Noise in Frequency Modulation-Dynamic Force Microscopy

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Abstract. Analytical expressions giving the noise power spectral densities of the signals of interest in frequency modulation-dynamic force microscopy are derived. They are validated by comparison with numerical simulations performed with a realistic virtual force microscope. Thermal noise as well as detection noise are considered. A tip-substrate interaction incorporating a van der Waals and a Morse potential is considered as an illustrative example.

1. Introduction

Frequency Modulation-Atomic Force Microscopy (FM-AFM) is a rather complex technique. Its complete analysis is difficult mainly because it includes non-linearities, which can be classified in two types: 1) the tip-substrate interaction is non-linear [1] because the oscillating amplitudes are large compared to its range; 2) the control system of the microscope includes itself non-linearities, in the form of multipliers, which make the analysis by usual linear control theory methods impossible. Nevertheless, a good understanding of the noise of the instrument is an important goal. It allows to precise the limits to the accuracy of the measurement set by the different kind of noise and what are the optimal settings to approach them. It can also help to avoid measurement artefacts and to compare different instrumental choices.

A virtual AFM was recently shown to provide a realistic numerical model of a real FM-AFM, including noise [2], but no analytical model has yet been proposed. The aim of this paper is to set analytical expressions for the noise in FM-AFM and to validate them by comparison with results produced by the virtual AFM.

This paper is a summary of a longer one, which is in preparation. For the detailed structure of the virtual AFM, we refer to [2].

2. Noise analysis of the FM-AFM oscillator

We briefly recall the structure of the control system of a FM-AFM illustrated in figure 1. The cantilever $C$ is maintained oscillating at its resonance frequency $\omega_c$ by a positive feedback loop which is constituted by an Automatic Gain Control (AGC) device and a Phase-Locked Loop (PLL)-based frequency demodulator. When properly set, the PLL outputs a signal $exc(t)$ at the resonant frequency $\omega_c$ with a phase shift of $\frac{\pi}{2}$ relative to the oscillation of the cantilever $z(t)$. The amplitude is measured by the Synchronous Demodulator (SD) of the AGC and compared with a pre-set value $A^\ast$. The resulting error signal is passed through a Proportional-Integral
controller (PI) giving \( w(t) \) called the damping signal, because it is proportional to the tip-substrate energy dissipation when the above mentioned phase shift of \( \frac{\pi}{2} \) is realized [3]. The Proportional gain \( P \) and Integral gain \( I \) allow to set the stability and the precision of the AGC regulation loop. When used in the constant frequency detuning imaging mode, the Automatic Distance Control loop (ADC) adjusts the tip-substrate distance \( D(t) \) in order to maintain the frequency detuning \( \Delta f(t) \) at a pre-set value \( \Delta f^* \). The error signal \( \Delta f^* - \Delta f(t) \), after being passed through a Proportional-Integral controller (PI\(_{adc} \)), acts on the tip-substrate distance \( D(t) \) via a piezoelectric transducer.

We consider only two noise sources, which are known to dominate in FM-AFM [5, 6]. (i) The thermal equilibrium noise of the cantilever, of two-sided Power Spectral Density (PSD) \( S_f = \frac{4k_B T}{Q} \) (in N².Hz⁻¹) where \( k \) and \( Q \) are the stiffness and quality factor of the cantilever, \( k_B \) the Boltzmann constant and \( T \) the temperature. Due to the equipartition of energy, the power of thermal noise should be shared equally between amplitude and phase noise. Thus, \( S_f = S_f^a + S_f^\phi \), with \( S_f^a = S_f^\phi = \frac{1}{2} S_f \). (ii) The noise of the deflection sensor \( S_z \). The amount and type of noise depends on the specific method used and of its detailed implementation. In the absence of more precise specifications, we will also consider that \( S_z^a = S_z^\phi = \frac{1}{2} S_z^\phi \).

