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An Observer Based Sample Detection Scheme for Atomic Force Microscopy

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Abstract—**In dynamic mode operation of Atomic Force Microscopes steady state signals like amplitude and phase are typically used for the detection and imaging of sample. Due to the high quality factor of the micro-cantilever probe the corresponding methods are inherently slow. In this paper we present a novel methodology for fast interrogation of sample that exploits the transient signals. A novel method is introduced for the detection of small time scale tip-sample interactions. Simulations and experiments show that the method results in significant increase in bandwidth and resolution as compared to the steady state data based methods.**

I. INTRODUCTION

There is significant demand on micro-cantilever based devices like the Atomic Force Microscope (AFM) for ultra-fast interrogation of the sample. The primary component of the AFM is a micro-cantilever with a sharp tip (see Figure 1(a)). In the static or contact mode operation, the deflection of the cantilever due to tip-sample interaction forces is monitored to infer sample characteristics. In the dynamic mode operation of the AFM, the micro-cantilever is oscillated using a dither piezo attached to the base of the cantilever. In typical operating conditions the tip settles down to a near sinusoidal periodic orbit. The periodic orbit gets modified due to changes in the cantilever tip-sample interaction forces.

Most of the current techniques rely on the steady state data of the cantilever tip position. This can result in very slow interrogation speeds due to the typical high quality factor of the micro-cantilever that lead to high settling times. Note that transient state data is not used for sample interrogation. However the signature of the sample characteristics is present in the transient of the micro-cantilever oscillations. Moreover these signatures can be considerably more pronounced in the transient than in the steady-state behavior. We show that sensing based on transient signal has the potential to detect events at extremely high rates. Such a technology has tremendous implications in numerous applications, for example, in micro-cantilever based retrieval of high density data and detection of the presence of chemical and/or biological molecules on a surface. Researchers at IBM (See Ref. [1]) have demonstrated areal densities of up to 500 Gb/in^2 in micro-cantilever based data storage devices; however, the reading is performed in contact mode which results in signal deterioration due to wear and, also needs to be corrected for thermal drift during extended periods of operation. Furthermore, the wear becomes more severe as the data rates are increased. In another application biologically modified cantilevers have been demonstrated to detect specific biological molecules (See Ref. [2]). Transient signal detection being a dynamic method is not afflicted by thermal drift and is highly non-invasive. Moreover, as will be shown later the data rates depend on the cantilever frequency.

A systems viewpoint of the AFM dynamics and observer based approach provide the basic analytical tools to analyze the transient signal. As is described later the proposed scheme also provides significant advantages with respect to *resolution*; particularly of events at the nanoscale that have very small time scales. The resolution depends on the quality factor of the micro-cantilever. However since the methodology does not depend on the steady state data, the sensing bandwidth depends on the resonant frequency of the micro-cantilever and is mostly independent of the quality factor of it.

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II. CANTILEVER MODEL

For many applications the micro-cantilever is well modeled as a flexible structure. A multi-mode model accurately captures the cantilever dynamics (see Ref. [3]). Typically a first or second mode approximation is enough to describe the dynamics. A first mode approximation of the cantilever dynamics is given by,

$$\begin{aligned} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} &= \begin{bmatrix} 0 & 1 \\ -\omega_0^2 & -2\xi\omega_0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} (\eta + w) \\ y &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + v \end{aligned}$$

where state x_1 denotes the cantilever-tip position and state x_2 denotes the cantilever-tip velocity. ω_0 and ξ denote the first resonant frequency of the micro-cantilever and the damping factor in the medium respectively. Note that $\xi = \frac{1}{2Q}$ with Q being the quality factor of the micro-cantilever. η is the thermal noise component, w describes all the external forces acting on the cantilever, y is the photodiode output that measures the deflection of the free end of the micro-cantilever and v is the measurement (photodiode) noise. We will denote the equivalent dither forcing by g and the tip-sample interaction force by $\phi(y)$ that depends on the tip position y. ϕ typically has characteristics of long range attractive force and short range strong repulsive force. In the above framework, we have $w = g + \phi(y)$. The cantilever model described above can be identified precisely using the thermal-noise response. We will assume a discretized model of the cantilever as

$$\begin{aligned} x_{k+1} &= Fx_k + G(\eta_k + w_k) \\ y_k &= Hx_k + v_k \end{aligned} \tag{1}$$

