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Electromechanical model of a resonating nano-cantilever-based sensor for high-resolution and high-sensitivity mass detection

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Abstract
A simple linear electromechanical model for an electrostatically driven resonating cantilever is derived. The model has been developed in order to determine dynamic quantities such as the capacitive current flowing through the cantilever-driver system at the resonance frequency, and it allows us to calculate static magnitudes such as position and voltage of collapse or the voltage versus deflection characteristic. The model is used to demonstrate the theoretical sensitivity on the attogram scale of a mass sensor based on a nanometre-scale cantilever, and to analyse the effect of an extra feedback loop in the control circuit to increase the Q factor.

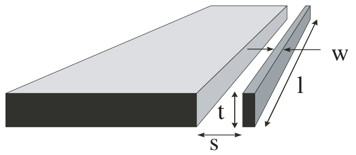
1. Introduction

Micro-electromechanical systems (MEMS) have wide application in the development of sensors for the detection of magnitudes in almost any domain [1]. A reduction of the dimensions of the mechanical transducer leads to a new generation of systems called nano-electromechanical systems (NEMS) [2], which represent an improvement on sensitivity, spatial resolution, energy efficiency and time of response. One particular kind of micromechanical device, which is based on a silicon cantilever, has been recently developed and used as a very sensitive detector of heat, surface stress or mass [3] or in molecular recognition [4]. As an example of NEMS, we have recently started the development of a mass sensor, based on a silicon nanometre-scale resonating cantilever, which is expected to achieve a mass sensitivity of around 10^{-19} g [5], which is high enough to detect changes in mass corresponding to a single biomolecule such as a medium-size protein, for example polypeptide chains[4]. In this sensor, the cantilever is driven electrostatically to the resonance by means of a lateral electrode, which is closely placed parallel to the cantilever. A capacitive read-out of the cantilever oscillation will be performed by means of a CMOS circuitry, which has been designed to be integrated monolithically with the nanocantilever-driver system. A knowledge as precise as possible of the electrical characteristics of the cantilever-driver system is crucial for a correct design of the CMOS circuitry.

In this paper we report on an electromechanical model of the cantilever-driver system, which allows us to derive the electrical specifications for the CMOS circuitry as dc and ac driving voltages and capacitive current levels at the resonance. The theoretical mass resolution of the cantilever will be also calculated by a simple first-order approximated expression. The Q factor and geometrical dimensions of the cantilever-driver system are the only inputs of the model. The validity of the model is based on the following assumptions. (a) The mass of the cantilever is homogeneously distributed, and the stress effect produced by the presence of a different material in the surface of the beam has not been considered. (b) The change of shape of the cantilever produced by the small torsions is approximated linearly. (c) The amplitude of the cantilever

[4] Polypeptide chains have molecular weights between 15 000 and 70 000 g mol^{-1}, which corresponds to weights per molecule between 0.25×10^{-19} and 1.16×10^{-19} g.

(*a*)



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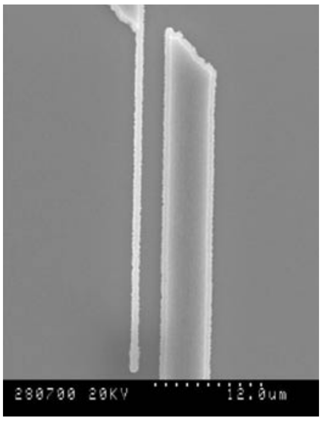


Figure 1. (*a*) Schematic drawing of the cantilever-driver structure with the definition of the dimensions. (*b*) SEM image of a nanofabricated cantilever. The material in which the cantilever is fabricated is polysilicon, the same as will be used for fabricating the integrated circuit.

oscillation at the resonance frequency is small enough to consider a linear oscillating regime.

The model is used to design an additional electronic feedback circuit that allows us to increase the 'effective' value of the Q factor.

