Frequency Response of Nanoelectromechanical Cantilevers Operating in Fluid

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***Abstract*-Nano-electro-mechanical resonators used for sensing, data storage, and nano-fabrication applications are often operated as feed-back control systems. To determine the transfer function of silicon cantilevers with a width of 5.0 μm, a thickness of 800 nm, and lengths of 10, 15, 30, and 45 μm, the damping in air and liquid was simulated numerically using an integrated fluid-structure solver. Bode diagrams and Nyquist plots of the cantilever transfer function indicate that the resonator will behave as a heavily damped system in liquid, and a lightly damped system in air. After experimental validation, ths computational method is expected to allow prediction of frequency response prior to fabrication of NEMS resonators.**

I. Introduction

As the applications of cantilever-based nano-systems [1] expand to include chemical sensing [2], medical instrumentation [3], data storage [4], atomic-force microscopy [5], and nano-fabrication [6] the need for sophisticated actuation and control will also increase. [7] This requires determination of the frequency response of the system, which will be heavily influenced by the damping. [8] When cantilevers operate in gas or liquid, the damping of the system is dominated by viscous losses. These losses can be computed using the Navier-Stokes equations on the cantilever cross-section. [9]- [12]

Navier-Stokes solvers have been successfully integrated with simplified structural models to estimate the frequency response of AFM cantilevers in liquid in the low kHz range. [13] The present work uses this computational approach to examine the frequency response of silicon NEMS cantilevers with natural frequencies in the high kHz range vibrating in air and water.

II. Computational Method

The cantilever geometry, with width b, thickness d, and length l, is shown as fig. 1:

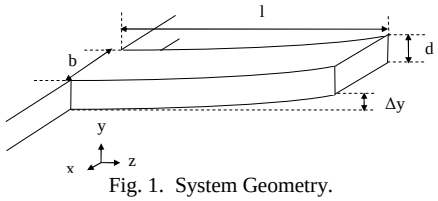

Fig. 1. System Geometry.

The natural frequency of the system ω_n will be given by

$$\omega_n = \frac{f_n}{2\pi} = \left(\frac{k_n}{l}\right)^2 \sqrt{\frac{EI}{m}} \tag{1}$$

where k_n is the vibrational mode constant, E is the Elastic modulus, I is the moment of inertia, and m is the cross-sectional mass. For a cantilever in the first mode if vibration, k_n is equal to 1.875. [14] The cross-sectional mass and the moment of inertia are given by:

$$m = \rho_s bd \tag{2}$$

$$E = bd^3/12 \tag{3}$$

where ρ_s is the density of the cantilever.

This geometry can be simplified to the 2-dimensional lumped-parameter model shown in fig. 2. The system consists of a cross-sectional effective mass attached to a spring with effective spring stiffness:

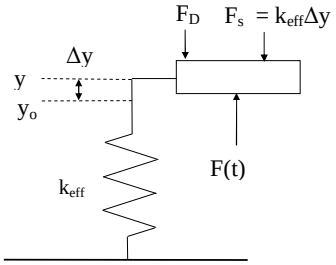

Fig. 2. Lumped-Parameter Model.

The equation of motion is then given by:

$$m\frac{d^2y}{dt^2} = F(t) - F_D - k_{eff}\left(y - y_o\right) \tag{4}$$

where F_D is the viscous drag force, and F(t) is the actuation force. This system will have a natural frequency given by:

$$\varpi_n = \sqrt{k_{eff}/m_{eff}}\ . \tag{5}$$

For a thermally actuated cantilever, the actuation force is assumed to be uniformly distributed across the cantilever length. Based on beam theory [15], the effective stiffness is:

$$k_{eff} = 8EI/l^4\ . \tag{6}$$

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The effective mass of the system is obtained by Rayleigh's method of setting the natural frequency of the lumped parameter oscillator given in (5) equal to the natural frequency of the cantilever given in (1). [16]

$$m_{eff} = 8m/k_n^4 . \quad (7)$$

The actuation force is given by a sinusoid with magnitude F_o and frequency ω:

$$F(t) = F_o \sin(\omega t) . \quad (8)$$

The viscous drag force is computed by solving the time-dependent Navier-Stokes equations on a 100 by 120 mesh around the cantilever, using a marker-and-cell CFD code. [17] The complete computational procedure is given by:

1. Solution of the velocity and pressure using a time-dependent Navier-Stokes algorithm.
2. Computation of the fluid force, spring force, and actuation force on the cantilever.
3. Computation of the acceleration, velocity, and position of the cantilever
4. Updating of fluid boundary conditions based on the new cantilever cross-section velocity.

