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Identification of Interaction Potentials in Dynamic Mode Atomic Force Microscopy

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***Abstract*— Atomic Force Microscopes (AFMs) are devices employed in many nanotechnology fields for nanoscale imaging and surface manipulation at the atomic level. The interaction potential between the cantilever tip and the sample is typically obtained using force curves. Each force curve involves an approach and retract phase and the entire process is relatively slow. In this paper we present the non-parametric identification of the tip-sample interaction potential that has the potential to significantly reduce the time when compared to force curves.**

I. INTRODUCTION

In recent years there has been a considerable progress in nanotechnology particularly propelled by instruments capable of providing atomic resolution. The Atomic Force Microscope (AFM) is one of the most widely employed instruments of this kind [1]. The instrument is composed by a microcantilever which can be excited through a dither piezo. The cantilever tip position can be measured using a laser beam and a photodiode. An AFM can work in many operating modes; however, in this paper, we are particularly focused on the so-called "tapping" or "dynamic" mode.
In such an operating mode, the AFM cantilever is periodically forced by a piezo placed under its support inducing a periodic oscillation influenced by the interaction forces between the cantilever tip and the sample. The topography is inferred by slowly moving the cantilever along the sample surface by the means of a piezoactuator and by measuring the magnitude and phase of the first harmonic of the cantilever deflection through an optical lever method as shown in Figure 1. Towards this aim, the experimentally observed quasi-sinusoidal nature of cantilever oscillation is exploited.

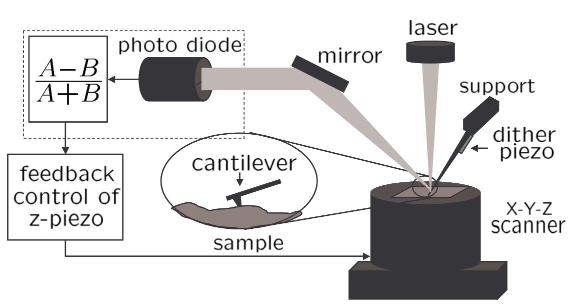

Fig. 1. A typical setup of an AFM is shown. The dither piezo forces the cantilever to oscillate at its resonance frequency with certain magnitude. The deflection of the cantilever is registered by the laser incident on the cantilever tip, which reflects into a split photo-diode. The xyz-piezo scanner is used to position the sample. The deflection signal is fedback to the z-piezo to track the sample profile. The xy-piezo moves the sample in a raster scanning pattern during imaging

In recent literature a Lure model [2] was introduced to model the tip-sample interaction. The Lure model is a feedback interconnection of a SISO linear system with a memoryless nonlinear block as depicted in Figure 2 . The linear block only describes the dynamical behaviour of

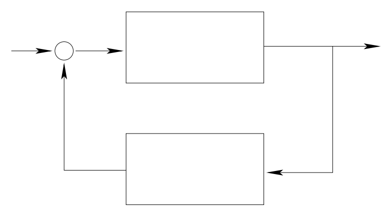

Fig. 2. Block diagram of a Lur'e system

the cantilever, while the nonlinear one represents the force interaction between the tip and the sample. The identification of the subsystem can be achieved indipendently in many manners [3] [4], while the identification of the nonlinear block is still a challenging task. Towards this aim, many techniques have been recently proposed. In [4] force curves are obtained by moving the sample relative to the cantilever in a quasi-steady state manner where the cantilever is not forced. The sample is moved slow enough that it can be assumed that the cantilever tip settles to the equilibrium point corresponding to the separation and previous initial conditions. However, the static force curves do not characterize the tip-sample interaction behavior when the cantilever is oscillating. Clearly, static force curves cannot characterize the damping and lossy processes of the sample, as such forces typically depend on the cantilever velocity and are absent when the velocity is zero. It is reasonable to think that the interaction force could show a distinct behaviour when then tip is continuosly moving, as it happens in the tapping operation mode. This motivates the development of tools to perform a "dynamical" identification in order to detect the forces acting on the cantilever [5]. In [6] power and harmonic balance is employed to determine the parameters of a piecewise linear model of the tip-sample interaction potential. In [7] the same technique has been extended and applied considering a wide class of Lennard-Jones-like potential functions. However, in all of the previous studies the employed techniques are parametric [8]. In this work a nonparametric approach is applied. Consequentely, there is no need to choose a specific class of functions to represent the potential. This approach is motivated by two considerations. First,the tip-sample interaction potential char-