III. Harnessing the Transient Data

Essentially in the above viewpoint the cantilever dynamics is separated as an independent system from the sample subsystem that affects the cantilever in a feedback manner. This systems view-point of the AFM (see Figure 1 (b)) provide the platform to design an observer (see Figure 2) that provides an estimate of the complete state x in the presence and absence of the sample.

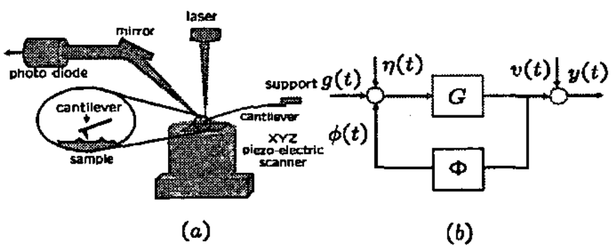

Fig. 1. (a) Schematic of an AFM. The main components are the micro-cantilever, an optical detection system and a sample positioning system. (b) In the systems perspective, the AFM dynamics is viewed as an interconnection of a linear cantilever system with the nonlinear tip-sample interaction forces in feedback.

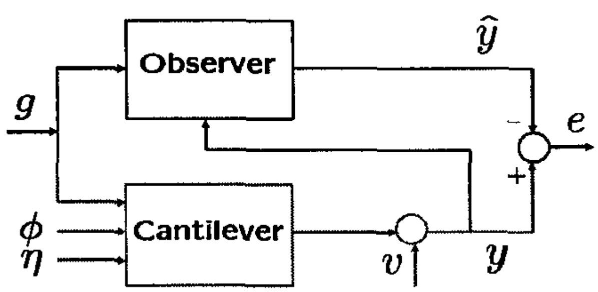

Fig. 2. The observer estimates the states to be $\hat{x}$. The actual state is x. By a choice of the observer gain L the error in the state estimate and the corresponding $e = y - \hat{y}$ go to zero when the micro-cantilever is freely oscillating. When the micro-cantilever is subjected to the sample force the micro-cantilever dynamics is altered whereas the observer dynamics remains the same. This is registered as a nonzero value in the error e.

The observer based state estimation facilitates fast detection using transient state data based methodology. The observer dynamics and the associated error dynamics is given by,

$$\overbrace{\begin{aligned} \hat{x}_{k+1} &=: F\hat{x}_k + Gg_k + L(y_k - \hat{y}_k); \hat{x}(0) = \hat{x}_0, \\ \hat{y}_k &= H\hat{x}_k \end{aligned}}^{Observer}$$

$\hat{x}_{k|j}$ is the estimate of variable x at time instant k based on input and output observation until time instant j and $\hat{x}_k$ denotes the case $j = k - 1$.

$$\overbrace{\begin{aligned} \tilde{x}_{k+1} &=: x_{k+1} - \hat{x}_{k+1} \\ &= Fx_k + G(g_k + \eta_k) - F\hat{x}_k - Gg_k - L\tilde{y}_k \\ &= (F - LH)\tilde{x}_k + G\eta_k - Lv_k, \\ \tilde{x}_0 &= x_0 - \hat{x}_0. \end{aligned}}^{State\ Error\ Dynamics}$$

The error process e is given by,

$$e_k = y_k - \hat{y}_k \tag{2}$$

and will be used for the detection of changes in tip-sample interaction.

