AFM improved the resolution dramatically and for atomic studies in vacuum the FM is now the preferred AFM technique [4].

Initially, the AM-AFM was used only in non-contact mode, but later, it was also used at a closer distance involving repulsive tip-sample interactions in intermittent contact mode AFM, or tapping mode [3, 4]. The tapping mode technique provides high resolution topographic images even for sample surfaces that are easily damaged, or difficult to image by other AFM techniques.
Recently, Phase-Locked Loops (PLLs) have advantageously been used in the demodulation process of FM-AFM [4, 5].

The PLL is a control system that synchronizes a local oscillator to an input signal, playing an important role in communication systems, computation and control. PLLs allow the correct order of information processing by efficiently generating and distributing clock reference signals.

Nevertheless, PLLs are inherently nonlinear devices, and behaviors such as bifurcations and chaos may arise [8, 9, 11, 12]. Additionally, ripple oscillations, such as the Double Frequency Jitter (DFJ), generated by the Phase Detector (PD), corrupts the synchronization quality [13, 14]. PLL design is critical to demodulation systems, and consequently, to the data recovery process.

In section 2 the mathematical model is derived and the main dynamical behavior characteristics of the analogical PLL is presented. The role of PLLs in Noncontact AFM is presented in section 3. In section 4 a design method for third-order PLLs is suggested, and finally, in section 5 the conclusions are presented.

2. PHASE-LOCKED LOOPS DYNAMICS

The PLL is a closed loop control system composed of a phase detector (PD), a low-pass filter $F(s)$ and a voltage controlled oscillator (VCO), that synchronizes the local VCO output to the incoming signal $v_i(t)$ (see Fig. 2). This is performed by adjusting the VCO frequency according to $v_o(t)$, which in turn is the filter response to the PD output $v_d(t)$.

![Figure 2 – PLL Block Diagram](image)

The input and output signals are expressed by:

$$v_i(t) = v_i \sin (\omega_M t + \theta_i(t))$$  \hspace{1cm} (1)

and

$$v_o(t) = v_o \cos (\omega_M t + \theta_o(t)),$$  \hspace{1cm} (2)

respectively, where $\theta_o$ is the estimate of the true phase to the input $\theta_i$, $v_i$ and $v_o$ are the amplitude of the signals. Since both input and output signals are supposed to have the same free-running angular frequency $\omega_M (rad/s)$, the phase error is defined as follows:

$$\vartheta(t) = \theta_i(t) - \theta_o(t).$$  \hspace{1cm} (3)

It can be noticed, from equations 1, 2 and 3, that for $\vartheta(t) = 0$ there is a static phase difference of $\pi/2 \ rad$ between input and output [8, 16].

The PLL is described by a differential equation of order $P + 1$ [15], considering that the order the filter $f(t)$ is $P$. First-order low-pass filters are widely used in PLL design due to its simplicity and reliable behavior in many different applications [8, 16]. In order to simplify the mathematical reasoning, the filter is considered to be the first-order all-pole given by:

$$F(s) = \frac{\alpha}{s + \beta}.$$  \hspace{1cm} (4)

The PD output is given by:

$$v_d(t) = k_d v_i(t) v_o(t),$$  \hspace{1cm} (5)

where $k_d$ is the PD gain.

The VCO frequency is controlled according to:

$$\frac{d}{dt}\theta_o(t) = k_v v_o(t),$$  \hspace{1cm} (6)

where $k_v$ is the VCO gain, and $v_o$ is the filter output given by the convolution:

$$v_o(t) = f(t) * v_d(t).$$  \hspace{1cm} (7)

The loop gain $G$ is defined as follows:

$$G = \frac{1}{2} k_d k_v v_i v_o.$$  \hspace{1cm} (8)

Considering the foregoing relations, the convolution theorem [18] and the trigonometric identity $\sin(A) \cos(B) = \frac{1}{2}[\sin(A - B) + \sin(A + B)]$, the dynamics of the phase error is given by:

$$\ddot{\vartheta}(t) = \beta \dot{\vartheta}(t) + \alpha G \sin (\vartheta(t)) = \ddot{\theta}_i(t) + \beta \dot{\theta}_i(t) - \alpha G \sin (2(\omega_M t + \theta_i(t)) - \vartheta(t)).$$  \hspace{1cm} (9)

The phase difference and the double frequency terms in equation 9 are responsible for the nonlinear behaviors observed in PLLs. The double frequency term, that generates the DFJ, is usually neglected since it is supposed to be cut by the low-pass filter [8, 15]. However, real PLLs present the DFJ, that appears as an oscillation around the synchronous state$^2$, even with the PLL in the lock-in and capture modes of operation [16]. In fact, the DFJ amplitude depends on the loop gain $G$ and on the filter frequency response [13, 14, 20].

