Real time estimation of equivalent cantilever parameters in tapping mode atomic force microscopy

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In this article, a method of imaging is developed, where during tapping-mode operation, equivalent resonant frequency and quality factor can be obtained in real time. It involves exciting the cantilever near its resonant frequency and two other frequencies chosen close to the resonant frequency. It is shown that changes in equivalent cantilever parameters can be registered for topography changes that are less than 1 nm in height and within 400 μs of the change occurring. The estimation time is two orders of magnitude better than current techniques. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3206740]

In the recent past, several ways of exciting the cantilever in an atomic force microscope (AFM) were developed with the aim of determining equivalent cantilever parameters.[1,2] All of these techniques rely on the fact that the cantilever interacting with the sample can be modeled as a spring-mass-damper system whose parameters, equivalent resonant frequency, ω_0', and quality factor, Q', vary depending on sample properties. There is an open question on the simplest excitation of the cantilever that can lead to a real time estimation of the equivalent cantilever parameters.

In the recently developed, band excitation (BE) method[1] and fast chirp methods,[2] the cantilever is excited with a continuous or discrete band of frequencies near the resonance. The cantilever input and output are recorded simultaneously and a second order model is fitted to the measured response. This gives the information about the equivalent resonant frequency and quality factor at each sample point with the image resolution limited by the image size, $(M\times N)$ pixels, where same procedure has to be carried out at each pixel. Also in the BE and fast chirp methods, the cantilever response to the input excitation has large amplitude variation which makes it difficult to obtain equivalent cantilever model parameters at one particular interaction level. These techniques provide the information at discretized levels in the vertical z direction in force spectroscopy experiments.

In this article, a technique is presented to estimate equivalent cantilever resonant frequency and quality factor during normal tapping mode operation. Further it is shown that an excitation by sum of three sinusoids is sufficient to extract equivalent cantilever parameters.

Cantilever dynamics in tapping mode can be modeled as a $G-\Phi$ interconnection[3] [see Fig. 1(a)] where $G(i\omega)$ is a second order approximation of the first mode of the cantilever beam and Φ models the nonlinear force exerted by the sample on the tip. It is through Φ that different sample properties like elasticity, height and charge get modulated onto interacting cantilever trajectories.

The $G-\Phi$ interconnection, with a one mode approximation of the cantilever dynamics, can be written as

$$\ddot{p}+\frac{\omega_0}{Q}\dot{p}+\omega_0^2p=\omega_0^2\left[g(t)+\frac{1}{k}\Phi(p,\dot{p})\right], \tag{1}$$

where $p(t)$ is the instantaneous cantilever position, ω_0 is the resonant frequency of the first mode, Q is the quality factor, k is the spring constant of the cantilever, $g(t)$ is the dither excitation, and $\Phi(p,\dot{p})$ is the nonlinear static memory-less tip-sample force. The model (1) with $\Phi=0$ will be termed as "sample-free" model of the cantilever where the cantilever experiences no forces from the sample. As the cantilever comes close to the sample, damping and tip-sample forces (Φ) affect cantilever dynamics. The related models are unknown but using averaging theory[4] it can be shown that the cantilever-sample interconnected system (1) can be modeled as an equivalent cantilever with the dynamics

$$\ddot{p}+\frac{\omega_0'}{Q'}\dot{p}+(\omega_0')^2p=(\omega_0')^2g(t), \tag{2}$$

where ω_0' is the equivalent resonant frequency and Q' is the equivalent quality factor. Thus in the presence of tip-sample interaction, $G-\Phi$ interconnection can be represented by an equivalent second order model $G_z(i\omega)$ [see Fig. 1(a)] that is determined by the parameters ω_0' and Q'.