The initial position of the micro-cantilever dynamics is hard to determine and thus it has to be assumed as unknown. Also, only the micro-cantilever position is available as a measured quantity, not the velocity. Thus the error between the observed state and the actual state of the micro-cantilever, when no noise terms are present ($\eta = v = 0$) is only due to the mismatch in the initial conditions of the observer and the micro-cantilever. It is evident that if the observer gain L is chosen so that the eigenvalues of the matrix $F - LH$ are in the open unit circle then the error $\tilde{x}$ due to the initial condition mismatch $\tilde{x}_0$ goes to zero with time. The system with one model is observable and therefore the eigenvalues of $F - LH$ can be placed anywhere. It can be shown that under the presence of the noise sources η and v the error process, e approaches a zero mean wide sense stationary stochastic process after the observer has tracked the state of the cantilever.

Now we provide the intuition behind the new methodology. When the observer has tracked the cantilever state and the cantilever is subjected to a force due to the sample, the cantilever dynamics get altered. There is a mismatch between the actual state of the cantilever and the estimated state of the observer. The observer sees the effects of the sample only through the cantilever position y which is the output of the photo-diode (see Figure 2). This introduces a lag (that is dependent on the gain L) between the time when the cantilever sees the sample's influence and when the observer realizes the sample's influence. This is registered as a change in the signal e which loses its stationarity. The magnitude of this error signal can be quite large even though the *magnitude of oscillation might not have changed significantly.*

Also, when the change in the tip-sample potential persists then the observer by utilizing the input y may track the altered behavior. Thus the error signal shows the signature at the initial part of the change but this deviation from stationarity might not persist even though the change in the tip-sample behavior persists. This is in contrast to the steady state methods where the information is available not in the initial part but after the cantilever has come to a steady state (for example in tapping-mode scheme this would mean an eventual lowered amplitude value when a step is encountered that persists).

There is considerable freedom on how fast the observer tracks the cantilever dynamics that is independent of the quality factor Q. Note that high quality factors are detrimental to high bandwidth in steady state methods; however required for high resolution. *By utilizing the observer based architecture presented in this article a method for effectively isolating the high bandwidth needs from the high resolution needs is obtained.*

IV. Impact Model Based Detection Based on the Transient Data

We assume that the sample's influence on the cantilever tip is well modeled as an impact condition. Intuitively this follows because the time spent by the cantilever tip under the sample's influence is negligible compared to the time it spends outside the sample's influence [4]. This hypothesis is particularly true for samples that have a small attractive regime. Under such an assumption the cantilever dynamics is described by the following discrete time state space model.

$$\begin{aligned} x_{k+1} &= Fx_k + G(g_k + \eta_k) + \delta_{\theta,k+1}\nu, \\ y_k &= Hx_k + v_k, \; k \geq 0 \end{aligned} \tag{3}$$

where $\delta_{i,j}$ denotes the dirac delta function, θ denotes the time instant when the impact occurs and ν signifies the magnitude of the impact. Essentially the impact is modeled as an instantaneous change in the state by ν at time instant θ. In this setting the time of impact and the resulting change in the state are unknown quantities. The profile of the change in the mean of the error signal due to the sample can be precalculated and one can then employ detection and estimation methods to search for the presence of such a profile in the error sequence to not only detect the samples presence but also estimate the sample parameters.

We assume that the input noise and the output noise are white and uncorrelated. Note that the input and output noise power Q and R can be measured experimentally. Given the following noise characteristic

$$E\left\{\begin{bmatrix}\eta_i \\ v_i \\ x_0\end{bmatrix}\begin{bmatrix}\eta_j \\ v_j \\ x_0 \\ 1\end{bmatrix}^T\right\} = \begin{bmatrix} Q_i\delta_{ij} & 0 & 0 & 0 \\ 0 & R_i\delta_{ij} & 0 & 0 \\ 0 & 0 & \Pi_0 & 0 \end{bmatrix}.$$

the optimal transient observer is a Kalman Filter (see [5]). Let the steady state Kalman observer gain be given by $L = L_K$. The error process is known as the innovation sequence when the optimal transient observer is employed. Moreover when the tip-sample interaction is absent, the innovation process asymptotically approaches a zero mean white process.

