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Frequency Domain Analysis of Robust Demodulators for High-Speed Atomic Force Microscopy

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Abstract—A fundamental but often overlooked component in the z-axis feedback loop of the atomic force microscope (AFM) operated in dynamic mode is the demodulator. Its purpose is to obtain a preferably fast and low-noise estimate of amplitude and phase of the cantilever deflection signal in the presence of sensor noise and additional distinct frequency components. In this paper, we implement both traditional and recently developed robust methods on a LabVIEW digital processing system for high-bandwidth demodulation. The techniques are rigorously compared experimentally in terms of measurement bandwidth, implementation complexity and robustness to noise. We conclude with showing high-speed tapping-mode AFM images in constant height, highlighting the significance of an adequate demodulator bandwidth.

I. INTRODUCTION

Since the invention of the atomic force microscope (AFM) [1] in the late 1980s, the instrument has established itself as a key enabling technology for nanoscale object and material property analysis for both research and industry. Dynamic imaging modes [2], in which the microcantilever is excited at one of its resonance frequencies, are especially suitable for the investigation of delicate matter and biological samples due to the low tip-sample forces. For these modes, a demodulator has to be employed in the z-axis feedback loop of the AFM, whose task is to determine amplitude and phase, preferably with a high measurement bandwidth and robustness to unwanted frequencies present in the cantilever deflection signal.

A number of demodulation techniques can be found in the existing literature, some of which have found regular use in commercial AFM systems. The available methods in the literature can be broadly classified as model-based and non-model-based variants each having distinct advantages with regards to measurement bandwidth, implementation complexity and robustness to noise. The RMS-to-DC converter [3], while being low in implementation complexity and limited to amplitude estimation, is prone to delivering biased estimates if higher eigenmode contributions and/or

higher harmonics are present in the signal such as during multifrequency AFM (MF-AFM) [4].

In contrast, the lock-in amplifier has been adopted as the industry wide standard, since it is extremely robust to other frequency components in the signal but is limited in its measurement bandwidth. Inspired by image-rejection mixers [5] and modulated-demodulated control [6], [7], a high-bandwidth lock-in amplifier was recently proposed and implemented to improve upon the measurement bandwidth [8]. However, it is still ultimately limited by the low-pass filter (LPF), which has to be employed in order to account for residual phase mismatches.

For high-speed AFM applications, such as for the study of fast biological processes [9], these two methods are not suitable and have led to the development of fast single wave detectors based on the peak-hold method [10], [11], Fourier technique [12] and real-time integration [13], [14]. While these methods possibly yield very fast estimates, they are inherently incompatible with MF-AFM methods due to the presence of multiple distinct frequency components close to the frequency of interest.

This fact has motivated the development of filters based on the system-theoretic modeling of the AFM deflection signal such as the time-varying Kalman filter [15] and Lyapunov filter [16], [17]. These approaches were shown to possess both, high measurement bandwidth and robustness to unwanted frequencies in the signal and can be readily extended to be capable of estimating multiple frequencies for MF-AFM [18], [19].

In this work, we aim to perform a thorough experimental analysis of demodulation methods for amplitude-modulation AFM which exhibit inherent robustness to additional frequency components. For this purpose, we have implemented the lock-in amplifier (LIA), high-bandwidth lock-in amplifier (HBW LIA), Kalman filter (KF) and the Lyapunov filter (LYAPF) on a widely used digital signal processing (DSP) system (LabVIEW). The techniques are experimentally compared in terms of their measurement bandwidth, noise performance, implementation complexity and robustness to other frequency components. We conclude by showing high-speed constant-height tapping-mode AFM experiments to highlight the case when the demodulator is the bandwidth bottleneck in the z-axis feedback loop.