The question of the sufficiency of the input excitation in determining the equivalent cantilever parameters is discussed next. A general discretized second order dynamics that represents the first mode approximated model of the cantilever is given as

$$e(n)=\vartheta(n)+b_1\vartheta(n-1)+b_0\vartheta(n-2),$$

$$u(n)=a_2g(n)+a_1g(n-1)+a_0g(n-2),$$

$$p(n)+b_1p(n-1)+b_0p(n-2)=u(n)+e(n), \tag{3}$$

where $p(n)$ and $g(n)$ denote the cantilever deflection and dither forcing at sampled time $t=nT_s$, where T_s is the sampling interval and $\vartheta(n)$ is zero mean white measurement noise with variance σ_ϑ^2. Thus to identify the dynamics in Eq. (3), five parameters, (b_1, b_0, a_2, a_1, and a_0), need to be identified. It is well known[5] that to identify $n=5$ parameters in real time $\lceil n/2\rceil=3$ sinusoids at the input are needed for identifying the second order model in Eq. (3). Any less richness of the input will lead to divergence in parameter estimates. The three sinusoids are chosen such that one sinusoid is at or

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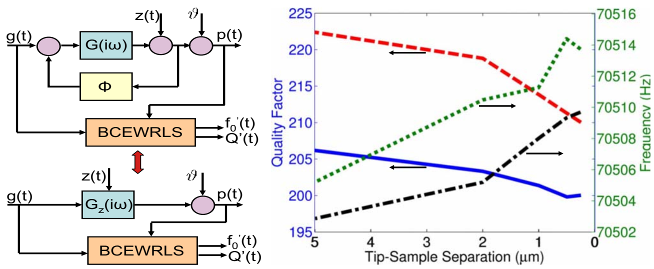
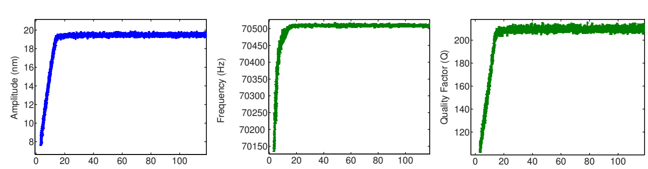


(a) (b)

FIG. 1. (Color online) (a) Modeling cantilever-sample interaction in tapping mode operation as a $G-\Phi$ interconnection where $G(i\omega)$ is the second order cantilever beam model and Φ is the nonlinear tip-sample force. $g(t)$, $z(t)$, ϑ, and $p(t)$ are the dither forcing, the sample height profile, the measurement noise and measured cantilever deflection, respectively. This interconnection can also be viewed as an equivalent second order system, $G_z(i\omega)$, which is dependent on sample height. BCEWRLS algorithm takes $g(t)$ and $p(t)$ as input and gives equivalent resonant frequency, f_0', and quality factor, Q', of the cantilever in real time. (b) Experimentally obtained equivalent resonant frequency f_0' and quality factor, Q', of the cantilever at different nominal tip-sample separations. Tip is not interacting with the sample. Blue-solid and black-dash-dot curves are obtained by a second order fit to the cantilever response to frequency sweep. Red-dash and green-dot curves are obtained by BCEWRLS scheme. This indicates that in most cases estimates of f_0 are accurate within +5 Hz and quality factor estimates are accurate to within +15 of actual values.

near the resonance as is the case in normal tapping mode operation. This will lead to a nominal periodic cantilever oscillations which ensures that the cantilever is interacting with the sample under operating condition found in conventional tapping mode operation. Other two sinusoids are chosen at $f_0 \pm 6$ kHz [with $f_0=(\omega_0/2\pi)$] because $G(i\omega)$ is a high Q system for operation in air and the forcing away from resonance of the cantilever will be heavily attenuated at the cantilever output. Indeed, if the cantilever forcing is $g(t)=A\sin\omega_0 t+B\sin(\omega_0+\Delta\omega_0)t+B\sin(\omega_0-\Delta\omega_0)t$ then the deflection of the sample-free cantilever is $p(t)=|G(i\omega_0)|\sin[\omega_0 t+\angle G(i\omega_0)]\{A+C\}$, where $C=2B[|G(i\omega_0+\Delta\omega_0)|/|G(i\omega_0)|]\cos\{\Delta\omega_0 t+[\angle G(i\omega_0+\Delta\omega_0)-\angle G(i\omega_0-\Delta\omega_0)/2]\}$ characterizes the change in the output amplitude due to the added excitation at frequencies $f_0+\Delta f_0$ and $f_0-\Delta f_0$ and $\angle G(i\omega)$ represents the phase between $g(t)$ and $p(t)$ at input frequency ω. Thus, we have $-2B[|G(i\omega_0+\Delta\omega_0)|/|G(i\omega_0)|]\le C\le 2B[|G(i\omega_0+\Delta\omega_0)|/|G(i\omega_0)|]$. Choosing amplitudes $B=A/2$ with $A\approx 25$ nm, quality factor, $Q\approx 225$ as representative tapping mode parameters, and $\Delta f_0\approx 6$ kHz, results in a total variation of 1 nm in the amplitude of output trajectory from the nominal tapping mode trajectory.