In order to illustrate the dynamical behavior of PLLs and the influence of the DFJ, simulations were conducted using Simulink built-in blocks and the “ode45 Dormand-Prince” integration method, considering $\alpha = \beta = 1, G = 1, \omega_M = 2 \pi rad/s, \theta_i(t) = 0$ and different initial conditions. The simulations are shown in the state space plots in Figs. 3 and 4.

Comparing Figs. 3 and 4 the effect of the DFJ on the trajectories becomes evident. Besides, for small phase errors, the double frequency term works as a forcing term producing an oscillation around the synchronous state.

The trajectories shown in the state space plots in Fig. 4, were simulated neglecting the double frequency term. In this

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$^1$The trigonometric identity is applied into equation 5 in order to transform the product of trigonometric functions into a sum. The term with $\sin(A - B)$ yields the phase difference term, and the term with $\sin(A + B)$ yields the double frequency term.

$^2$The synchronous state is an equilibrium point of equation 9 when the double frequency term is neglected [9].
case, the remaining sine term in equation 9, or the phase difference term, generates periodically spaced equilibrium points, alternating stable and unstable. This feature generates cycle-slips and prevents the PLLs to overcome large initial phase errors. In spite of that, for most of the applications, cycle-slips represent no concern.

Second-order PLLs are extensively used in applications related to recovering clock signals for synchronous demodulation in telecommunication networks. In some situations even higher order PLL loops are used, despite the possibility of producing bifurcations and chaos [12, 21, 22].

3. PHASE-LOCKED LOOPS IN NONCONTACT AFM

In the FM-AFM the cantilever is driven to oscillate with both amplitude and frequency constants. However, tip and sample interaction forces are directly related to changes in the amplitude and frequency over the oscillation cycle while the surface is scanned [4, 24]. These changes are measured and used as feedback signals to the control system.

The role of PLLs is to demodulate the FM signal from the photodiode. The demodulated signal can be obtained by choosing the correct PLL output, and, as shown in Fig. 5, the FM output is the signal $v_c(t)$.

The signal $v_c(t)$ is used as feedback for FM-AFM, in order to keep the cantilever frequency at a given setpoint $\Delta\omega_0 \text{rad/s}$. Additionally, and since the PLL must be synchronized with the cantilever oscillation, its output $v_o(t)$ is used to synthesize the control signal in the amplitude control loop, also in order to keep the amplitude at a given setpoint $A_0$.

The block diagram of the FM-AFM control system can be seen in Fig. 6. The deflection $z(t)$ of the cantilever is measured using a laser beam that incides on the top of the cantilever and is reflected into an array of photodiodes (Fig. 1). The photodiode output is used by the amplitude control loop and by the distance control loop. The distance control loop controls the mean distance between tip and sample. While the sample is scanned the tip and sample interactions are frequency modulated in the photodiode output signal. The PLL demodulates the signal obtaining the frequency offset of the cantilever.

The PLL output ($v_c(t)$) is compared to the frequency setpoint $\Delta\omega_0$, generating the error signal to the distance con-
controller that actuates on the PZT scanner\(^3\) in order to maintain the cantilever frequency shift induced by the tip surface interaction at the frequency setpoint. The control signal of the distance control loop is used to generate topographical images [4–6].

The amplitude control loop uses a peak detector as a means to determine the amplitude \(A\) of the cantilever oscillation from the photodiode signal. In the sequence \(A\) is compared to the amplitude setpoint \(A_0\) generating the error signal to the amplitude controller. The amplitude control signal is used to generate the dissipation images.

As it can be noticed, the PLL performance is vital to FM-AFM. Nevertheless, little attention is drawn to PLL design and performance in atomic force microscopy literature. Perhaps because designing stable third-order PLLs, in contrast to second-order, demand some effort [10].

4. THIRD-ORDER PLL STABILITY AND DESIGN

Stable operation with second-order PLLs is simple and reliable because the open loop transfer function presents two poles and one zero, and if the poles and zeros are properly located the loop is stable [8].

In [10] the conditions for stability of third-order PLLs in one-way master-slaves networks are determined, and the results can be applied for single PLLs. Here, the filter considered is the all-pole second-order:

\[
F_1(s) = \frac{\alpha_0}{s^2 + \beta_1 s + \beta_0}. \tag{10}
\]

Considering the filter \(F_1\) (equation 10), the other relations in section 2, and dropping the double frequency term, the dynamics of the phase error is given by:

\[
\ddot{\vartheta} + \beta_1 \dot{\vartheta} + \beta_0 \vartheta + \alpha_0 G \sin (\vartheta) = \ddot{\theta}_1 + \beta_1 \dot{\theta}_1 + \beta_0 \theta_1. \tag{11}
\]

The stability analysis is performed considering the first term in the Taylor’s series expansion around the equilibrium points which are hyperbolic [9, 10, 12, 21].