2. Geometrical dimensions and mechanical properties

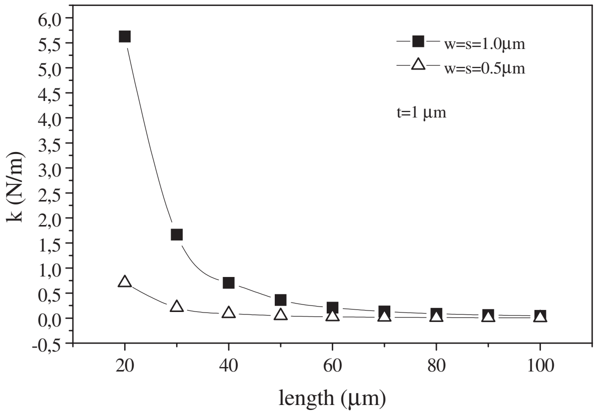
The mechanical properties of the cantilever are completely defined by (i) the Young modulus and density, which for silicon are $E = 180$ GPa and $\rho = 2.33 \times 10^3$ kg m^{-3} respectively, and (ii) five inputs that depend on the specific cantilever:

- (a) The dimensions of the cantilever, length (l), thickness (t) and width (w), and the gap between the cantilever and the driver (s) (figure 1).
- (b) The Q factor, which has to be determined experimentally [5], and depends on several factors that account for the viscoelastic damping. These factors are ambient (UHV, liquid, air) and geometrical configuration (distance to the driver, for example).

The elastic constant, k, and the resonance frequency, f_{res}, of the cantilever are derived directly from these parameters using the following expressions [6]:

$$k = \frac{E}{4}\frac{w^3}{l^3}t \ (\mathrm{N\ m^{-1}}) \qquad (1)$$

$$f_{\mathrm{res}} = 0.16\sqrt{\frac{E}{\rho}}\frac{w}{l^2} \ (\mathrm{Hz}). \qquad (2)$$



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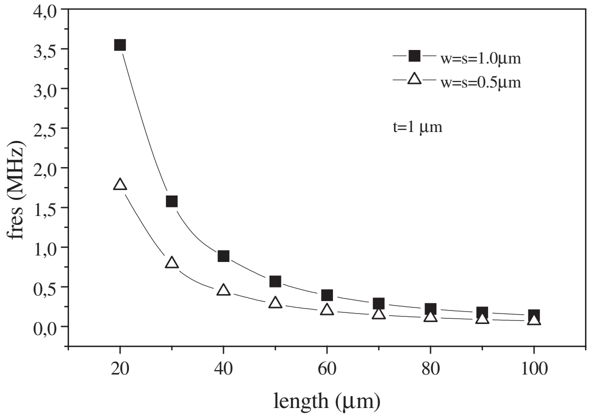

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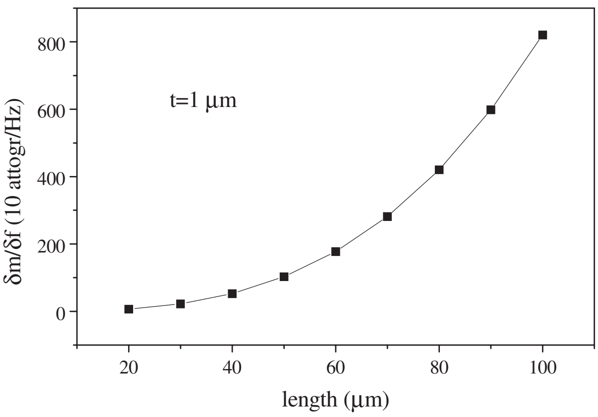

(*c*)

Figure 2. Elastic constant (*a*), resonance frequency (*b*) and mass sensitivity (*c*) of cantilevers with a thickness of 1 μm and different lengths.

Figures 2(*a*) and (*b*) show the dependence of the elastic constant and the resonance frequency on the cantilever length, for two different cantilever widths. A width of 500 nm corresponds to the limit of resolution of the lithography technique used to fabricate the cantilever-driver structures [5].

The cantilever-driver transducer can be used for mass detection if the small changes in resonance frequency produced by small changes in the cantilever mass are measured. A simple estimation of the theoretical minimum mass detectable, δm, can be found by assuming that the mass which we want to

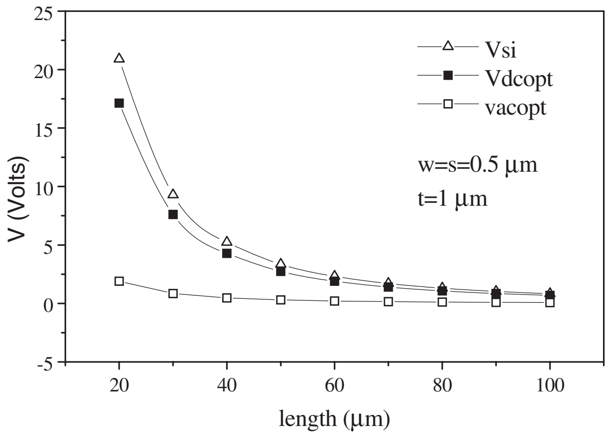

Figure 3. Snap-in voltage (V_{si}), dc voltage (V_{dcopt}) and ac voltage (V_{acopt}) as a function of the cantilever length. These values are used to determine the small-signal electrical model of the cantilever. A value of $\gamma = 25$ has been used in the calculations.