With a Kalman Observer and an impact model when the sample is encountered (given by the model in (6)), the innovation sequence e_k (see [6]) can be written as,

$$\begin{aligned} e_k &= y_k - \hat{y}_k \, , \\ &= \Upsilon_{k;\theta}\; \nu + \gamma_k \, , \end{aligned} \tag{4}$$

where $\Upsilon_{k;\theta}$ is a known dynamic state profile with unknown arrival time θ defined by

$$\Upsilon_{k;\theta} = \begin{bmatrix} H \\ H(F - L_K H) \\ H(F - L_K H)^2 \\ \cdot \\ \cdot \\ \cdot \\ H(F - L_K H)^{k-\theta} \end{bmatrix} \tag{5}$$

and $\{\gamma_k\}$ is a zero mean white noise sequence and is exactly the measurement residual had the jump not occurred.

Thus determining when the cantilever is "hitting" the sample and when not is equivalent to deciding whether the dynamic profile is present in a zero mean white process or not. This problem can be formulated in the framework of binary hypothesis testing given by,

$$\begin{aligned} H_0 &\;:\; e_k = \gamma_k, \; k = 1, 2, \ldots, n \\ versus & \\ H_1 &\;:\; e_k = \Upsilon_{k;\theta}\; \nu + \gamma_k, \; i = 1, 2, \ldots, n \end{aligned} \tag{6}$$

where γ_k is a zero mean white gaussian process, $e_k = \gamma_k$ is the observed innovation and $\Upsilon_{k;\theta}\;\nu$ is a known *dynamic profile* with unknown arrival time θ and unknown magnitude ν.

A number of detection and estimation methods exist in Statistical Signal Processing literature. A suboptimal version of the generalized likelihood ratio test ([6]) is used to detect the dynamic profile in the innovations. Let $\hat{\theta}(n)$ and $\hat{\nu}(n)$ denote the most probable time of arrival (tip-sample interaction) and magnitude (the size of tip-sample interaction) based on the available observed data. Thus the estimation problem is to compute the maximum likelihood estimates (MLE's) $\hat{\theta}(n)$ and $\hat{\nu}(n)$ based on the observed data $e_1, \ldots, e_n$. The likelihood ratio is computed as,

$$l(n;\theta) = d^T(n;\theta)C^{-1}(n;\theta)d(n;\theta) \tag{7}$$

where $C(n;\theta) = \sum_{k=\theta}^{n} \Upsilon_{k;\theta}^T \Sigma^{-1} \Upsilon_{k;\theta}$ and $d(n;\theta) = \sum_{k=\theta}^{n} \Upsilon_{k;\theta}^T \Sigma^{-1} Y_k$. Σ is the error covariance of γ. The likelihood ratio is compared with a threshold value as $l(n;\hat{\theta}_n) \gtrless_{H_0}^{H_1} \epsilon$ to arrive at a decision whether the dynamic profile is present or not (equivalent to deciding whether a tip-sample interaction has occurred or not. The threshold ϵ is chosen to provide a suitable tradeoff between false alarm rate and missed alarm rate [7]. The false alarm and detection probabilities are given by $P_F = P_0(\Gamma_1) = \int_\epsilon^\infty p(l = L|H_0)dL$, and $P_D(\nu,\theta) = P_1(\Gamma_1) = \int_\epsilon^\infty p(l = L|H_1,\nu,\theta)dL$ respectively. $p(l = L|H_0)$ is Chi-squared (χ^2) density with n degrees of freedom and $p(l = L|H_1)$ is a non-central χ^2 density (see [8]) with non-centrality parameter $\nu^T C(n;\theta)\nu$. Thus P_D is dependent upon values of θ and ν. In practice the search is carried out on a data window of finite length M and assuming $\hat{\theta} = 1$. It is a suboptimal solution of GLRT and performs satisfactorily for the detection case. Note that the expressions for false alarm probability P_F and the detection probability remain unchanged with degree of freedom M. For specified P_F or P_D, the threshold value ϵ can be computed from the tables in [8] and vice versa. To compute P_D, ν is taken as the minimum jump that is required to be detected and θ as the size of the data window M. The window size is decided from the effective duration of the dynamic profile.