Equation 11 can be transformed into state equations defining:

\[
\begin{align*}
\dot{x}_1 &= \vartheta, \\
\dot{x}_2 &= \dot{\vartheta}, \\
\dot{x}_3 &= \ddot{\vartheta},
\end{align*}
\]

resulting:

\[
\begin{align*}
\dot{x}_1 &= x_2, \\
\dot{x}_2 &= x_3, \\
\dot{x}_3 &= -\beta_1 x_3 - \beta_0 x_2 - \alpha_0 G \sin (x_1).
\end{align*}
\]

The equilibrium points of the state equation 13 are \(x^* = [\pm k\pi, 0, 0]\), for \(k = 0, 1, 2, \ldots\), and for odd values of \(k\) the equilibrium points are unstable for any parameter combination [9, 10, 13]. Consequently, stable equilibrium points correspond to even values of \(k\) and their stability can be determined by the eigenvalues of the jacobian matrix [12, 18].

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\(^3\)Piezoelectric tubes (PZT) are used in AFMs to position the sample that is being scanned. The scanner combines in a single tube piezo electrodes that expands and contracts orthogonally, for \(x\), \(y\) and \(z\) directions, to be actuated in a raster pattern [25].
The characteristic polynomial obtained from the jacobian matrix of equation 13 is given by:

\[ P(\lambda) = \lambda^3 + \beta_1 \lambda^2 + \beta_0 \lambda + \alpha_0 G. \] (14)

Applying the Routh-Hurwitz criterion [18] on equation 14 and considering that all the coefficients of the characteristic polynomial are positive numbers, all the roots have negative real parts if:

\[ G < \frac{\beta_1 \beta_2}{\alpha_0}, \] (15)

Writing the filter coefficients according to \( \alpha_0 = \beta_0 = \omega_n^2 \) and \( \beta_1 = 2 \xi \omega_n \), results that:

\[ G_{\text{max}} < 2 \xi \omega_n, \] (16)

where \( G_{\text{max}} \) is the superior limit for the loop gain \( G \), \( \omega_n \) is the natural frequency and \( \xi \) is the damping ratio of the filter. Relation 16 associates the dynamical characteristics of the filter to the stability of the loop.

4.1. Third-order PLL design

In [5] a virtual FM-AFM was simulated considering a PLL with loop gain \( G_p = 8.2938 \times 10^3 \), a VCO free running frequency of \( \omega_M = 1.6965 \times 10^6 \) and a second-order all-pole loop filter given by:

\[ F_p(s) = \frac{1}{(55 \times 10^{-6} s + 1)(160 \times 10^{-6} s + 1)}. \] (17)

In order to compare the performance of the PLL designed here with the one in [5] the corner frequency of the filter is chosen to be \( \omega_n = 1.5708 \times 10^4 \text{rad/s} \). The damping ratio of the filter is set to \( \xi = 0.7 \), and the transfer function of the filter becomes:

\[ F_1(s) = \frac{2.4674 \times 10^8}{s^2 + 2.1991 \times 10^4 s \+ 2.4674 \times 10^8}. \] (18)

According to relation 16 the loop gain must satisfy \( G_{\text{max}} < 2.1991 \times 10^4 \). The loop gain is determined in order to produce the best settling time, which is achieved with

\[ G = 4.3982 \times 10^3, \] (19)

as it can be seen in the root locus in Fig. 7.

As it can be noticed, the loop gain \( G \) was chosen five times less than \( G_{\text{max}} \), resulting in a satisfactory gain stability margin. The Bode diagrams of the open loop transfer functions of the designed PLLs are shown in Fig. 8, and the step responses in Fig. 9.

Comparing the performance of the systems it can be seen that both generate a well damped response with a settling time considerably small for the PLL with the filter \( F_1 \).

In Fig. 8 it is shown that at frequency \( 3.39 \times 10^6 \text{rad/s} \) — which is the double of the free running frequency of the VCO — the attenuation is of approximately \(-150 \text{dB}\).

Since the results obtained in [5] are considered satisfactory even with this strong attenuation, it suggests that the bandwidth of the PLL could be wider, improving the transient response of the PLL and consequently the demodulation process. Nevertheless, this must be verified experimentally, due to the lack of published works regarding to design requisites for FM-AFM.

5. CONCLUSION

The role of PLLs in FM-AFM was clarified, and the dynamics of PLLs was put into the perspective of the atomic
force microscopy. Also a simple method to design PLLs assuring stability was discussed. However, the design must be verified experimentally due to the lack of publications concerning the performance requirements of the FM-AFM control system.

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REFERENCES