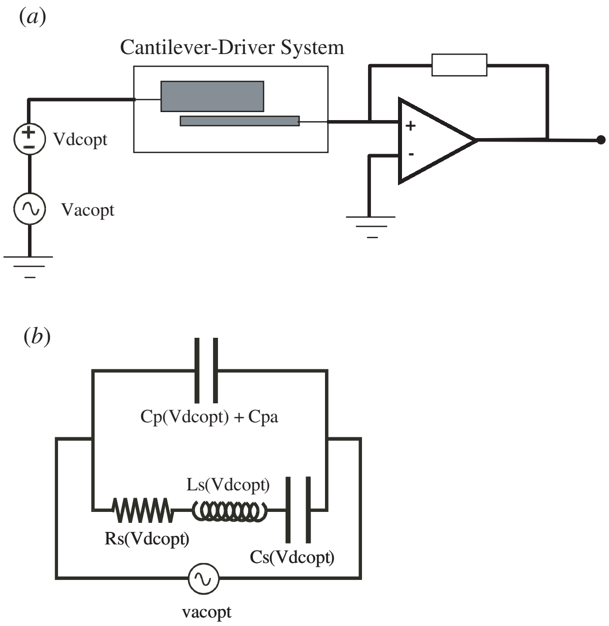

Figure 4. (*a*) Schematic of the experimental set-up to excite the oscillation of the cantilever and acquire the resulting current. (*b*) Small-signal electromechanical model of the oscillating cantilever-driver system.

measure is added to the cantilever, producing no change in the elastic constant (k), but only a shift in its resonant frequency (δf):

$$\delta m = 26k\left[\frac{1}{(f_{res} - \delta f)^2} - \frac{1}{f_{res}^2}\right] \text{ (g)}. \tag{3}$$

A linear approximation of the previous expression leads to a simpler function for the mass resolution, which can be expressed in terms of mass per frequency unit:

$$\frac{\delta m}{\delta f} = 56\frac{k}{f_{res}^3} \text{ (g Hz}^{-1}\text{)}. \tag{4}$$

Figure 2(*c*) shows the dependence of this mass resolution per unit frequency on the cantilever length.

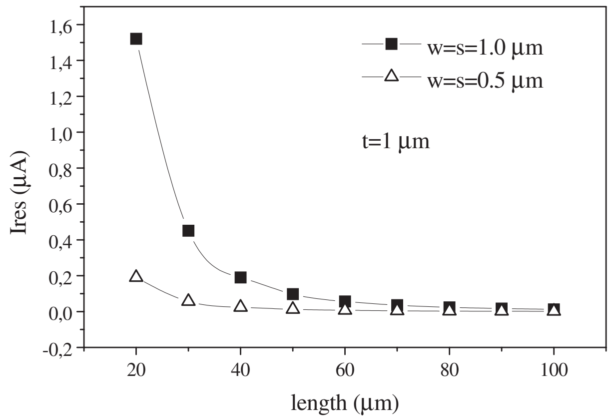

Figure 5. Current flowing through the cantilever-driver structure at the resonance peak as a function of cantilever length. Other parameters used in the calculation are $Q = 50$, $\chi = 0.1$ and $\gamma = 25$.

We can also deduce from figure 2(*c*) that mass resolution is improved by decreasing the cantilever length. Thus, a theoretical mass resolution of 6.5×10^{-18} g Hz^{-1} can be obtained with a cantilever 20 μm long and 1 μm thick.

3. Response of the cantilever to an applied voltage

An exact solution of the cantilever deflection, x, as a function of the applied voltage, can only be found by complex numerical methods, because the nonlinear differential equation which describes this deflection has no analytical solution [7]. However, a simple linear approximation [8] can provide a static voltage versus deflection function, $V(x)$, which is good enough for our purposes. This approximation is based on the assumption that the cantilever sustains a linear deformation shape and that the electrostatic force is uniform along its lateral surface. Then, the voltage corresponding to each equilibrium value of the deflection is easily calculated by finding a minimum to the total potential energy of the system, which consists of the electrostatic energy stored in the cantilever-driver capacitance and the elastic energy stored in the cantilever. The resulting expression is

$$V(x) = \sqrt{\frac{0.533E}{\varepsilon}\frac{w^3}{l^4}\frac{x^3(s-x)}{x-(s-x)\ln\left|\frac{s}{s-x}\right|}} \text{ (V(m))} \tag{5}$$

where ε is the medium permittivity.