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acteristics, even qualitatively might not be known making a parametric approach very difficult. Towards this purpose we adopt the framework presented in [8]. The main advantage lays in the fact that the shape of the nonlinearity is directly derived from measured signals which need to be extensively processed, though. In the studied case, we extensively use the Lur'e structure of the model and the assumption that the force can be expressed through a single-valued nonlinear function. This is a limitation and in future studies we will extend the study to tip-sample interaction models where dissipation is included.
The paper is structured as follows: first, a brief introduction to the AFM model is presented; then the proposed identification technique is briefly described and finally experimental results are reported.

II. AFM MODEL

For sake of completeness, in this section we briefly describe the AFM model we employ in our identification scheme.

A. Cantilever model

AFM cantilevers have their lengths in the range of $-$ μ . When operating in tapping mode, common values for the tip oscillation amplitudes are of the order of $-$, that is less than $^{-}$ times the cantilever length. Thus, it is reasonable to model an AFM cantilever as a linear elastic beam as depicted in Figure 3. The cantilever is well

Fig. 3. Schematic representation of a microcantilever as an elastic beam

modelled as

$$\omega \quad \sum^{\infty} \frac{}{-\omega \qquad \xi\,\omega \quad \omega \quad \omega} \quad \omega \qquad (1)$$

where is the coordinate along the cantilever, ω is the modal frequency and ξ , are the corresponding damping factor and gain [9]. We will employ capital letters to indicate the Fourier transform of the time signal. Assuming the tip located at a distance , we define the tip vertical displacement as the measured variable and as the equivalent load acting on the tip. So, we limit ourselves to the equation

$$\omega \quad \sum^{\infty} \quad \omega \quad \omega \qquad (2)$$

where

$$\omega \qquad \frac{}{-\omega \qquad \xi\,\omega \quad \omega \quad \omega} \qquad (3)$$

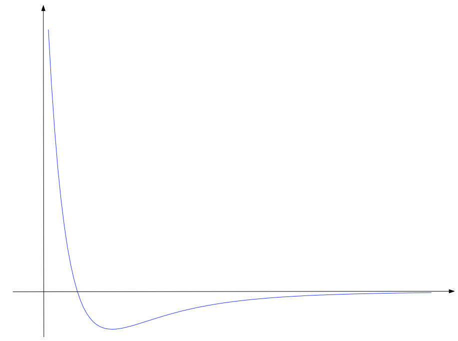


Fig. 4. Qualitative behaviour of static interaction force between the AFM tip and the sample as a function of the relative distance . The force is strongly repulsive for small values of while it is weakly attractive for large ones, converging to as approaches ∞

Every term ω in (2) represents an elastic "mode" of the beam and the cantilever transfer function is given by the sum of all its modes

$$\omega \quad \sum^{\infty} \quad \omega \qquad (4)$$

A single-mode approximation is considered sufficient for most applications, where it is assumed that a cantilever behaves like a simple spring-mass-damper system, that is

$$\omega \qquad \omega \qquad \omega \simeq \frac{}{-\omega \qquad \xi\,\omega \quad \omega \quad \omega} \qquad \omega \qquad (5)$$

However, as will be seen later, multi-mode models can be required when it is important to give a more detailed description at higher frequencies.