2.1. Analytical formulation

We start from the simplest situation, where the cantilever is oscillating at a large distance from the substrate. The tip-substrate interaction is then negligible and the ADC is opened. We indicate only the starting point and the result of the calculation. Details will be published elsewhere. The displacement \( z(t) \) of the tip can be modeled as an amplitude and phase modulated carrier [4]: \( z(t) = A_c[1 + m(t)] \sin[\omega_c t + \phi(t)] \). With \( m(t) = m_0 \cos(\Omega t + \theta_0) \), \( \phi(t) = \phi_0 \sin(\Omega t + \theta_0) \) and assuming small maximum deviations \( \phi_0 \) and \( m_0 \), we get:

\[
z(t) \approx A_c \sin(\omega_c t) + \delta z_a \{ \sin[(\omega_c + \Omega) t + \theta_0] + \sin[(\omega_c - \Omega) t - \theta_0] \} \\
+ \delta z_{\phi} \{ \sin[(\omega_c + \Omega) t + \theta_0] - \sin[(\omega_c - \Omega) t - \theta_0] \}
\]

with \( \delta z_a = A_c \frac{m_0}{\omega_c} \) and \( \delta z_{\phi} = A_c \frac{\phi_0}{\omega_c} \). The crossterm in \( \phi_0 m_0 \ll 1 \) is neglected.

Starting from this expression for \( z(t) \), the damping signal \( w(t) \) at the output of the AGC can be calculated as well as the excitation signal at the output of the PLL (figure 1). Then the excitation force \( F(t) = exc(t).w(t) + \delta F(t) \) is applied to the cantilever through the transfer function:

\[
Cl(\omega) = \frac{z(\omega)}{F(\omega)} = \frac{1}{k(\frac{\omega_c^2 - \omega^2}{\omega_c^2} + \frac{j\omega}{Q\omega_c})}
\]

Near resonance, \( \omega = \omega_c + \Omega \), with \( \Omega \ll \omega_c \) and \( Cl(\omega_c + \Omega) = C(\Omega) \approx \frac{1}{k(\omega_c^2 + \Omega^2)} \). Neglecting the second order noise terms - in \( \delta z_a \delta z_{\phi} \) one finally gets \( PSD_w(\Omega) \), the PSD of the damping signal, and \( PSD_{\Delta f}(\Omega) \), the PSD of the frequency detuning signal:

\[
PSD_w(\Omega) = 4 \left| \frac{2F_{agc}(\Omega)}{1 - 2jC(\Omega)F_{agc}(\Omega)} \right|^2 \left| C(\Omega) \right|^2 S_z^\phi + S_z^a \tag{1}
\]
PSD\(\Delta f(\Omega) = 4\nu^2 \frac{H(\Omega)}{1 - j\frac{k}{Q}C(\Omega)H(\Omega)}^2 (|C(\Omega)|^2 S^\phi_f + S^\phi_z)\) (2)

with the transfer function of the AGC \(F_{\text{agc}}(\Omega) = \frac{-1}{1 + j\frac{f}{\tau_D}(P + \frac{I}{f})}\) and the transfer function of the PLL \(H(\Omega) = \frac{K_v}{j\Omega(1 + j\tau_1)(1 + j\tau_2) + K_v}\). \(\tau_D\) is the time constant of the lowpass filter of the SD, \(P\) (resp. \(I\)) is the gain of the proportional (resp. integral) branch of the P-I controller of the AGC. \(K_v\) is the loop gain of the PLL, \(\tau_1\) and \(\tau_2\) the time constants of the second order lowpass filter of the PLL [2].

The noise of the damping signal depends on the thermal phase noise and the detection amplitude noise while the frequency detuning noise depends on the thermal amplitude noise and the detection phase noise. This results from the fact that, for noise or small displacements from equilibrium, the two feedback loops of the control system work independently.

**2.2. Numerical simulations**

Figure 2 shows \(PSD_w(\nu)\) and \(PSD_{\Delta f}(\nu)\) obtained by numerical simulation compared with their analytical expressions (1) and (2) for different amounts of detection noise. When the detection noise is small (\(S_z = 0\) or \(2 \times 10^{-28}\) m² Hz⁻¹), the spectra are close to their thermal limit in the measuring bandwidth, indicated by horizontal dotted lines. In this situation, the integrated noise scales as \(\nu^2\). The dissipation noise thermal limit is given by \(\lim_{\Omega \to 0} [PSD_w(\Omega, S_z = 0)] = 4S^\phi_f\). This value agrees with that given in [7], within a numerical factor of the order of unity and with [8], within a factor of 2. For the parameters of figure 2, it gives, when expressed in energy per oscillation cycle \(4S^\phi_f\nu^2 \Omega^2 = 10^{-6}\) (eV/cycle)² Hz⁻¹, resulting in a variance of \(2 \times 10^{-4}\) (eV/cycle)² when integrating from - 100 Hz to + 100 Hz. The dissipation sensitivity is then 14 meV/cycle, comparable to the best experimental data obtained so far [9]. The frequency detuning noise thermal limit is given by:

\[
\lim_{\Omega \to 0} [PSD_{\Delta f}(\Omega, S_z = 0)] = \frac{f^2k_BT}{2\pi kA^2_cQ}\]