V. SIMULATION RESULTS

To test the efficacy of the proposed technique of utilizing the innovation signal characterization, extensive simulations were performed with cantilever parameters obtained from experimental data. The parameters of the simulation are: first resonant frequency of $f_0 = 74KHz$, the quality factor $Q = 130$, the value of the forcing γ was chosen such that the free oscillating amplitude was 80 nm with the sinusoidal forcing $g(t) = \gamma \cos \omega_0 t$ ($\omega_0 = f_0/(2\pi)$). We will use the term *cycle* to mean $1/f_0$ seconds. The simulations assumed that thermal-noise and the photo-diode sensor noise can be characterized as band-limited white-noise with zero mean and known variance. The input and the output noise power used were in conformity with the experimental values. The simulation was performed using an attractive and repulsive spring-damper model (see Figure 3) for the tip-sample interaction that has been shown to reproduce close fidelity to experimental data (see [9]).

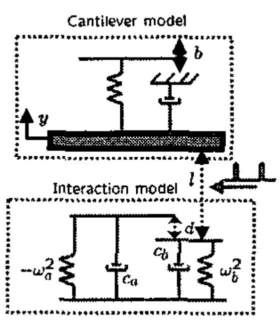

Fig. 3. The cantilever is modeled by the single mode approximation. The tip-sample interaction is modeled by a repulsive spring and an attractive spring with stiffness $\omega_b = 3.03rad/\mu s$ and $\omega_a = 0.351rad/\mu s$ and damping coefficients $c_b = 0.5rad/\mu s$ and $c_a = 0.0042rad/\mu s$ respectively that are offset by a distance $d = 1.695$ nm [9]. This mimics the repulsive and attractive feature of the tip-sample interactions.

Consider Figure 4 that shows the simulation results when the cantilever is subjected to two short pulses of 25 μs duration separated by 100 μs. It is evident from the innovation sequence that the pulse at 4000 μs is registered as

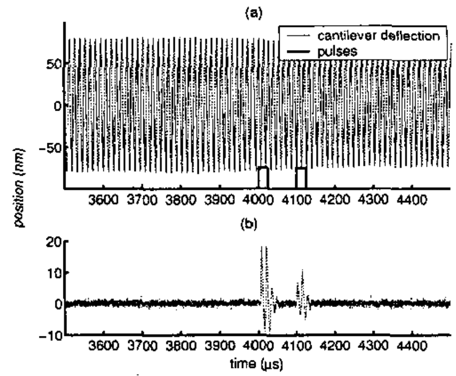

Fig. 4. Shows simulation results when the cantilever is subjected to pulses of 25 μ s duration. (a) The cantilever deflection and the pulses encountered are shown. The hits being very weak, the cantilever oscillation doesn't change significantly. (b) But the innovations capture the two pulses distinctly. When the cantilever is not encountering the pulses the innovation process is zero mean and white whereas dynamic profiles appear in the innovations due to the pulses.

a large deviation from the zero-mean white nature. As soon as the cantilever moves away from the pulse the innovation sequence recovers the zero-mean white nature within 25 $\mu s \approx 2/\ f_0 seconds$. This implies a bandwidth of approximately $f_0/4$ Hz. Note that the second pulse introduced at 4100 μs is registered again by the innovation sequence *even though* the transient of the cantilever dynamics due to the first hit has not died out. Similarly, the other pulse are also registered. Note that it is not clear how such hits can be inferred from even the amplitude demodulated signal as during the transient, signature of the pulses is impossible to infer.

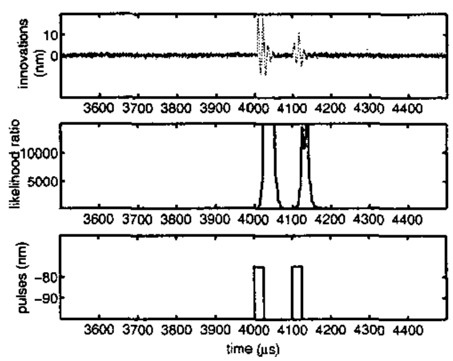

Fig. 5. The suboptimal version of the generalized likelihood ratio test was employed to detect the dynamic profiles present in the innovations.