B. Interaction force model

Microscopic bodies have complicated interactions that can be repulsive or attractive depending on the relative distance as shown in Figure 4. Attractive forces are mainly due to Van der Waals forces, but some other phenomena like the surface tension of the moisture film can play a significant role on the cantilever behaviour. The strong repulsive forces are caused by overlap of similar charges that occurs at small distances.
We will assume a "memoryless" expression for the force , where the dependence is only on the relative distance of the two bodies and the associated derivatives

C. Tapping AFM model

Under the assumptions presented in sections II-A and II-B the whole system can be represented in the Lur'e structure depicted in Figure 5. where, apart an additive term, the tip position can be assumed as the tip-sample relative distance, is the cantilever transfer function, is the known periodic excitation generated by the dither piezo, $\dot{}\ \ddot{}$ is the interaction force and ξ is an additive

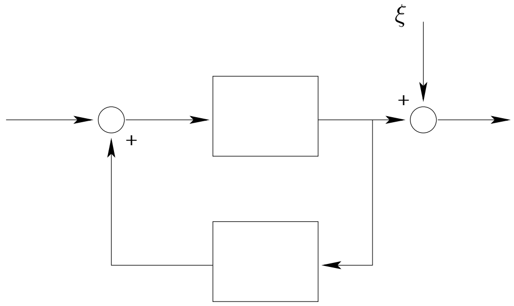


Fig. 5. Lur'e structure of the AFM model

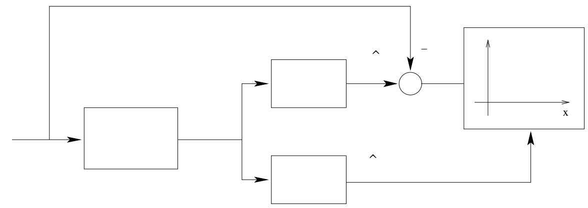


Fig. 6. Schematic representation of the force identification technique

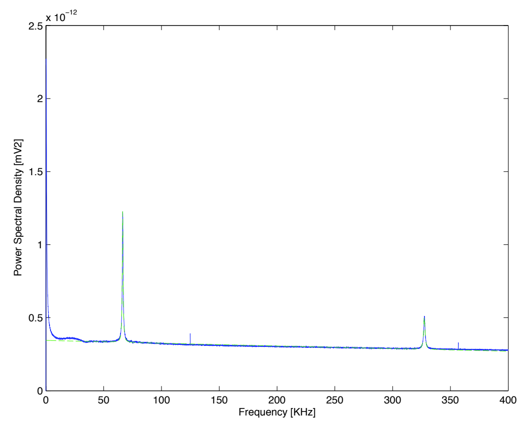


Fig. 7. The system thermal response (solid line) is very well fitted by a two-mode model (dashed line)

output noise corrupting the photodiode measurement . It may be convenient to write the system equations as

$$\dot{\ } \quad \ddot{\ } \quad \xi \tag{6}$$

III. IDENTIFICATION TECHNIQUE

We consider an AFM model as the one defined in (6). We use the notation ω to indicate the power spectral density of a signal . We assume that and $_\xi\ \omega$ can be estimated or are a-priori known. Moreover, we assume that the system has entered a steady state regime, so all deterministic signals are periodic.
An estimate $\hat{\ }$ and an estimate $\hat{\ }$ of can be sought using deconvolution filters and that process the measured signal Thus we have

$$\hat{\ }\ \omega \quad \omega \quad \omega \qquad \hat{\ }\ \omega \quad \omega \quad \omega \tag{7}$$

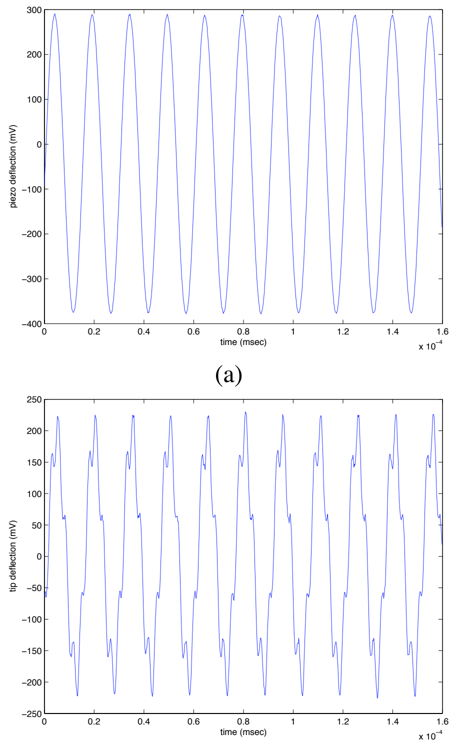
The use of a non-causal Wiener Filter in (7) leads to