II. SUMMARY OF DEMODULATION METHODS

The following subsections aim to provide a short summary of existing and novel demodulation methods, their imple-

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Fig. 1. Blockdiagram of the z-axis feedback loop for tapping-mode AFM highlighting the high-frequency section of the control loop.

mentation and properties. For the standard feedback loop in tapping-mode AFM shown in Fig. 1, the demodulator acts as a crucial link between the high-bandwidth response of the cantilever $y(t)$ and the low-bandwidth feedback signal $A(t)$. For this purpose, we consider a signal with carrier sine wave with frequency ω and (with respect to the carrier frequency) slowly varying amplitude $A(t)$ and phase $\phi(t)$ of the form

$$y(t) = A(t) \sin(\omega t + \phi(t)). \quad (1)$$

The model can be linearly parametrized by applying trigonometric identities, where the state vector $\mathbf{x} = [x_1 \ x_2]^T$ represents the in-phase and quadrature components

$$y(t) = [\cos(\omega t) \ \sin(\omega t)] \mathbf{x} = \mathbf{c}(t)\mathbf{x}. \quad (2)$$

A. Lock-In Amplifier

The lock-in amplifier [20]–[22] mixes the input signal (1) with in-phase and quadrature sinusoids to obtain

$$\begin{aligned} y_i(t) &= y(t) \sin \omega t \\ &= \frac{1}{2} \underbrace{A(t) \cos \phi(t)}_{x_1} - \underbrace{\frac{1}{2} A(t) \cos(2\omega t + \phi(t))}_{\text{LPF}} \end{aligned} \quad (3)$$

and

$$\begin{aligned} y_q(t) &= y(t) \cos \omega t \\ &= \frac{1}{2} \underbrace{A(t) \sin(\phi(t))}_{x_2} + \underbrace{\frac{1}{2} A(t) \sin(2\omega t + \phi(t))}_{\text{LPF}}. \end{aligned} \quad (4)$$

Amplitude and phase estimates can be calculated by

$$\begin{aligned} A(t) &= \sqrt{x_1^2 + x_2^2} \\ \phi(t) &= \arctan\left(\frac{x_2}{x_1}\right). \end{aligned} \quad (5)$$

Note, that the mixing process generates harmonics at ω (for a DC offset present in the input signal) and at 2ω , which need to be removed by employing a low-pass filter with $\omega_{\text{lpf}} \ll \omega$. Thus, the order and cut-off frequency of the LPF directly determines the noise performance and bandwidth of the estimates. In order to limit the noise to 1% of the signal, i.e. a -40 dB suppression of the 2ω component, a 2nd order LPF would limit the bandwidth to a cut-off frequency approximately a decade below the carrier frequency. A LIA described by the equations (3)–(5) can be realized digitally with two direct digital synthesizers (DDS) to create the

reference sine and cosine signals, two multipliers, two LPFs, and an output block with square root functionality and an arctan calculation method such as polynomial approximation or the CORDIC algorithm [23] to calculate the phase.

B. High-Bandwidth Lock-In Amplifier

The high-bandwidth lock-in amplifier [8] is a novel extension to the standard LIA technique which employs phase cancellation to precisely cancel the 2ω term. Compared to the standard LIA, this demodulation scheme essentially requires two additional multipliers, which operate on the input signal shifted by -90° . Their output products

$$\begin{aligned} y_{i,\perp}(t) &= \frac{1}{2} A(t) [\sin(\phi(t)) + \sin(2\omega t + \phi(t))] \\ y_{q,\perp}(t) &= \frac{1}{2} A(t) [\cos(\phi(t)) - \cos(2\omega t + \phi(t))] \end{aligned} \quad (6)$$

are added to the output products of the LIA mixers which in theory exactly cancels their 2ω components. While good results have been achieved with an analog implementation of this technique in [8], in practice, exact phase cancellation will not occur due to circuit mismatches. As such, post-mixing low-pass filters still have to be employed, however as the 2ω terms are heavily attenuated, the bandwidth of the filters can be increased. On a digital implementation, the standard LIA implementation has to be extended with two additional multipliers, two summing stages and a Hilbert transform filter to realize the -90° phase shift [24].

C. Kalman Filter

A linear time-invariant (LTI) state-space model of the signal described by (1) can be obtained by choosing position $\bar{x}_1 = y(t)$ and velocity $\bar{x}_2 = \dot{y}(t)$ as the state variables and $y = \bar{x}_1$ as the output. Due to the sparse nature of the resulting state matrix, especially when modeling higher resonance frequencies, this model is generally ill-conditioned for the use in an observer like the Kalman filter which requires an inversion. This problem is circumvented by applying a time-variant transformation such that a time-variant but numerically well-conditioned state-space representation can be obtained [15]. In its discretized form, this model is given