The system time step is set by the maximum allowable time step for the fluid solver. The system achieves equilibrium within 5 to 10 cycles. For each cycle, the maximum displacement, and the phase difference between the maximum displacement and the maximum force are recorded.

III. RESULTS

A. *Maximum Displacement*

The frequency response of three silicon cantilevers was simulated. All cantilevers simulated have a width of 5 μm and a thickness of 800 nm. The cantilever lengths were 10, 15, 30, and 45 μm. These cantilevers dimensions are of the same order as those proposed for integration into nano-electro-mechanical systems for bio-detection. [1], [18] The elastic modulus used was 160 GPa, and the density was 2400 kg/m^3. [19] This yields natural frequencies of 6.63 x 10^7, 2.95 x 10^7, 7.36 x 10^6, and 3.27 x 10^5 s^{-1}.

The cantilever damping was simulated using two fluids: water at 293 K, and air at 103 kPa and 293 K. For water, this corresponds to a density ρ_f of 999.4 kg/m^3, and a viscosity μ of 1.007 x 10^{-3} kg/m-s. For air, this corresponds to a density ρ_f of 1.22 kg/m^3, and a viscosity μ of 1.81 x 10^{-5} kg/m-s. [20]

Because of the small scale of the system, a slip boundary condition was used in the CFD computation, with a momentum accommodation coefficient of 0.85. [21] This incorporates the continuum break-down effects encountered in nano-systems at atmospheric pressure. For the given cantilevers, the system was swept using a force with magnitude F_o of 10 μN/m, with values of ω/ω_n ranging from 0.10 to 7.0 in liquid, and 0.5 to 5.0 in air.

B. *Simulation results for cantilevers in water*

The peak displacement versus frequency is shown in fig. 3. These results show that the simulation predicts displacements in the nm range, indicating that the physical parameters chosen for the simulation are physically realistic.

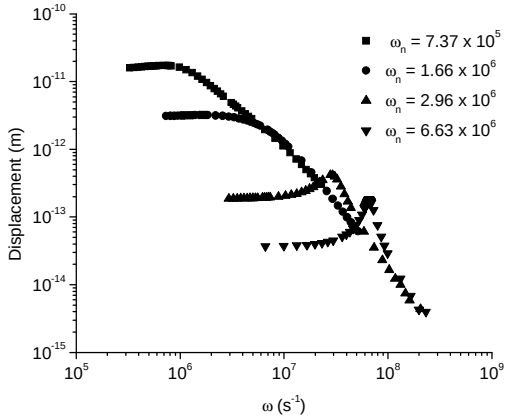

Fig. 3. Displacement versus Frequency for Cantilevers in Liquid.

The displacement results can be normalized to obtain the system gain using (9):

$$G(\omega) = 20 \cdot \log_{10}(k_{eff}\, y_{\max} / F_o) . \quad (9)$$

A plot of the gain as a function of the normalized frequency s is shown as fig. 4:

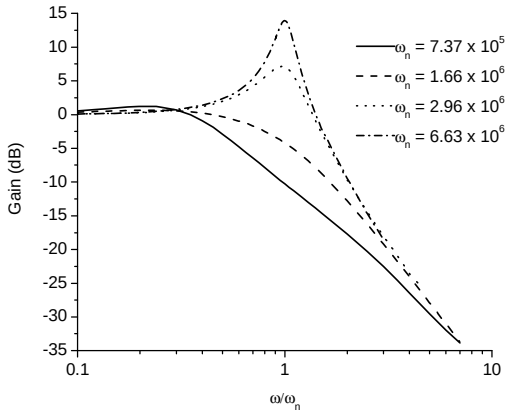

Fig. 4. Gain versus Frequency for Cantilevers in Liquid.