(a) (b) (c)

FIG. 2. (Color online) Experimentally obtained (a) amplitude, (b) estimated f_0', and (c) estimated Q' response during z-force curve experiment. Δ amplitude=12 nm, Δf_0=350 Hz, and ΔQ=110. There are two different slopes in f_0' estimate curve. Both f_0' and Q' decrease with decrease in tip-sample separation.

On identification of plant at several points on the force curve, it was observed that the coefficients a_2, a_1, and a_0, which capture the delays in the system, do not change much and contribute to the response of system at frequencies considerably away from the cantilever resonance. These coefficients are attributed to the dither piezo dynamics or beam dynamics which is not affected by sample properties. Subsequently values of a_2, a_1, and a_0 are fixed to the sample-free model values. It must be noted that even though $\vartheta(n)$ is uncorrelated noise process, $e(n)$ is not uncorrelated noise process. Equation (3) can be written as

$$z(n)=\underbrace{\begin{bmatrix} b_1 & b_0\end{bmatrix}}_{\theta}\underbrace{\begin{bmatrix}-p(n-1)\\ -p(n-2)\end{bmatrix}}_{\phi(n)}+e(n), \tag{4}$$

where θ represents the vector of unknown parameters and $z(n)=p(n)-a_2 g(n)-a_1 g(n-1)-a_0 g(n-2)$. At any time instant $t=nT_s$, past data $z(k)$, and $\phi(k)$ for $k=0,1,\ldots n$ are available. An estimate $\hat{\theta}_{\mathrm{LS}}(n)$ can be computed by solving the standard exponentially weighted least-squares problem

$$\min_{\hat{\theta}_{\mathrm{LS}}(n)} \Sigma_{k=1}^{n}\lambda^{n-k}[z(k)-\hat{\theta}_{\mathrm{LS}}(n)\phi(k)]^2. \tag{5}$$

It is well known[5] that Eq. (5) can be solved recursively in an updated manner with $\hat{\theta}_{\mathrm{LS}}(n)$ computable from $\hat{\theta}_{\mathrm{LS}}(n-1)$ alone using exponentially weighted recursive least-squares (EWRLS) method. When $e(n)$ is uncorrelated, it can be shown[5] that $\hat{\theta}_{\mathrm{LS}}(n)\rightarrow\theta$, the true parameter, with the multiple sine excitation. However, $e(n)$ is correlated as $e(n)$ given in Eq. (3) is dependent on $\vartheta(n)$, $\vartheta(n-1)$, and $\vartheta(n-2)$. This leads to the estimate $\hat{\theta}_{LS}(n)$ converging to θ within a bias. Recently,[6] a bias compensated recursive least-squares was reported that provides an unbiased estimate when the noise is correlated. Bias compensated EWRLS (BCEWRLS) method is developed instead since a handle on convergence rate of the parameter estimates is required. At time instant $t=nT_s$, assuming $z(n)$, $\phi(n)$, $\hat{\theta}_{\mathrm{LS}}(n-1)$, $P(n-1)$, $J(n-1)$, and $\hat{\theta}_C(n-1)$ are available, the corresponding updated values are found as

