Calculation of Resonant Frequencies of Silicon AFM Cantilevers

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Abstract. A theoretical study of the quality and the validity range of different numerical and analytical methods of calculating of the frequency shift in measurement using microcromechanical sensor is presented. This work considered a calculating method for natural frequency in comparison with experimentally measured oscillation frequencies of microcromechanical sensor immersed in air and/or viscous medium. The numerical methods for solving the equation of resonance oscillation of the console fixed on one side are considered for calculating the natural oscillation frequencies of standard AFM cantilevers.

1. Introduction

At present micromechanical sensors are commonly used. Their repeatability, resolution and stability are remarkable [1]. Micromechanical sensors mostly use the resonance mode of cantilever oscillations for higher sensitivity which allows measuring of wide range of physical quantities (pressure, vacuum degree, temperature, humidity, acceleration, flux etc), in different environmental conditions. Such sensors based on cantilever oscillations could operate both in air and different viscous media (water, medium, oil etc.). However, their operation in liquids is hampered by a significant decrease in the quality factor of the cantilever oscillations which in turn leads to a significant decrease in the sensor sensitivity.The oscillation frequency of the micromechanical consoles depends both on the physical parameters of the console and on the media properties. In some cases, by optimisation the physical parameters of the console, one could providean operable of the micromechanical sensor in a liquid medium. In this paper we consider methods of modelling the resonance oscillations and calculating the natural frequencies. The results of calculation we compare with the experimentally measured oscillations frequencies of cantilevers immersed in air and a viscous medium.

2. Resonance frequency in vacuum

In the general case a cantilever is a rectangular beam fixed on one of the sides to a rigid base. Such an oscillator has several resonance modes [2]. The quality factor (amplitude) of oscillations is the possibility to detect any of the modes and is determined by the cantilever geometry. There is a number of applications where alongside the main mode, for example, the torsion mode increases the sensitivity of the sensor [3], however, in practice, most sensors operate using the first oscillation mode. Therefore, in this paper, we consider only the first mode of resonant oscillations of cantilever sensors. The resonance frequency can be calculated as [4]:

$$f_0 = \frac{1}{2\pi}\left(\frac{k}{m_0}\right)^{\frac{1}{2}}, \quad (1)$$

where m_0 is mass of cantilever, k is elastic coefficient which is associated with the geometrical parameters of the cantilever and the Young's modulus, E, as:

$$k = \frac{EWT^3}{4L^3}, \quad (2)$$

where L, W, T are the cantilever length, width and thickness, correspondingly.

In many applications of cantilever sensors, the frequency shift, Δf, is measured under the influence of a change in the cantilever mass, Δm, related with, e.g., some objects attached to the cantilever (absorbed molecules, biological objects, films, etc.) From expression (1) it is easy to obtain that[5]:

$$\Delta f = -\frac{f_0}{2m_0}\Delta m \quad (3)$$

The application of this analytical expression is very limited, since it involves the uniform distribution of the attached mass over the entire surface of the cantilever. In addition, the value of the attached mass should be less than the mass of the cantilever.The case when the attached mass is concentrated only at the end of the cantilever is taken into account in the following analytical expression for calculating the resonant frequency of the cantilever [6]:

$$f = \frac{\lambda^2 T}{2\pi L^2}\left(\frac{E}{12\rho(1+4\gamma)}\right)^{\frac{1}{2}}, \quad (4)$$

$\gamma = \Delta m/m_0$; ρ – cantilever material density; λ – dimensionless parameter dependent on γ as $\lambda(\gamma)=1.875/(1+4\gamma)$.

Eqs. (1) and (4) allows one to calculate the resonant frequency of a cantilever with a rectangular geometry. At the same time most commercially available cantilevers, such as those used in AFMs, have a complex geometry different form rectangular. To calculate the resonant frequencies of such cantilevers the authors use software package COMSOL Multiphysics 5.3a. Calculation of the natural frequencies in the “Eigenfrequency” module is carried out by finite difference method.The calculation consists of the following steps: 1) creation of the console geometry; 2) setting the initial conditions; 3) construction of a mesh on the cantilever; 4) start the calculation to find a solution.