Fig. 2. FM-AM frequency response of the robust demodulators showing the tracking bandwidth and equivalent filter order for different bandwidth settings.

by

$$\begin{aligned}
 \mathbf{x}_{k+1} &= \mathbf{x}_k + \mathbf{w}_k \\
 y_k &= \mathbf{c}_k^T \mathbf{x}_k + v_k \\
 E[\mathbf{w}_k \mathbf{w}_k^T] &= \mathbf{Q} \\
 E[v_k v_k^T] &= R \\
 E[\mathbf{w}_k v_k^T] &= 0.
 \end{aligned} \tag{7}$$

where $\mathbf{c}_k = [\cos(\omega k T_s) \ \sin(\omega k T_s)]$, $\mathbf{w}_k, v_k, \mathbf{Q}, R$ are process noise, measurement noise and their respective covariance matrices and T_s is the sample period. Here, $\mathbf{Q}$ and R have an adverse effect on the Kalman gain and therefore the tracking bandwidth. If R is chosen as $R = \sigma^2$, where σ is the standard deviation of the Gaussian noise in the sensor signal $y(t)$, $\mathbf{Q}$ remains the only tuning variable. The recursive implementation follows the standard equations of the Kalman filter [25], [26]. The calculations in the prediction steps are heavily simplified due to the time-varying system representation, enabling a high-bandwidth implementation on an FPGA [19]. Amplitude and phase are recovered by employing the output equations (5).

D. Lyapunov Filter

The Lyapunov filter is an online adaptive estimator based on the linear parametrization of the LTI transfer function of the signal (1) for which the estimation error relates to the parameter error through a strictly positive real (SPR) transfer function $W(s)$ [27]. This SPR property is exploited in designing the update law via a Lyapunov stability proof to show boundedness of the error. An additional persistency of excitation property [27] guarantees exponential convergence of the parameters. The estimator can be written as [17]

$$\begin{aligned}
 \dot{\mathbf{x}} &= \gamma \mathbf{c}(t)^T W(s) (y - \hat{y}) \\
 \hat{y} &= \mathbf{c}(t) \mathbf{x}
 \end{aligned} \tag{8}$$

where γ is a constant gain parameter for tuning the bandwidth and $\hat{y}$ is the estimated signal. A digital implementation

TABLE I
SUMMARY OF IMPLEMENTED DEMODULATION METHODS

Method	Max. F_s [kHz]	Max. F_3 dB [kHz]	Tuning	Order
LIA	431	70.0	LPF f_{lpf}	4
HBW LIA	417	52.6	LPF f_{lpf}	4
KF	300	50.5	$\mathbf{Q}$	1
LYAPF	327	50.0	γ	1

of the Lyapunov filter requires two DDS compilers, multipliers, discrete filters and discrete integrators. Amplitude and phase are recovered by employing the output equations (5).

III. EXPERIMENTAL RESULTS

A. Implementation and Experimental Setup

The demodulators were implemented digitally on a common digital signal processing system (National Instruments USB-7855R with Kintex-7 70T FPGA) using dedicated LabVIEW DSP blocks in order to ease reproducibility. When left free-running, the resulting sampling rate of the LabVIEW system is representative of the implementation complexity and as such is used as a comparison parameter and stated in Table I. Here, the LIA as the simplest method achieves the highest sample rate, followed by the HBW LIA, LYAPF and KF. It must be stressed that the difference of only 27 kHz between LYAPF and KF is not in line with their respective implementation complexities. However, the small difference can be associated with the highly hardware optimized implementation of the KF [15], [19], which does not use any continuous states or LabVIEW specific blocks. In order to make a clear comparison between the demodulation methods, a fixed sample rate of $f_s = 300$ kHz was chosen for the experimental verification.

B. Tracking Bandwidth

To determine the tracking bandwidth, a laboratory function generator (Agilent 33521A Waveform Generator) providing a carrier frequency of $f_c = 50$ kHz is amplitude modulated by

Fig. 3. Relationship between the respective demodulator tuning variable and achievable tracking bandwidth.

a swept sine signal. This FM-AM concept directly reveals the low pass filter characteristic of the demodulators and allows for a direct extraction of the -3 dB tracking bandwidth.