$$\frac{}{\xi} - \omega \left(- \frac{\xi}{} \right) - \omega \qquad \frac{}{\xi}\ \omega \left(- \frac{\xi}{} \right) \omega \tag{8}$$

Both and cannot be computed since is not known. However, can be estimated directly from data, so a good approximation is possible. Since the identification is not being done in real-time it is possible to invert the system even if it has non-minimum phase zeros.
Note that the signal $\hat{\ }$ $\hat{\ }$ $-$ provides an estimate of along the trajectory . Thus, the plot of $\hat{\ }$ as a function of $\hat{\ }$ gives the interaction force plot in a straighforward way. The nonparametric identification scheme is represented by Figure 6.

IV. EXPERIMENTAL RESULTS

In this section we report experimental results obtained applying the methods we described in the previous section.
In Figure 7 the identification of based on the thermal response is shown. We can distinguish two different sharp peaks, the first at and the second at .
We employ a two mode model for the reconstruction of the tip-sample interaction potential. A one mode model does not yield good results. As a byproduct of the thermal tuning we also obtain the Power Spectral Density $_\xi\ \omega$.
For identification purposes it was found that the tip-sample offset has to be such that the cantilever deflection exhibits relatively large higher harmonics.
If the separation is too large, the higher harmonics become small and get consequently corrupted by the output noise (we assume that the thermal noise is neglegible). Similarly, a very small offset leads to a small oscillation amplitude and again to small energy coupled with high order components.
A theoretical study to detect the optimal separation is outside of the goals of this paper even if it could be an interesting subject for future investigations.
The signals and have been acquired at a sampling rate and oversampled by a factor . In Figure 8, we have reported the measured data. The two noncausal Wiener filters and have been designed as previously described in order to find the signals $\hat{\ }$ and $\hat{\ }$. The plot of $\hat{\ }$ $\hat{\ }-$ as a function of $\hat{\ }$ is presented in the Figure 9. As it can be noted, the obtained plot has a shape very close to the expected graph of Figure 4, but it is does not represent a single-value function. This cannot be attributed to the noise alone, but, more likely, it shows the presence of a hysteresis cycle in the tip-sample interaction. In future works much effort will be spent in obtaining a better identification with a model capable to explain also such hysteresis phenomena.



(a)

(b)

Fig. 8. (a) Input forcing signal
(b) Output measured by the photodiode system

V. Conclusions

A method to identify the interaction potential between the cantilever tip and the sample in an AFM has been illustrated. The main advantage lies in the fact that the method is nonparametric, so it does not rely on the choice of a particular model class for the identification. Since no restrictive assumptions are made on the interaction force it is possible to investigate a larger class of tip-sample potentials.

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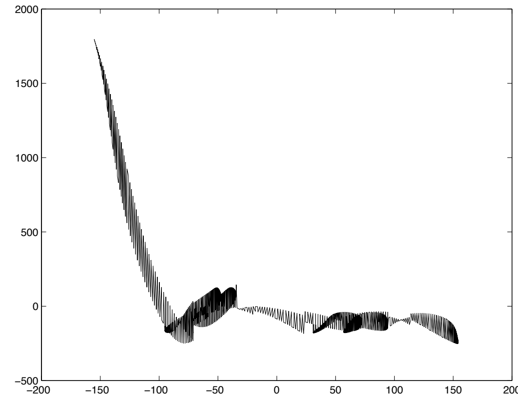

Fig. 9. The graph obtained plotting the estimated force ˆ as a function of ˆ

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