The dynamic profile which appears in the innovations is detected using the suboptimal generalized likelihood ratio test using a window size of 128 points. The results are shown in Figure 5. From likelihood ratio test the step is detected in 23.94 μs ($1/f_0 = 13.5/\mu s$) with a false alarm rate of 0.1 % (threshold $\epsilon = 1681.3$ and data window size $M = 128$). The test with a data window size $M = 100$ and threshold $\epsilon = 1460$ can detect a minimum step size of 0.25 nm with 90% detection probability. Note that the speed of detection of the pulses scales with the resonant frequency of the micro-cantilever; simulations indicate a bandwidth of $f_0/4$ when trying to decipher pulse like features. Thus the bandwidth can be further improved if cantilevers with higher resonant frequencies are employed (cantilevers with gigahertz frequencies have been fabricated). *This shows that MHz bandwidth readouts are attainable with transient signal method.* Note that high quality factor of the microcantilever required for better resolution does not limit the bandwidth in the proposed technique.

VI. Experimental Results

Experiments were performed to further verify the efficacy of the new transient signal based approach. The slowness of the piezo (the Z component of the X-Y-Z scanner for sample positioning (see Figure 1(a))) dynamics makes it difficult to generate a waveform as shown in Figure 4. An alternative approach is to make use of the piezo dynamics to generate a similar waveform. The frequency response of the piezo was obtained using an HP control system analyzer and a model was fit to the response. The model response is compared with that obtained experimentally in Figure 6.

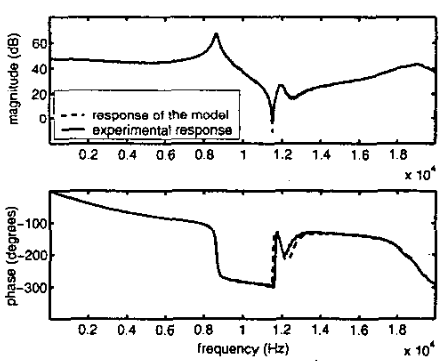

Fig. 6. The experimental frequency response of the Z-piezo is compared with that of the model.

Simulations were performed using the model to obtain the input signals to the piezo which generate pulses similar to the those in Figure 4.

Figure 7 shows the response of the piezo to a voltage pulse of amplitude 0.5V, period 1000 μs and on time 500 μs. The piezo dynamics results in the occurance of 4 peaks separated by approximately 100 μs during the on time. The maximum width of each peak is approximately 35 μs. This signal resembles the sample profile used in the simulations (see Figure 4).

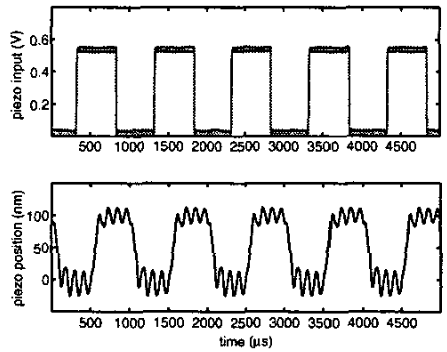

Fig. 7. An input voltage pulse of amplitude 0.5V, period 1000 μs and on time 500 μs results in the above piezo response. The four peaks during the on time are separated by approximately 100 μs.