The geometry of NSG10 cantilever fabricated by NT-MDT which was additionally corrected in accordance with preliminary obtained SEM images of the real cantilever was used as a base calculations. Experimentally the frequency of the cantilever vibrations was measured using an adaptive holographic interferometer [7] and was amounted to 168.2 kHz which is well corresponded to the simulation results. The cantilever performs its vibrational movements which accompanied with the loss of vibrational energy. This energy is dissipated in the form of heat on the defects in the cantilever structure, flows into the base to which the cantilever is fixed. When the cantilever is placed in a liquid the vibrational energy is dissipated into the medium due to the presence of viscous friction. Similar energy losses should be taken into account while using the COMSOL Multiphysics module “Viscous damping”. However, the “Eigenfrequency” module does not support a calculation of resonant frequencies in liquids. To simulate oscillations and calculate the resonant frequencies of the cantilever in liquids, we propose the using of “FSI Analysis” module (Fluid Structure Interaction) [8]. At the same time, this model assumes a strong influence of fluid flows on the deformation of the cantilever, but limits the geometry of the cantilevers: the cantilever thickness should be much less than length. Thus, resonance frequencies for commercial AFM cantilevers cannot be calculated using the "FSI analysis” module.

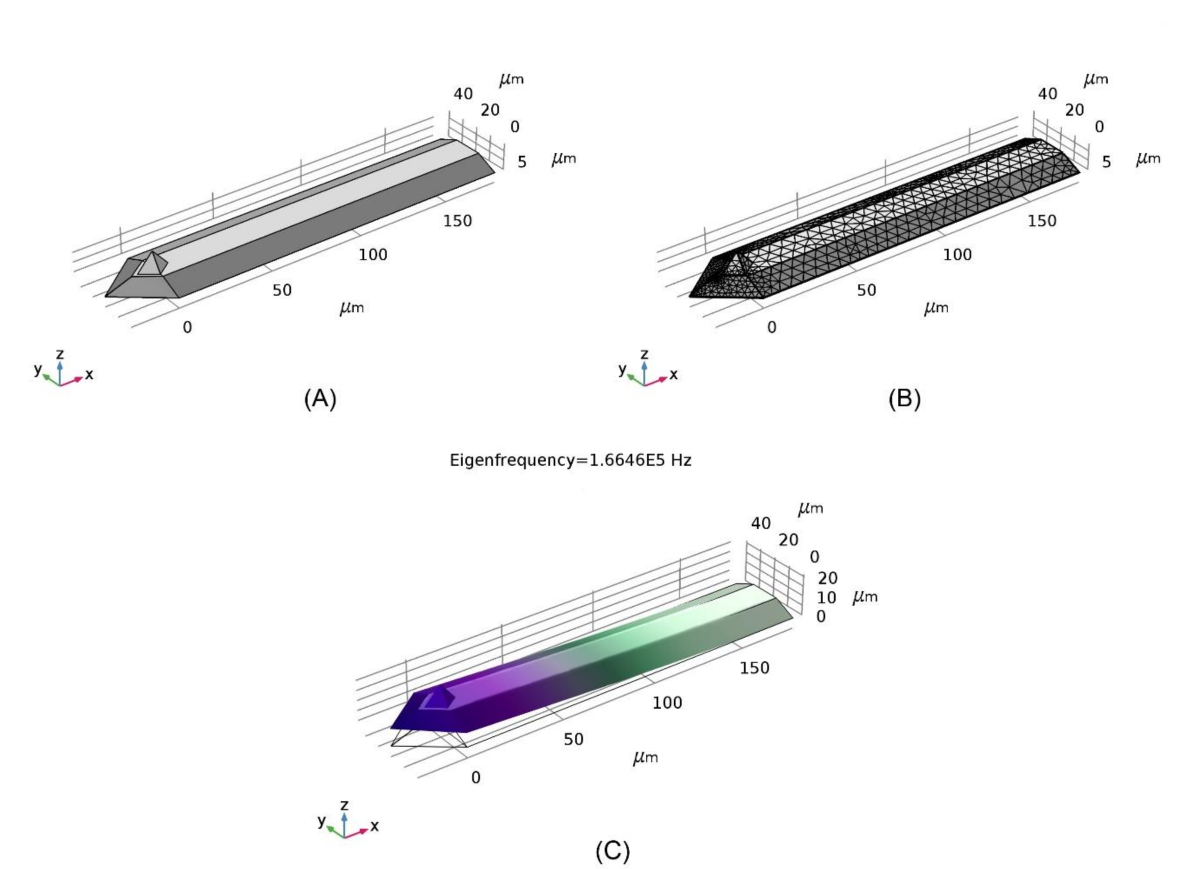

Figure 1. Simulation of the AFM cantilever oscillations in the COMSOL Multiphysics interface: (A) – geometry of trapezoid-shaped AFM cantilever; (B) – mesh for calculating the physical model; (C) – simulation result of the first cantilever oscillation mode.

3. Resonance frequency in liquid

The natural oscillations frequencies of cantilever are reduced when cantilever is immersed in a fluid. The fluid also affects resonance mode shapes and provides additional vibration damping. In the case of immersed cantilevers, an approximate analytical solution is frequently used to estimate the natural frequencies based on the fluid properties, cantilever geometry and the structure-only natural frequencies. The analytical expression accounts for the “added mass” of the fluid that is displaced by the beam as it vibrates [9]. Our calculations of the oscillation frequency using one of these analytical solutions are shown below.