The maximum voltage that can be applied to the structure is the snap-in or collapse voltage: if the applied voltage to the structure exceeds that value, the cantilever will collapse into the driver and will remain in that position irreversibly. The collapse voltage corresponds to the first unstable deflection and can be calculated by finding a minimum of the first derivative of the total potential energy. The values of the snap-in deflection and voltage are

$$x_{si} = 0.44s \text{ (m)} \tag{6}$$

$$V_{si} = \sqrt{0.22\frac{E}{\varepsilon}\frac{w^3 s^3}{l^4}} \text{ (V)}. \tag{7}$$

The voltage applied between driver and cantilever is determined by linearity criteria: an optimal total voltage, V_{opt},

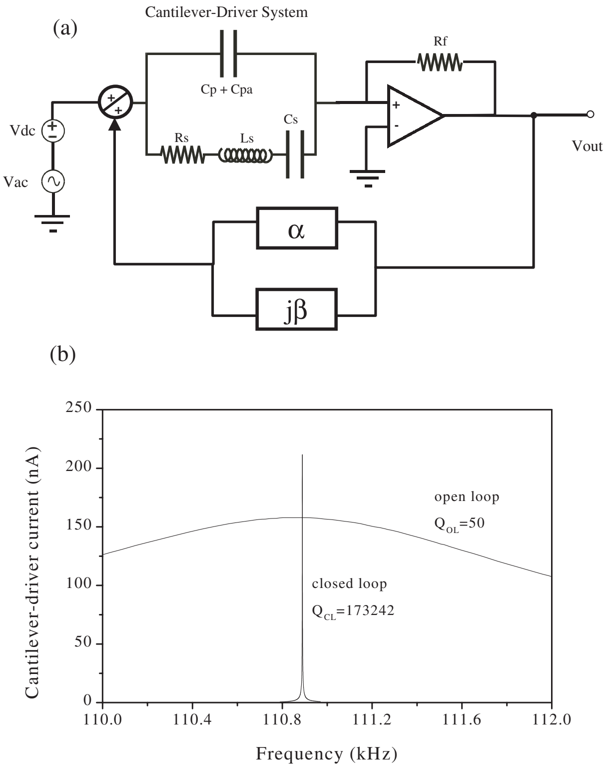

Figure 6. (*a*) Schematic diagram of the inclusion of the additional feedback to enhance the Q factor. (*b*) Simulation of the frequency response of the cantilever oscillation with and without the use of the additional feedback. In order to compare closed- and open-loop responses, the parasitic current component has been subtracted from the open-loop characteristic and the input voltage has been decreased in the closed-loop operation. Dimensions of the cantilever are $l = 80\ \mu$m, $w = 0.5\ \mu$m, $t = 0.6\ \mu$m, $s = 0.5\ \mu$m, $f_{res} = 110.9$ kHz and $k = 0.0066$ N m^{-1}.

is defined as that corresponding to a deflection, x_{opt}, which is a fraction of the gap(s), defined by the parameter γ. The following equations summarize the definition of V_{opt}:

$$x_{opt} = \frac{\gamma}{100} s \text{ (m)} \tag{8}$$

$$V_{opt} = V(x_{opt}) \text{ (V)}. \tag{9}$$

By choosing a small enough value for γ (e.g. 25) the linearity of the motion equation can be satisfied. Each time V_{opt} is calculated, it is verified that its value does not exceed the snap-in voltage value, V_{si}. Finally, the optimal voltage, V_{opt}, is distributed between a dc component, V_{dcopt}, and an ac component, V_{acopt}, by means of a χ factor:

$$V_{acopt} = \chi V_{opt} \text{ (V)}. \tag{10}$$

In figure 3, the values of the ac and dc voltages calculated for cantilevers with different lengths are shown. In the same figure it can be appreciated that neither voltage ever exceeds the critical snap-in voltage.

4. Small-signal electromechanical model

In the previous section, we deduced the expressions that allow the calculation of the mechanical properties and the optimal applied voltages for the cantilever-driven systems. In this section, an equivalent model of the cantilever-driver system in a linear regime is derived (figure 4). Similar models are used to describe the dynamic electromechanical behaviour of resonating piezoelectric-material-based devices such as quartz crystal balances.