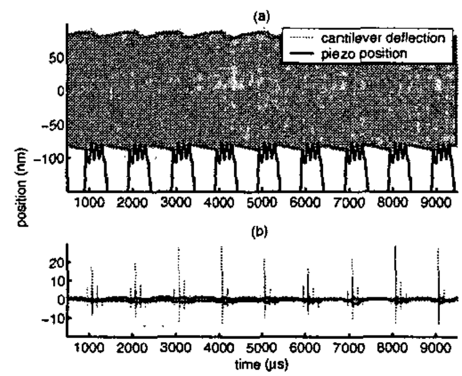

Fig. 8. (a) The cantilever deflection signal is plotted against the pulse shape generated using the piezo dynamics. It is difficult to detect when the cantilever tip interacts with the peaks looking at the deflection signal. (b) The innovation process on the other hand bears the signature of the hits. Every time the tip interacts with the sample the innovations loose the zero mean white nature

The cantilever is oscillated at the first resonant frequency of 70.1 kHz. The amplitude of oscillation was approximately 80 nm and the oscillating tip was approximately 100 nm away from the sample surface. The piezo is actuated with the voltage pulse mentioned above. The oscillating cantilever interacts with the resulting peaks. The objective is to detect these peaks using the transient signal scheme. A two mode model was obtained for the cantilever with the first resonance at 70.1 kHz and the second resonance at 445 kHz. This model is used to build the Kalman filter and obtain the innovation sequence. The resulting innovation sequence is shown in Figures 8 and 9.

The innovations become non-white when there is a hit and a dynamic profile appears. This dynamic profile is detected using the scheme descibed in section IV. The resulting likelihood ratio is shown in Figure 10. Using the likelihood ratio it is possible to accurately detect the hits as predicted

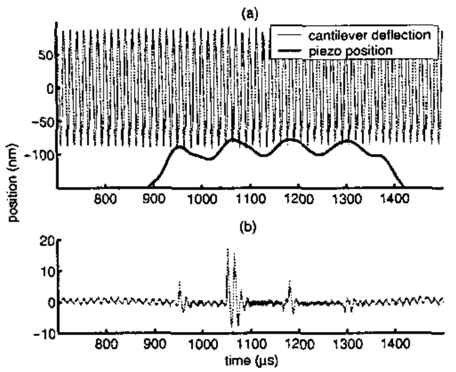

Fig. 9. The innovations show signatures of all four hits due to the four peaks. The dynamic profile is clearly seen when the hits occur.

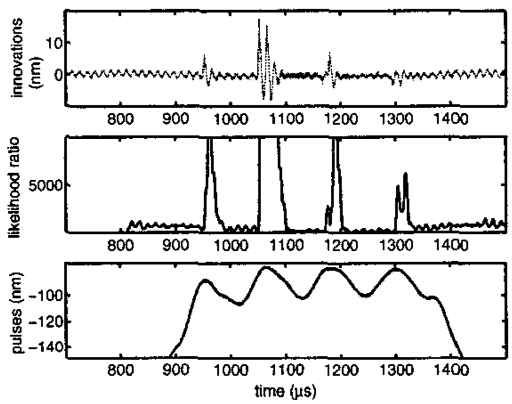

Fig. 10. This figure shows the innovations and likelihood ratios along with the piezo movement. Clearly the likelihood ratios provide a highly accurate way of detecting the hits.

by the simulations proving the efficacy of the transient signal based detection scheme.

VII. Conclusion

Note that all present schemes employ steady-state data. It is fair to say that this article presents for the first time transient signal methods. The simulation and experimental results presented indicate the huge potential of such principles. In this article a framework for ultra-fast interrogation of sample in Atomic Force Microscopy is proposed which utilizes the tip-deflection data during the transient state of the micro-cantilever probe. The systems perspective has facilitated the development of this methodology. The micro-cantilever and its interaction with the sample is modeled. A first mode approximation model of the cantilever is considered and a Kalman filter is designed to estimate the dynamic states. The tip-sample interaction is modeled as an impulsive force applied to the cantilever in order to detect the presence of sample. The dynamics due to tip-sample interaction is calculated in the innovation sequence and a likelihood ratio test is performed to obtain the decision rule to infer the presence of sample. Experimental results tally with the simulation results verifying the proposed methodology and the sample-detection scheme. Simulations show a bandwidth of $\frac{f_0}{4}$ (f_0 being the natural frequency of the micro-cantilever) in detecting small time scale tip-sample interactions. In this method high quality factor does facilitate high resolution but it does not limit the bandwidth as in steady state data based methods.

VIII. Acknowledgments

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