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Real-time stochastic response analysis as a tool for monitoring cantilever mechanical properties☆

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ABSTRACT

Microcantilever-based sensors are very promising devices for biochemical applications. They are usually operated in two modes. In the first one, a microcantilever static bending induced by the surface stress is observed. In the second mode, resonant frequency shift caused by mass loading is measured. The second mode requires an external force to excite cantilever vibrations. There is a possibility to use a stochastic excitation signal to estimate frequency shift as well as other interesting mechanical properties, such as effective spring constant or damping. Cantilever thermal self-vibrations or artificially generated white noise are very convenient examples of such a stochastic excitation signal.

In the paper a real-time stochastic response analysis (RTSA) technique is presented. It is based on autoregressive moving average (ARMA) process modeling. Estimated model parameters are used for calculation of the eigenfrequency, quality factor and effective spring constant of a given vibration mode. The description of the entire procedure is presented, along with the results of simulations. The results confirm validity of the proposed ARMA model and show expected estimation errors for an illustrative set of cantilevers.

The proposed algorithm is also applied to monitor the quality factor and resonant frequency of an electromagnetically-actuated microcantilever. The stochastic signal used to excite the cantilever is generated by a very simple white noise generator. The RTSA enables simultaneous monitoring of the cantilever resonant frequency and quality factor.

The proposed solution is an interesting option in applications, in which simplicity and cost of the measurement system are key issues.

1. Introduction

Microcantilevers are known to be very promising biochemical sensors [1,2,3]. They can be operated in two modes. In the first one, the static bending caused by the surface stress induced by adsorbed molecules is observed. In the second one, vibrations of a cantilever are analyzed and dynamic mechanical properties of the microcantilever are estimated. In the latter one, the mass of adsorbed molecules can be estimated on the basis of resonant frequency shift. It is also possible to measure properties of the surrounding fluid, such as density [4] or viscosity [5], on the basis of both the resonant frequency shift and the quality factor measurements. The resonant frequency is usually measured by a phase locked loop (PLL) circuit or a self-excited resonator [6]. These methods ensure great frequency resolution but monitor only resonant frequency. The quality factor is estimated on the basis of the cantilever frequency response, which may be measured by network analyzers [7,5] or by analysis of the power spectrum of cantilever thermal vibrations [8,9]. There are also solutions based on step response analysis [10]. They ensure high precision measurements of the quality factor. Usually, static and dynamic modes are used independently but there are some reports about mixing these two approaches [8,9,11].

The stochastic excitation is usually an undesirable phenomenon, the influence of which must be minimized [12]. In some cases, however, this random signal carries useful information. We present an approach based on real-time stochastic response analysis (RTSA) incorporating autoregressive moving average (ARMA) modeling. Recently, similar system identification techniques were applied to fault diagnosis of microelectromechanical systems (MEMS) [13]. In the presented approach, we analyzed the thermo-mechanical noise of the cantilever and the response of the cantilever excited by band-limited white noise. The advantages of this solution are the simplicity of the circuitry and the use of numerical procedure

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that is better suited for implementation in modern digital signal processing devices (e.g. field programmable gate arrays (FPGA) and digital signal processors (DSP)) due to less memory requirements and straightforward elementary calculations. It is also important that the proposed algorithm does not estimate quality factor on the basis of the amplitude of the resonant response of a microcantilever. Therefore, the results are not affected by changes of the microcantilever's effective spring constant. In the presented work we focus on the stochastic response of the simple harmonic oscillator (SHO) system, which is frequently used as a model of dynamic response of MEMS devices. In the work of Sader [19], it was shown that this model is valid as long as the quality factor $Q>>1$. Below this limit the SHO model is invalid due to dissipative effects in fluid that surrounds the device. In the paper, the simulations and experiments were carried out under conditions where the SHO is valid.

2. Methodology

A single mode of cantilever vibrations is modeled by a damped harmonic oscillator model. It is expressed by the following differential equation

$$\frac{k}{(2\pi f_0)^2}\ddot{x}(t) + \frac{k}{2\pi f_0 Q}\dot{x}(t) + kx(t) = \gamma(t) \tag{1}$$

where k is the effective spring constant, f_0 is the eigenfrequency, Q is the quality factor, x is the cantilever deflection and γ is the excitation force. Single and double dots indicate the first and the second derivative. According to the Nyquist fluctuation-dissipation theorem, when a cantilever vibrates thermally, the power spectrum of the thermal fluctuation force is constant and equal to

$$\Gamma_{th}(f) = \frac{2k_B T k}{\pi Q f_0} \tag{2}$$

where k_B is the Boltzmann constant and T is the temperature in thermal equilibrium state. The modulus of the cantilever frequency response is defined by the following equation

$$H(f) = abs[X(f)/\Gamma(f)] = \frac{{f_0}^2}{k\sqrt{\left({f_0}^2 - f^2\right)^2 + \frac{{f_0}^2 f^2}{Q^2}}} \tag{3}$$

where abs indicates the modulus of a complex number, while $X(f)$ and $\Gamma(f)$ are Fourier transforms of the cantilever's deflection and the excitation force, respectively. The power spectrum of cantilever vibrations is computed as the product of the power spectrum of the thermal fluctuation force and the squared modulus of the cantilever's frequency response

$$X_{th}(f) = \Gamma_{th}(f)H^2(f) = \frac{2k_B T {f_0}^3}{\pi Q k}\frac{1}{\left({f_0}^2 - f^2\right)^2 + {f_0}^2 f^2 Q^{-2}} \tag{4}$$