During vibration of a cantilever in a liquid, an external force arises which resists its movement. This force is denoted by F_{fluid} and is as follows [9]:

$$F_{fluid} = -g_1\dot{\omega} - m_f\ddot{\omega}, \tag{5}$$

where $\omega=\omega(x, t)$ is the deflection at an arbitrary place x on the axis of the cantilever. g_1 is the damping coefficient of the fluid, and m_f is the mass of the added fluid per unit length of the cantilever. From this formula, the resonant frequency f_r of a cantilever immersed in a viscous liquid can be expressed [10]:

$$f_r = f_0 \frac{1}{\left(1+\frac{L\cdot m_f}{m_0}\right)^{1/2}} \left(1-\frac{1}{2Q_{tot(liq)}}\right)^{1/2} \tag{6}$$

where $Q_{tot(liq)}$ is the general figure of merit of the submerged cantilever, it reflects both the cantilever's own losses and those caused by interaction with the liquid. The frequency f_0 can be expressed as follows:

$$f_0 = \frac{1}{2\pi}\left(\frac{\lambda}{L}\right)^2\left(\frac{\sum_i \widehat{E}_i I_i}{W\sum_i \rho_i h_i}\right)^{1/2}. \tag{7}$$

Equation (7) is derived from the classical theory of beam bending. The parameters ρ_i and h_i are the density and thickness of the corresponding layers of the composite cantilever. I_i represents individual moments of inertia of different layers relative to the neutral axis of the beam. $\widehat{E}_i$-elementary Young's modulus. Since the quality factor $Q_{tot(liq)}$ of the cantilever immersed in the liquid also shows the cantilever's intrinsic losses due to interaction with the liquid, we can express it as the sum of two main components:

$$\frac{1}{Q_{tot(liq)}} = \frac{1}{Q_{\text{int}}} + \frac{1}{Q_{fluid}} \tag{8}$$

Q_{int} is the proper quality factor of the cantilever, Q_{fluid} is the loss caused by the liquid. One can neglect the contribution of own losses and replace the overall quality factor in the formula. This follows from the fact that losses caused by the liquid dominate the cantilever's own losses. Then we get $Q_{tot(liq)} \approx Q_{fluid}$. Using the results of J.E. Sader [11] Q_{fluid}can be written as:

$$Q_{fluid} = 2\pi f_0 \frac{\left(1+\frac{L\cdot m_f}{m_0}\right)^{1/2}}{\frac{L\cdot g_1}{m_0}} \tag{9}$$

