Modelling of Non-Uniform Piezoelectric Micro-Cantilever in Different Environments

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Abstract: In recent years, Atomic Force Microscopy (AFM) has been known as a powerful and efficient tool for surface imaging in different environment. To enhance image quality and more precise prediction of Micro-cantilever (MC) behaviour, accuracy in the MC modeling and simulation and detecting the MC sensitivity to geometric parameters has great importance. To model the vibration motion of the AFM non-uniform piezoelectric MC, Timoshenko beam theory is used in order to consider the effect of shear effect in air and liquid environment. In addition, the effect of the forces imposed by the ambient and sample surface is considered. Frequency response has been studied in the air and different liquid environments and the obtained results have been compared with experiential results as well as with results obtained from Euler-Bernoulli beam theory that is reflective of higher precision exercised in the modeling in respect to Euler-Bernoulli beam theory. Efast statistical method, which is found efficient and quick in the survey of linear and nonlinear models and takes the inter-parameter coupling effect into consideration besides calculating the sensitivities unique to each of the factors, has been applied in order to analyse the geometrical parameters' effects on the MC natural frequencies in the air and water environments.

Keywords: Different Environments, Efast Method, Finite Element Method, Piezoelectric MC, Timoshenko Beam Theory

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1 INTRODUCTION

Atomic force microscopy (AFM) is one of the most powerful tools for imaging surfaces at the Nano-scale. A cantilever with a sharp tip located at its free end, plays a significant role in the AFM performance. The MC dynamic behaviour is very complex and difficult. Therefore, presenting more accurate dynamic models which lead to a simpler and better prediction of the system behaviour is of great importance.
In this regard, utilizing MC with a piezoelectric layer which improves imaging speed and accuracy was first raised by Tortonese et al (Tortonese et al. 1991). Mahmoodi and Jalili investigated piezoelectric MC frequency response in far from the surface with regard to the geometric discontinuity effect (Nima Mahmoodi and Jalili 2007). Wolf and Gutilba analyzed the MC frequency response with an overall piezoelectric layer in the air environment (Wolf and Gottlieb 2002). Mahmoodi et al. analyzed the natural frequency of the MC with a piezoelectric layer based on multi-scale method (Mahmoodi, Daqaq, and Jalili 2009). Song and Bhushan considered the effect of hydrodynamic forces imposed by the liquid to the MC in analyzing the system vibration (Song and Bhushan 2007). Vasquez et al, experimentally investigated the density and viscosity effects of a glycerol solution on the MC frequency responses in the far from the surface (Vazquez et al. 2008).
Furthermore, Naik et al, dealt with experimentally analyzing the MC dynamic response in a liquid environment and in the vicinity of the sample surface(Naik, Longmire, and Mantell 2003). According to the high significance of the sensitivity analysis, there has been a lot of research so far conducted in this regard. Rezazadeh has dealt with the sensitivity analysis of the amplitude and natural frequency based upon the MC's geometric parameters by using the Euler-Bernoulli theory (Razzazade 2013). Lee and Chang studied the flexural vibrations of cracked MC AFM in terms of contact stiffness and tip length (Lee and Chang 2012). Farrokhpayam has studied the flexural vibrations sensitivity of the rectangular MC floated in a liquid environment in terms of the surface stiffness variations based on the Euler-Bernoulli beam theory (Farokh Payam 2013). Korayem and Ghaderi by use of Sobel's sensitivity analysis method investigated the geometric parameters effect and some of the environmental parameters on the first MC natural frequency and amplitude in the noncontact mode (M. H. Korayem and Ghaderi 2013).
It is tried in this study to upgrade the accuracy of MC modelling by considering the rectangular cross-section and the MC shear changes effect by using the Timoshenko's beam theory. Due to the MC modelling, mass, stiffness and damping matrices have been obtained by equations discretization based on Galerkin method. The effect of added mass and hydrodynamic damping on MC's frequency response have been investigated in water environment, and the results have been compared with the experimental results in the air and water.
Finally, Efast sensitivity analysis method has been used to analyse the effect of the parameters such as length, width and thickness of the layers and the coupling effect existing between them on the MC frequency in various vibration modes in the water environment and air. This paper is organized as follows: Section 2 presents governing equation of motion. Section 2.1 briefly presents the discretization of governing equation. Section 2.2 represents frequency response and Newmark algorithm. Simulation results are presented in Section 3 and sensitivity analysis results are explained in Section 4. Section 5 reports the summary and conclusions.

2 MC GOVERNING EQUATION OF MOTION BASED ON THE TIMOSHENKO BEAM THEORY

The AFM piezoelectric MC includes four layers as it is shown in Fig. 1. A silicon MC, piezoelectric layer and two layers of electrode are modelled based on the Timoshenko beam theory by considering the geometric discontinuities.