This two-sided PSD is in agreement with the one-sided expression calculated by Albrecht et al [10]. For the parameters of figure 2, it amounts to \(3.2 \times 10^{-7}\) Hz² Hz⁻¹, resulting in a variance of \(6.4 \times 10^{-4}\) Hz². The frequency detuning sensitivity is then of the order of 0.025 Hz. When the detection noise dominates (figure 2b with \(S_z = 2 \times 10^{-24}\) m² Hz⁻¹), \(PSD_{\Delta f}(\nu)\) increases as \(\nu^2\) from 10 Hz to 1 kHz leading to an integrated noise scaling as \(\nu^2\) as explained by Giessibl [5].
Figure 3 shows how the settings of the AGC influence the PSDs. As expected, $PSD\Delta f(\nu)$ is not affected by these settings, since the two feedback loops work independently. For $P = 0.1 \text{ N.m}^{-1}, I = 10 \text{ N.m}^{-1}\text{s}^{-1}$, a peak appears on $PSD_w(\nu)$. It corresponds to a tendency of the AGC loop to oscillate (“ringing”) at the peak frequency. For $P = 0.01 \text{ N.m}^{-1}, I = 0.5 \text{ N.m}^{-1}\text{s}^{-1}$, the loop operates near critical damping.

The agreement between analytical and simulated spectra is quite good, showing that the approximations involved in the derivation of expressions (1) and (2) are valid for the considered parameters.

3. Introducing the tip-substrate interaction

We consider in the following the tip-substrate interaction potential as a sum of a van der Waals and a Morse contribution. An approximate analytical expressions can be derived for the frequency detuning considering the tip trajectory as sinusoidal, a very good approximation due to the high $Q$ of the cantilever. Following equation (29) in reference [5], one writes the following integral for the frequency detuning:

$$\Delta f = \frac{f_c^2}{k A_c^2} \int_0^{1/f_c} F_{\text{tip-sample}}[z(t)] z(t) \, dt$$

with the cantilever oscillation $z(t) = A_c \sin(2\pi f_c t)$ and the force $F_{\text{tip-sample}}$ between the tip and the sample such as:

$$F_{\text{tip-sample}}[z(t)] = \frac{H R_1}{6(D + z(t))^2} - 2 E_b k (1 - e^{-\kappa(D+z(t)-\sigma)}) e^{-\kappa(D+z(t)-\sigma)}$$

$D$ is the distance between the tip at rest and the surface. The other parameters are explained in figure 4. $\Delta f(D)$ obtained with the virtual AFM is compared in figure 4 with this analytical expression, showing a very good agreement.

Let us consider an amplitude fluctuation $\delta A_c$ and a distance fluctuation $\delta D$. Due to the nonlinear character of the interaction, these fluctuations will induce a frequency fluctuation:

$$\delta \Delta f = \frac{\partial \Delta f}{\partial A_c} \delta A_c + \frac{\partial \Delta f}{\partial D} \delta D = \alpha(A_c, D) \delta A_c + \beta(A_c, D) \delta D$$