Fig. 4 shows that the cantilever operating in liquid is a heavily damped system, with a large shift in the resonant frequency away from the natural frequency of the system. This is confirmed by computing the quality factor of the system, as shown in table (1). The quality factors of less than one are similar to previous experimental results for long cantilever resonators in liquid. [5]

Table (1) shows a large gain the quality factor as the resonator natural frequency increases. This is consistent with previous experience operating cantilevers at higher frequencies [5] and higher-order modes. [22] These results show that the quality factor is proportional to the natural frequency of the system raised to the 1.4, which suggests that the damping is frequency dependent.

TABLE I
RESONANT FREQUENCY AND QUALITY FACTORS FOR CANTILVERS IN LIQUID

Natural Frequency f_n (MHz)	Natural Frequency ω_n (s^{-1})	Resonant Frequency ω_r (s^{-1})	ω_r/ω_n	Q
10.6	6.63×10^7	6.62×10^7	0.9985	10.15
4.69	2.94×10^7	2.85×10^7	0.969	4.56
1.17	7.37×10^6	1.67×10^6	0.226	0.58
0.521	3.74×10^6	7.88×10^5	0.211	0.23

A plot of the phase difference between the peak force and the peak displacement is shown as fig. 5. Together, fig. 4 and fig. 5 constitute the Bode plots of the resonators when operating in liquid.

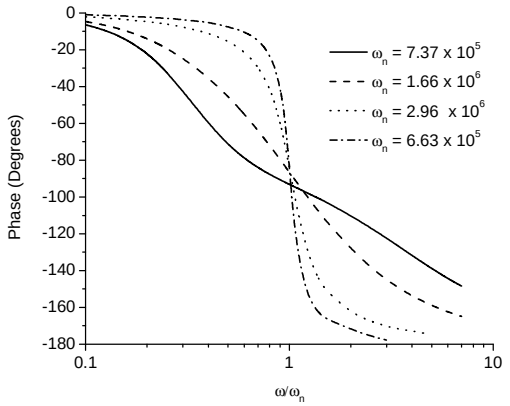

Fig. 5. Phase versus Frequency for Cantilevers in Liquid.

The data in fig. 4 and fig. 5 can be used to prepare the Nyquist diagram of the system. This result, shown in fig. 6, can be used to evaluate the stability of proposed control algorithms for the system.

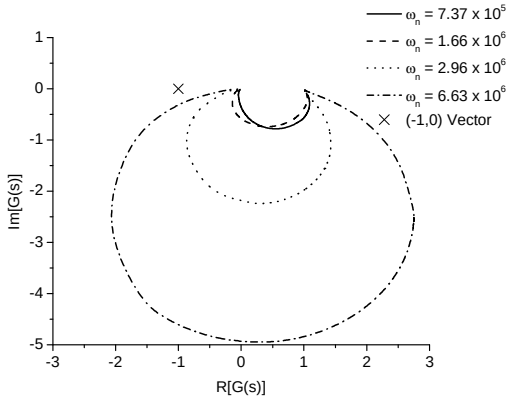

Fig. 6. Nyquist Diagram for Cantilevers in Liquid.

C. Simulation results for cantilevers in air

The analysis performed for the resonators using water as a working fluid is repeated using air as a working fluid. The maximum resonator displacements obtained through numeric simulation are show as fig. 7:

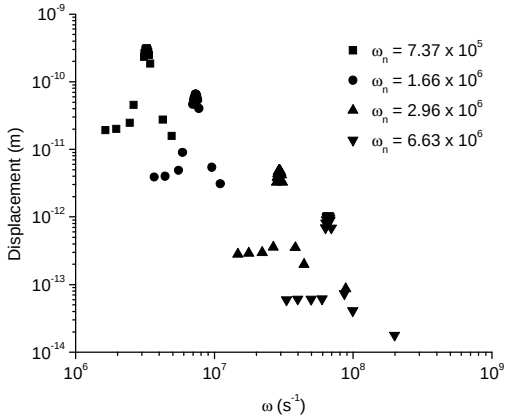

Fig. 7. Displacement versus Frequency for Cantilevers in Air.