$$\hat{\theta}_{\mathrm{LS}}(n)=\hat{\theta}_{\mathrm{LS}}(n-1)+P(n)\phi(n)l(n),$$

$$l(n)=[z(n)-\phi'(n)\hat{\theta}_{\mathrm{LS}}(n-1)],$$

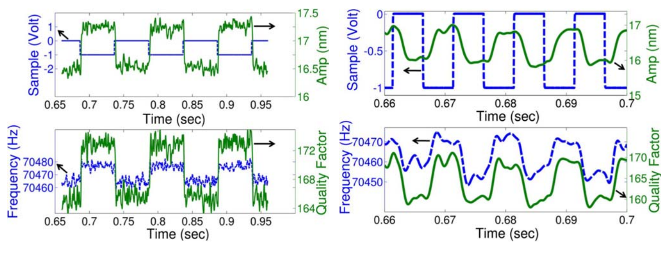
$$P(n)=\frac{1}{\lambda}\left[P(n-1)-\frac{P(n-1)\phi(n)\phi'(n)P(n-1)}{\lambda+\phi'(n)P(n-1)\phi(n)}\right]$$

$$J(n)=\lambda\left[J(n-1)+\frac{[z(n)-\phi'(n)\hat{\theta}_{\mathrm{LS}}(n-1)]^2}{\lambda+\phi'(n)P(n-1)\phi(n)}\right],$$

$$\hat{\theta}_C(n)=\hat{\theta}_{\mathrm{LS}}(n)+\frac{\hat{\sigma}^2(n)}{1-\lambda}(1-\lambda^n)P(n)\hat{\theta}_C(n-1),$$

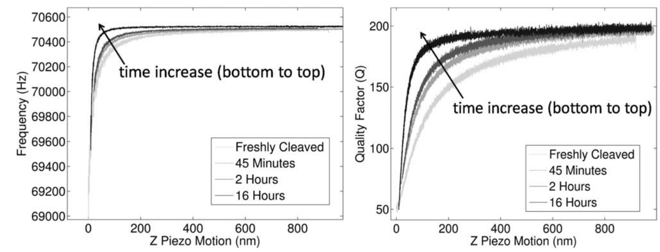
$$\hat{\sigma}^2(n)=\frac{(1-\lambda)}{(1-\lambda^n)}\frac{J(n)}{1+\hat{\theta}_C'(n)\theta_{\mathrm{LS}}(n)}, \tag{6}$$

where $\lambda=0.995$ is the exponential forgetting factor, $\hat{\theta}_{\mathrm{LS}}(n)$ is the parameter estimate of θ at time instant $t=nT_s$ using



(a) (b)

FIG. 3. (Color online) Experimentally obtained Sample Profile (top-blue-dash curve), Amplitude (top-green-solid curve), f_0' estimate (bottom-blue-dash curve), Q' estimate (bottom-green-solid curve) while imaging ≤ 1 nm square profile at (a) 10 Hz and (b) 100 Hz. ≤ 1 nm steps are clearly visible in f_0' and Q' estimates.



(a) (b)

FIG. 4. Experimentally obtained (a) f_0' estimate and (b) Q' estimate during force spectroscopy experiment done on a freshly cleaved mica surface and then subsequently at 45 min, 2 h, and 16 h. Localization of surface forces within 20 nm of the sample surface occurs after 16 h of cleaving a mica surface.