The results are presented in Fig. 2 where four different tracking bandwidths are shown for each demodulator. The absolute maximum achievable tracking bandwidths are stated in Table I. Apart from the tracking bandwidth, the equivalent demodulator filter order (determined from the amplitude reduction per decade for the slowest bandwidth setting) can also be determined from this plot and is stated in Table I. Here, the LIA achieves the highest bandwidth, however at the expense of passing through large $2f_c$ and $4f_c$ components, as is visible from the spikes in Fig. 3(a). Comparing Fig. 3(a) with Fig. 3(b), the elimination of the harmonic peaks due to the phase cancellation of the HBW LIA is clearly visible. The KF and LYAPF achieve a bandwidth of around 50 kHz which corresponds to tracking within one cycle of the carrier signal.

C. Demodulator Tuning

By plotting the tuning parameter against the experimentally determined tracking bandwidth in Fig. 3, the region of linear relationship of each technique is determined. The tuning variables are the low-pass filter cut-off frequencies f_{lpf} for the LIA and HBW LIA, assumed covariance Q for the KF, and feedback gain γ for the LYAPF. All methods achieve a linear relationship for the lower end of tracking bandwidths on a double logarithmic scale. At the upper range of the tracking bandwidths, the relationship function for the KF flattens out revealing the proximity to the bandwidth limitation. Also noticeable is a slight deviation from the linear trend for the LYAPF associated with a peaking at the carrier frequency due to recovery of the carrier signal itself.

D. Robustness to Other Frequency Components

To determine the robustness to other frequency components, we perform a carrier frequency sweep while a specific frequency is modeled at $f_c = 50$ kHz and the demodulation bandwidth is set to a fixed value of 1 kHz. The off-mode rejection is calculated as the difference between the gain at the modeled frequency (0 dB) and at 40 kHz as highlighted in Fig. 4. It can be seen, that the LIA and the HBW LIA yield the best off-mode rejection of around -42.0 dB

Fig. 4. Off-mode rejection of the demodulators for a carrier frequency of $f_c = 50$ kHz and a tracking bandwidth of 1 kHz. From the folding artifact located at f_f , the effective sampling rate can be deduced as $f_s = f_c + f_f$.

owing to the fourth-order low-pass filters employed. This result emphasizes the fact that these methods should be used when maximum suppression of other distinct frequency components in the deflection signal is of priority. The KF and LYAPF yield an off-mode rejection of around -19.5 dB. Because the frequency sweep is performed beyond the sample frequency f_s of the implemented filters, a folding artifact is observed at $f_f = f_s - f_c$ which can be used to extract the exact sample frequency.

E. Noise Evaluation

To determine the noise performance, the RMS noise of the amplitude estimate of the demodulators is evaluated as a function of tracking bandwidth and compared against the performance of an ideal second-order low-pass filtered (Stanford Research SR560 Low Noise Preamplifier) white noise process. For this purpose, a laboratory function generator, providing a carrier frequency of 50 kHz is amplitude modulated by a 40 kHz bandwidth-limited white noise signal with an amplitude of $10 \text{ mV}_{\text{rms}}$ to dominate any additional noise introduced by the DSP system. This approach also allows for a direct comparison with an ‘ideal demodulator’, resembled by low-pass filtered white noise of equal magnitude. The acquisition front end of a micro system analyzer (Polytec MSA-050-3D) is used to capture time-domain data sampled at $f_s = 2.56 \text{ MHz}$ for $T = 13.11 \text{ s}$. We use the total

Fig. 5. Tracking bandwidth vs. total integrated noise for each demodulator and for a low-pass filtered white noise process as reference, color-coded according to Fig. 4

integrated noise (TIN) as the performance metric, which for a given system G assuming a white noise input is given by [28]

$$\sigma(G) = \sqrt{\int_0^{f_{bw}} A |G(j\omega)|^2 df} \quad (9)$$

where f_{bw} is the measurement bandwidth and A is the power spectral density of the white noise. The TIN is obtained by integrating the noise density estimate from DC to $f_s/2$ using Welch's method with 16 averages.