These results can be used to obtain the gain, as shown in fig. 8:

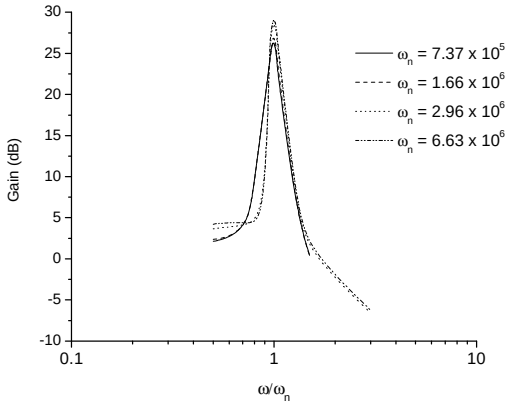

Fig. 8. Gain versus Frequency for Cantilevers in Air.

The frequency shifts and the quality factor obtained are shown in table (2). The quality factors in air are typically orders of magnitude higher than the estimated quality factors in water for the same resonator, which agrees with experimental results. [4], [23]

TABLE II
RESONANT FREQUENCY AND QUALITY FACTORS FOR CANTILVERS IN AIR

Natural Frequency f_n (MHz)	Natural Frequency ω_n (s^{-1})	Resonant Frequency ω_r (s^{-1})	ω_r/ω_n	Q
10.6	6.63×10^7	6.62×10^7	0.9992	19.9
4.69	2.94×10^7	2.93×10^7	0.9985	15.8
1.17	7.37×10^6	7.32×10^6	0.9937	10.8
0.521	3.74×10^6	3.71×10^6	0.9916	10.4

These results show that the quality factor is proportional to the natural frequency of the system raised to the 0.23, again indicating frequency-dependent damping. However, the relative resolution of this technique for determining quality factor is less than other techniques that compute Q directly by computing the energy loss at resonance. [12]

A plot of the phase difference between the peak force and the peak displacement is shown as fig. 9. Together, fig. 8 and fig. 9 constitute the Bode plots of the resonators when operating in air.

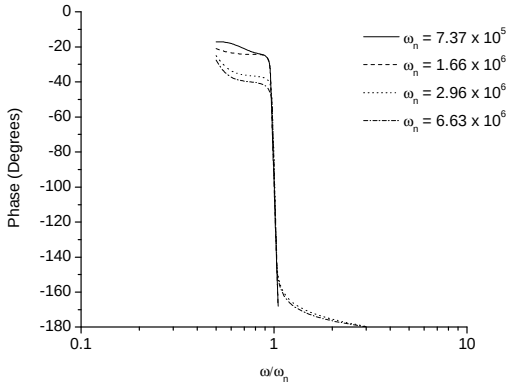

Fig. 9. Phase versus Frequency for Cantilevers in Air.

The large computational cost of performing simulations of cantilevers vibrating in air prevented reconstruction of the entire Nyquist diagram. Selected points of the Nyquist diagram for the system operating in air are shown as fig. 10:

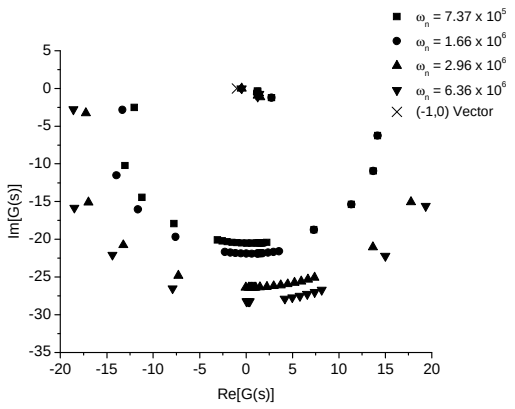

Fig. 10. Nyquist Diagram for Cantilevers in Air.

IV. CONCLUSIONS

For cantilevers operating in air, the frequency response is relatively unaffected by the natural frequency of the system. For cantilevers in water, there is a large difference in the frequency response at higher frequencies, due to increased damping. However, the high computational cost of simulating resonators operating in air limited comparisons off behavior away from the resonance frequency.

These results predict the dynamic response and the frequency shift from resonance without use of empirical expressions such as added mass. If the results for the frequency response are experimentally validated, then capturing the dynamic response by simulation will allow optimization of NEMS for integration with feed-back control without trial-and-error experimental design.

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