Liquid ratios, g_1 and m_f:

$$g_1 = \pi\eta\,\text{Re}\cdot\Gamma_i(\text{Re}), \tag{10}$$

$$m_f = \frac{\eta\cdot\text{Re}}{2 f_r}\Gamma_r(\text{Re}) \tag{11}$$

where η is the viscosity of the liquid; Re is the Reynolds number of the fluid flow around the cantilever which is given by

$$\text{Re} = \frac{\pi\rho_f W^2 f_r}{2\eta}; \tag{12}$$

ρ_f - fluid density; Γ_r and Γ_i are the real and imaginary parts of the "hydrodynamic function":

$$\Gamma(\text{Re}) = \Omega(\text{Re})\left[1+\frac{4j\cdot K_1\left(-j\left(j\,\text{Re}\right)^{1/2}\right)}{\left(j\,\text{Re}\right)^{1/2}\cdot K_0\left(-j\left(j\,\text{Re}\right)^{1/2}\right)}\right], \tag{13}$$

where $K_0(\ldots)$ and $K_1(\ldots)$ are modified Bessel functions. The Reynolds number is proportional to the oscillation frequency, which represents an unknown parameter that will be calculated here. This means that we need to perform a self-consistent calculation of f_r. The resonant frequency of the cantilever in air is used as the initial value f_r for the Eq. (12). Then, the obtained *Re* value is used to calculate g_1 and m_f. Thus we obtain a new resonant frequency f_r of the cantilever in the liquid. Then we find a new Reynolds number. This iterative process continues until self-consistency is achieved.

To facilitate calculations, an algorithm for finding the resonant frequency of a cantilever in a liquid was implemented in MATLAB. With its help, the theoretical resonant frequency of the cantilever in the following liquids was calculated. For the cantilevers considered in this work, the difference in the resonant frequency in air and vacuum differs insignificantly and, as a rule, is less than the error of frequency measurement. In most cases few iterations are usually enough for obtaining good accuracy of resonance frequency calculation. In our case the change of calculated of resonance frequency became less than 0.01 % already after 4 iterations.

4. Experimental measured resonant frequencies

For experimental measuring of the resonant frequencies of cantilevers we used an adaptive holographic interferometer based on two-wave interaction of waves in a photorefractive crystal [12, 13]. The cantilever was placed in a flow cell and installed in the reference beam of the interferometer. To excite natural oscillations of the cantilever, the Nd:YAG pulsed laser operated at a wavelength of 532 nm with a pulse duration of 5 ns and a pulse repetition rate of 20 Hz was used. The average laser pulse energy (200 μJ) was chosen so that the recorded longitudinal vibrations of the cantilever did not exceed a quarter of the wavelength of the laser used in the interferometer (1064 nm). The signal demodulated by the interferometer was detected by a photodetector and recorded in digital oscilloscope. The obtained signal was processed using FFT conversion to finding the eigenfrequencies. Calculated and experimentally measured frequencies of the first resonance mode for various cantilevers surrounded by air and water are summarised in the Table 1.

Table 1. Theoretically calculated and experimentally measured frequencies of the first resonance mode of various cantilevers placed in water and in air.

	Cantilever **C1** (lenth:180; width:40; thickness:7)	Cantilever **C2** (lenth:120; width:32; thickness:15)	Cantilever **C3** (lenth:240; width:40; thickness:2)
in air (modelling)	181.5 kHz	290.0 kHz	19.8 kHz
in air (measured)	178.2 kHz	277.1 kHz	8.2 kHz
in liquid (modelling)	72.1 kHz	108.3 kHz	7.5 kHz
in liquid (measured)	69.3 kHz	102.9 kHz	4.8 kHz

Analyzing the obtained data from the Table 1, we can conclude that the methods described above for calculating resonant frequencies are in good agreement with experimental results. The frequency differences for the C3 cantilever can be explained by the small cantilever thickness, due to which the structural defects that inevitably appear during manufacture at the factory have a significant effect on the resonant frequency.

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