The static capacitance of the cantilever-driver system, C_0, increases when a dc voltage is applied. The new capacitance, C_p, is

$$C_p = C_0\,(1 + \kappa(V_{dc})) \text{ (F)} \tag{11}$$

$$C_0 = \varepsilon \frac{lt}{s} \text{ (F)} \tag{12}$$

where κ is the so-called electromechanical coupling parameter, which can be calculated by

$$\kappa = \frac{\varepsilon}{2k} \frac{lt}{s^3} V_{dc}^2. \tag{13}$$

The model also describes the current component induced by the dc voltage applied to the vibrating cantilever by a series $R_s L_s C_s$ branch [9, 10] in parallel to C_p:

$$C_s = 1.798 \kappa C_0 \text{ (F)} \tag{14}$$

$$L_s = \frac{1}{2\pi C_s f_{res}} \text{ (H)} \tag{15}$$

$$R_s = \frac{1}{Q} \sqrt{\frac{L_s}{C_s}} \text{ }(\Omega). \tag{16}$$

An additional parasitic capacitance, C_{pa}, connected in parallel is also included in the model; this can occasionally be useful to model the parasitic capacitance associated with contact pads and wires.

The total current that flows between driver and cantilever is finally determined by firstly calculating the impedance of $R_s L_s C_s // C_p // C_{pa}$ at the bias point defined by V_{dcopt}, and then computing the current induced through this impedance when V_{acopt} is applied.

Figure 5 shows the value of the current through the cantilever-driver system at the resonance frequency. This figure indicates that the value of the current resonance peak can be increased by lowering the length of the cantilever and increasing its width.

5. Increase of the effective Q factor of the cantilever-driver system

Equation (4) shows that the minimum mass change that it is possible to detect will depend on the minimum change of the resonance frequency that the electronic circuit can elucidate. This, in turn, will depend on the quality factor of the cantilever, because low quality factors imply that the variation of amplitude with frequency is small. In consequence, high quality factors are required. Experimental visual characterization of the cantilever [11] reveals that the quality factor of the system under ambient conditions is around 50, and it increases to 10 000 for operation in vacuum.

Recently, the use of an additional electronic feedback has been proposed to increase the quality factor of the cantilever used in tapping mode operation [12], which is specially indicated for operation in liquid. As, under these conditions, the cantilever, in conjunction with mechanical excitation optical detection systems, behaves as a second-order system, the additional feedback loop consists of a phase shifter (90°) and an amplifier. In the case of the cantilever-driver system that we report here, according to figure 4, the equivalent circuit is a third-order system. Then, the analysis is more complicated and the feedback circuit must be designed accordingly.

Figure 6(a) shows the small-signal electrical model of the cantilever together with the current/voltage converter and the feedback circuit. The open-loop transfer function has the following expression:

$$H(jw) = -R_F \times \frac{C_p R_s w^2 + j[C_p L_s w^3 - (1 + \frac{C_p}{C_s})w]}{(L_s w^2 \frac{1}{C_s}) - jR_s w}. \quad (17)$$

In order to increase the quality factor of the system, the feedback loop section of the circuit has to have the form $G(s) = \alpha + j\beta$. The values that provide a maximum of the closed-loop transfer function at the resonance frequency ω_o are the following:

$$\beta = -C_p R_F \omega_o \quad (18)$$

$$\alpha = C_s R_F \omega_o - 1. \quad (19)$$

These values are used to obtain an initial estimation of the parameters α and β. Careful analysis of the closed-loop transfer function shows that the quality factor can be further increased if we excite the cantilever at a frequency slightly different from the resonance frequency. In figure 6(b), we show the dramatic increase of the quality factor if the optimized values of α and β are used. The enhancement factor of the Q factor is 3500. The additional feedback loop makes feasible the operation of the system in a liquid environment, where the Q factor is expected to be very low, and, in consequence, applications of the system to detection of single biomolecules might be possible.

6. Conclusions

A simple linear model for characterizing the electromechanical behaviour of a resonating cantilever-driver system has been derived. The model allows us to calculate static magnitudes such as the collapse voltage and deflection of the cantilever, as well as dynamic quantities such as the current flowing through the vibrating cantilever-driver capacitance. Simple expressions used to determine the mass resolution of the cantilever have been also included in the model. The model is currently being used to determine the electrical specifications of the CMOS circuitry, that will be integrated together with the resonating nano-cantilever in the framework of a European project called NANOMASS [13]. Finally, by using an additional feedback loop, the Q-factor of the system can be increased enough to achieve the maximum sensitivity, even under liquid operation. We are currently evaluating alternative approaches to the electrical excitation and capacitive detection used here in order to expand the applicability of the system.

Acknowledgment

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