EWRLS, and $\hat{\theta}_C(n)$ is the bias compensated $\hat{\theta}_{\mathrm{LS}}(n)$. Note that in Eq. (6), the estimate $\hat{\theta}_{\mathrm{LS}}(n)$ at time $t=nT_s$ can be obtained from past estimate $\hat{\theta}_{\mathrm{LS}}(n-1)$ and an update term that depends on certain gain $P(n)\phi(n)$ and the instantaneous error term $[z(n)-\phi'(n)\hat{\theta}_{\mathrm{LS}}(n-1)]$. $P(n)$ represents the variance of the error in the parameter estimates $[\theta-\hat{\theta}_{\mathrm{LS}}(n)]$ and $J(n)$ represents the least square error in Eq. (5) that is being minimized at any given instance. $\hat{\sigma}^2(n)$ is an estimate of the variance of noise $e(n)$ at any instance. The algorithm is initialized with $\hat{\theta}_{\mathrm{LS}}(0)=\left[\begin{smallmatrix}0\\0\end{smallmatrix}\right]$, $P(0)=\left[\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right]\times 10^6$, $J(0)=0$, and $\hat{\theta}_C(0)=\left[\begin{smallmatrix}0\\0\end{smallmatrix}\right]$. The advantage of Eq. (6) is that it requires a small amount of memory since only current estimated values need to be stored and can be implemented on hardware for real time operation with ease. f_0' and Q' can be calculated from estimated b_1 and b_0 values in closed form.

To study the efficiency of the method, experiments were performed on Multimode AFM (Veeco Inc.) with AC240 cantilever (Asylum Research Inc., $f_0=71500$ Hz, $Q=206$, and $k=2$ N/m). Sample-free model was identified using frequency sweep method wherein excitation frequency ω of $g(t)=A_0 \sin \omega t$ was varied from 0–100 kHz and $p(t)$ was recorded. Magnitude and phase information about $G(i\omega)$ was obtained by evaluating ratios between steady state amplitude and phase of output versus input excitation, respectively. f_0 and Q were extracted by a second order fit around resonance. The same sample-free model parameters were extracted in real time with BCEWRLS scheme using Eq. (6). Dither and deflection signals were sampled simultaneously at 500 kHz. Eq. (6) was then computed offline to get estimates of f_0' and Q'. Comparison [see Fig. 1(b)] indicates that in most cases estimates of f_0 are accurate within +5 Hz and quality factor estimates are accurate within +15 of actual values identified using the frequency sweep method. Rate of convergence of parameters is lesser than 400 μs. This means the sample can have a spatial frequency up to 2.5 kHz. These convergence rates are faster than conventional imaging signals like amplitude and phase of the cantilever deflection. This property, together with the recursive least-squares algorithm Eq. (6), makes it possible to estimate equivalent cantilever model in real-time in the sense that they can be computed in a time scale smaller than the time scales of amplitude and phase of the cantilever oscillations. The rate of convergence can be tuned by the exponential forgetting factor λ at the expense of increased variance in the error in estimating parameters. It is seen that the rate of convergence will be faster with smaller height changes in sample profile. Equivalent cantilever parameters were identified during force curves done at 1 Hz to observe how $G_z(i\omega)$ modifies with sample height. Equivalent resonant frequency f_0' and quality factor Q' are experimentally estimated together with amplitude and phase (see Fig. 2). Modified plant parameters were estimated when the deflection amplitude varied from sample-free amplitude (≈ 25 nm) until 8 nm. A reduction in equivalent resonant frequency and quality factor was observed as expected with an increase in tip sample interaction. A sample with periodic features, which are less than 1 nm in height (see Fig. 3), was imaged in tapping mode at 10 Hz and 100 Hz frequency. Controller gains were kept sufficiently small so that the controller just cancelled the sample slope and the z-piezo drifts. It is evident that the algorithm presented in the paper can generate f_0' and Q' estimates in real time providing simultaneous images of amplitude, phase, f_0', and Q'. Experimental results [see Figs. 3(a) and 3(b)] indicate that the method has an estimation resolution of better than 1 nm and can be used during normal tapping mode operation without any dependence on the image pixel size. Force spectroscopy experiments were done on a freshly cleaved mica sheet, and then subsequently after 45 min, 2 h, and 16 h. It was observed that due to the presence of negative charges on a freshly cleaved mica sheet, the resonant frequency and quality factor started decreasing at a distance of ≈ 1 μm from the sample indicating the presence of long distance forces in addition to the van de Waals forces. It took roughly 16 h for this charge to neutralize. Changes in resonant frequency and quality factor after 16 h were localized to within 20 nm from the sample surface indicating the presence of only short range forces (see Fig. 4).

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