with $\alpha = \frac{\partial \Delta f}{\partial A_c}$ and $\beta = \frac{\partial \Delta f}{\partial D}$. These couplings can be taken into account by considering the expression of $z(t) = A_c [1 + m(t)] \sin(\omega_c t + \phi(t))$. The amplitude fluctuation is given by $\delta A_c(t) = A_c m(t) = A_c m_0 \cos(\Omega t + \theta_a)$. The distance fluctuation is imposed as $\delta D(t) =$
Figure 4. Circles: $\Delta f(D)$ obtained with the virtual AFM with the following parameters: $P = 0.1$ N.m$^{-1}$, $I = 10$ N.m$^{-1}.s^{-1}$, $A^* = 20$ nm and without noise. Interaction parameters, for the van der Waals contribution: Hamaker constant $H = 1$ eV, tip radius $R_1 = 10$ nm, for the Morse contribution: depth of the potential minimum $E_b = 2.15$ eV, equilibrium atomic bond distance $\sigma = 0.235$ nm and decay of the potential $\kappa = 15.5$ nm$^{-1}$. Continuous line: analytical expression. Dotted lines: $-\alpha(D)$. Dashed lines: $\beta(D)$. $-\alpha$ and $\beta$ are distinct but not distinguishable at the scale of the figure.

$\delta D_0 \cos(\Omega t + \theta_d)$. The couplings $\alpha$ and $\beta$ generate a new phase modulation contribution $\phi^{\text{int}}(t)$ such that $\phi(t) = \phi_0 \sin(\Omega t + \theta_a) + \phi^{\text{int}}(t)$ with:

$$\phi^{\text{int}}(t) = \frac{\delta \Delta f}{\nu} = \frac{\alpha A_c m_0}{\nu} \cos(\Omega t + \theta_a) + \frac{\beta \delta D_0}{\nu} \cos(\Omega t + \theta_d)$$

Then:

$$z(t) = z_0(t) + \delta z^{\text{int}}_A \{\cos[(\omega_c + \Omega)t + \theta_a] + \cos[(\omega_c - \Omega)t - \theta_a]\} + \delta z^{\text{int}}_D \{\cos[(\omega_c + \Omega)t + \theta_d] + \cos[(\omega_c - \Omega)t - \theta_d]\}$$

where $\delta z^{\text{int}}_A = \frac{\alpha A_c^2 m_0}{2\nu} \delta z_a$ and $\delta z^{\text{int}}_D = \frac{\beta A_c^2}{2\nu} \delta D_0$. Starting from this expression of $z(t)$, the calculation proceeds as in section 2.1. Expression (1) for $\text{PSD}_w(\nu)$ stays unchanged, because it does not depend on the position phase noise while expression (2) for $\text{PSD}_{\Delta f}(\nu)$ becomes:

$$\text{PSD}_{\Delta f}(\nu) = 4 \nu^2 \left| \frac{H}{1 - j \frac{k}{\beta} C H + \beta F_{\text{adc}} H} \right|^2 \left[ C \left| S_f^a + S_z^\phi \left( \frac{\alpha A_c}{\nu} \right)^2 \right| \frac{C}{1 - 2j C F_{\text{adc}}} \left| S_f^\phi + |F_{\text{adc}}|^2 S_z^a \right| \right]$$

with $F_{\text{adc}}(\Omega) = P_{\text{acc}} + \frac{I_{\text{acc}}}{\beta t}$ the transfer function of the ADC. Due to the interaction, the four noise sources ($S_f^a, S_f^\phi, S_z^a, S_z^\phi$) contribute now to the frequency noise. Finally, the PSD of the distance $D$ is given by:

$$\text{PSD}_D(\nu) = |F_{\text{adc}}|^2 \text{PSD}_{\Delta f}(\nu) = 4 \nu^2 \left| \frac{\beta F_{\text{adc}} H}{1 - j \frac{k}{\beta} C H + \beta F_{\text{adc}} H} \right|^2 [\text{noise source terms}]$$

The results displayed in figure 5 show good agreement between simulated and calculated data. It is seen that the frequency noise scales approximately as $\alpha^2$; it is dominated by the non-linear contribution. It increases when the tip is closer to the substrate, except at very short distances, when $\alpha^2$ begins to decrease due to the repulsive interaction (figure 4). $\Delta f$ shows a more complex behaviour due to the $1/\beta^2$ dependance when $\beta F_{\text{adc}}$ is kept constant as in figure 5.
Figure 5. (a) $PSD_{\Delta f}(\nu)$, (b) $PSD_D(\nu)$ with $\beta P_{adc} = 0.2$ and $\beta I_{adc} = 400$.

4. Conclusions
The analytical expressions for the Power Spectral Densities of the different signals produced by FM-AFM presented here open many possibilities. We plan to use them to compare and to optimize different instrumental choices, for instance for which kind of measurement a tuning fork is a better choice than a cantilever.

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