After calculating the inverse Fourier transform of the power spectrum of cantilever vibrations, the autocorrelation function (5) of the thermal noise is obtained.

$$\begin{aligned} R_{th}(\tau) &= E[x_{th}(t)x_{th}(t-\tau)] \\ &= \frac{k_B T}{k}\frac{2Q}{\sqrt{4Q^2-1}}\exp\left(-\frac{\pi f_0}{Q}\tau\right)\cos\left[\pi f_0\frac{\sqrt{4Q^2-1}}{Q}\tau - \varphi\right] \\ \varphi &= \arctan\left[\frac{1}{\sqrt{4Q^2-1}}\right] \end{aligned} \tag{5}$$

where E means the expected value. For large values of quality factor Q, the angle φ is almost zero. The assumption $Q>>1$ is the limit for applicability of the simple harmonic oscillator (SHO) model. Below this limit dissipative effect of fluids makes the SHO model invalid [19].

The Laplace transform of Eq. (1) is the cantilever transmittance

$$H(s) = X(s)\Gamma(s)^{-1} = \frac{1}{k}\frac{(2\pi f_0)^2 Q}{Qs^2 + 2\pi f_0 s + (2\pi f_0)^2 Q} \tag{6}$$

If this transmittance is treated as transmittance of an analog filter, it is possible to design a digital filter by the impulse invariance method (IIM) [18]. The impulse response of such a filter is the same as the impulse response of its analog prototype. The transmittance of the digital filter designed by the IIM on the basis of $H(s)$ is expressed by the following equation

$$\begin{aligned} H(z) &= \frac{bz^{-1}}{1 + a_1 z^{-1} + a_2 z^{-2}} \\ b &= \frac{2\pi f_0}{f_s k}\frac{2Q}{\sqrt{4Q^2-1}}\exp\left[-\frac{\pi f_0}{f_s Q}\right]\sin\left[2\pi\frac{f_0}{f_s}\frac{\sqrt{4Q^2-1}}{2Q}\right] \\ a_1 &= -2\exp\left[-\frac{\pi f_0}{f_s Q}\right]\cos\left[2\pi\frac{f_0}{f_s}\frac{\sqrt{4Q^2-1}}{2Q}\right] \\ a_2 &= \exp\left[-\frac{2\pi f_0}{f_s Q}\right] \end{aligned} \tag{7}$$

where f_s is the digital filter sampling frequency.

If a_1 and a_2 are known and Q is large enough, it is possible to determine f_0 and Q from the absolute value and argument of the poles of the digital filter transmittance. The poles may be easily calculated as the roots of the quadratic function $z^2 + a_1 z + a_2$. The cantilever's resonant frequency and its quality factor may be calculated from the following equations

$$\begin{aligned} f_0 &\cong \frac{|\arg(p)| f_s}{2\pi} \\ Q &= \frac{-\pi f_0}{f_s \log[abs(p)]} \end{aligned} \tag{8}$$

where p is one of the roots of the quadratic function. It is assumed that cantilever thermal vibrations are modeled by a filtered sequence of samples generated randomly from Gaussian distribution with standard deviation determined on the basis of $\Gamma_{th}(f)$ (see Eq. (2)) and expressed by the following relation

$$\sigma_{\Gamma th} = \sqrt{\frac{k_B T k f_s}{\pi f_0 Q}} \tag{9}$$

We show (see Figs. 2 and 3) that such a sequence has approximately the same statistical properties as the continuous stochastic process of thermal vibrations of a real cantilever.

In real measurements, cantilever thermal vibrations are superimposed on noise, which may be assumed to be white only near the resonant frequency. In the presented solution, an additional digital bandpass filter is used. Its purpose is to remove all other interferences. The width of the passband of the bandpass filter depends on the predicted changes of the resonant frequency and quality factor. The resonance peak must be placed inside the passband. The broad passband increases the impact of the white noise on the estimation procedure but larger changes of eigenfrequency and quality factor are possible. Narrow passband decreases the impact of white noise but smaller changes of SHO parameters are allowed. On the basis of our experience, the width equal to 0.1 of sampling frequency may be the rule of thumb. If the quality factor is low (e.g. due to fluid viscosity), this rule may be inappropriate. In such a case, a cantilever with higher stiffness could be designed or higher vibration eigenmodes could be used, which usually results in higher quality factors. It is also possible

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