The results are shown in Fig. 5. It can be seen that the LIA follows the trend of the reference filtered white noise process for low tracking bandwidths but exhibits an exponentially growing TIN when the tracking bandwidth approaches the carrier frequency. This fact is due to the increasing $2f_c$ component in the amplitude estimate due to inadequate filtering. On the contrary, the HBW LIA does not show this increase owing to its phase cancellation. However, the addition of the phase shifted mixing products increases the noise for lower tracking bandwidths. The KF and LYAPF show an equal trend with respect to the reference filtered white noise process with increasing tracking bandwidth until the non-linearity of the LYAPF becomes visible for the very high bandwidths. At frequencies approaching DC, the methods approach a constant value which limits the minimum estimated noise due to residual DC-offsets and $1/f$ -noise. Over the bandwidth of interest, the demodulators adequately follow the reference of the low-pass filtered white noise with slight increased noise which can be attributed to their limited and bandwidth-dependent off-mode rejection as discussed in the previous section. Although the responses roll-off around the modeled frequency, at 1 kHz tracking bandwidth, the maximum attenuation is only 30 dB for LYAPF and KF and 42 dB for LIA and HBW LIA, which may be passing noise from the out-of-band frequencies. This experiment highlights that the amplitude noise needs to be taken into account when

Fig. 6. (a) Frequency response of the DMASP cantilever in open-loop (blue) and for various controller gains to reduce the quality factor from 222 down to 8. (b) Tracking bandwidths of the DMASP cantilever determined via amplitude modulation for selected frequency responses shown in (a).

stating the maximum tracking bandwidths of these methods. As such, the LIA can only be used up to a tracking bandwidth of 38 kHz (compared to 70 kHz as stated in Table I) before the harmonic distortion makes this demodulator unusable. On the contrary, the LYAPF and KF, despite being of first order, show excellent noise performance over the entire bandwidth of interest.

F. AFM Imaging

To demonstrate the effect of insufficient demodulator bandwidth in a high-speed tapping-mode AFM experiment, a NT-MDT NTEGRA AFM equipped with a Bruker DMASP piezoelectric cantilever was used and imaging was performed in constant height. This approach circumvents the common z-axis actuator bandwidth limitation since the z-axis controller bandwidth is reduced to the point where the sample features entirely appear in the amplitude error image and therefore any imaging artifacts are due to either insufficient demodulator or cantilever bandwidth. In order to render the demodulator the bottleneck, we employ a piezoelectrically actuated cantilever with fundamental resonance frequency of $f_1 \approx 50$ kHz. The integrated actuation allows for model-based quality factor control [29] to reduce the quality factor to $Q_1 = 8$, resulting in an experimentally verified tracking bandwidth of 3.3 kHz, adequately matching the first order approximation $f_1/(2Q_1)$ [9], as can be seen in Fig. 6.

AFM images of a calibration grating (NT-MDT TGZ3) with periodic features of heights $h \approx 500$ nm were obtained at a speed of $627.45 \mu\text{m/s}$, scanner rate of 30 Hz and area of $10 \mu\text{m} \times 10 \mu\text{m}$ and are shown in Fig. 7. It can be seen that for small demodulator bandwidths in Fig. 7(a)-(c), the sample features are not accurately tracked. By setting a larger demodulator bandwidth (here using the Lyapunov filter), the sharp sample features are properly tracked in Fig. 7(d)-(f).

Fig. 7. 3D, 2D image and crosssection of (a)-(c) LIA with $f_{lpf} = 200$ Hz and (d)-(f) Lyapunov filter with $\gamma = 60k$ at an imaging speed of $627.45 \mu\text{m/s}$.

IV. CONCLUSION

In this work, we have performed a frequency domain analysis of the lock-in amplifier and three novel demodulation techniques, namely the high-bandwidth lock-in amplifier, Kalman filter and Lyapunov filter. The methods were implemented on a common DSP system and experimentally assessed with respect to their tracking bandwidth, noise performance, complexity and robustness to other frequency components. The results highlight the superiority of the Kalman filter and Lyapunov filter when it comes to maximizing the tracking bandwidth without introducing excessive noise in the estimate due to inadequate filtering of the mixing products which commonly arise in a lock-in amplifier implementation. While the high-bandwidth lock-in amplifier eliminates these mixing products via phase cancellation, it introduces additional noise at low frequencies due to the summation of the phase shifted signals. If maximum noise suppression away from the carrier frequency is the priority, the lock-in amplifier can still be regarded as the method of choice as it shows large off-mode rejection and the lowest noise at low tracking bandwidths.

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