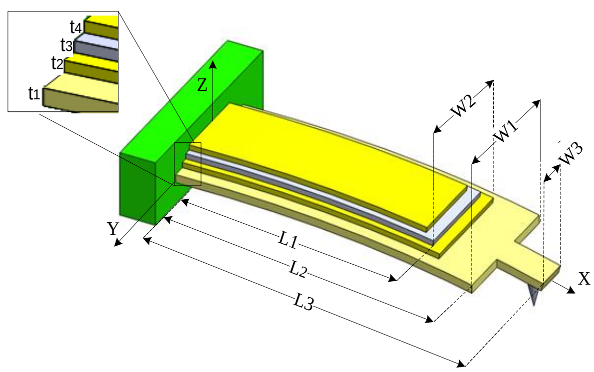

Fig. 1 schematic of AFM non-uniform piezoelectric MC

To extract MC equations of motion, there is made use of Hamilton's Principle. In this regards, the kinetic energy and potential energy for each of the four layers are obtained. It is worth mentioning that the electrical field effects have been taken into consideration for obtaining the potential energy of the piezoelectric layer [14]. The governing equations of motion have been extracted as presented in equation (1) through being influenced by the overall system energy as well as the exertion of external forces and then being put into Hamilton's Principle [15]. In these equations, δ denotes the impact function.

$$\rho I\left(\frac{\partial^2\psi}{\partial t^2}\right)+\left(EI+I_p\left(\frac{e_1e_5}{2\lambda_{33}}+\frac{e_1^2}{\lambda_{33}}\right)\right)\left(\frac{\partial^2\psi}{\partial x^2}\right)+\beta\left(\psi+\frac{\partial w}{\partial x}\right)+I_p\left(\frac{e_1e_5}{4\lambda_{33}}\right)\left(\frac{\partial^3 w}{\partial x^3}\right)+\gamma\delta(x-L_1)=0 \quad (1)$$

$$\rho A\left(\frac{\partial^2 w}{\partial t^2}\right)+\beta\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial\psi}{\partial x}\right)+I_p\left(\frac{e_1e_5}{4\lambda_{33}}\right)\left(\frac{\partial^3\psi}{\partial x^3}\right)+C\left(\frac{\partial w}{\partial t}\right)-F_{ts}(L_3,t)=0 \quad (2)$$

Where:

$\beta = KAG$

$\gamma = e_1.V.W_3.\left(t_1+t_2+\frac{t_3}{2}-z_n\right)$

$w(x,t)$ is the bending displacement, $\psi(x,t)$ is the torsion amount of the cross-section. Also, ρ_i،I،E،e_i،λ ،A،G،V and k are indicative of every layer's density, inertia moment, elasticity modulus, piezoelectric constant, Lame constant, cross-section area, shear modulus , voltage and shear coefficient, respectively, for which a value equal to 0.83 has been obtained regarding the rectangular cross-section. Constant coefficients relevant to each section of piezoelectric MC have been presented in table (1); additionally,e_1, e_5, and λ_{33} are -0.51 C/m^2, -0.45 C/m^2 and -7.88 F/m, respectively.

Table 1 Coefficients of Equation (1) for each section of MC

Beam section	α	η	ρI	β	ρA
$0<x<L_1$	$\sum_{j=1}^{4}\alpha_j$	$\sum_{j=1}^{4}\eta_j$	$\sum_{j=1}^{4}\rho_j I_j$	$\sum_{j=1}^{4}\beta_j$	$\sum_{j=1}^{4}\rho_j A_j$
$L_1<x<L_2$	α_c	η_c	$\rho_c I_c$	β_c	$\rho_c A_c$
$L_2<x<L_3$	α_{tip}	η_{tip}	$\rho_{tip} I_{tip}$	β_{tip}	$\rho_{tip} A_{tip}$

According to the distance between the tip and the sample surface, the external force effect on the MC free end (F_{ts}) which includes the Van der Waals(F_{vdw}), capillary (F_{cap}) and contact force (F_{DMT}) have been shown in equation (3).

$$F_{ts}=\begin{cases}-\dfrac{HR}{6d_{ts}^2} & d_{ts}>d_{on}\\ -\dfrac{HR}{6d_{ts}^2}-\dfrac{4\pi\gamma_w R}{1+\frac{d_{ts}}{h}} & a_0<d_{ts}<d_{off}\\ -\dfrac{HR}{6a_0^2}-\dfrac{4\pi\gamma_w R}{1+\frac{a_0}{h}}+\dfrac{4}{3}E^*\sqrt{R}(a_0-d_{ts})^{\frac{2}{3}} & d_{ts}<a_0\end{cases} \quad (3)$$

In the above equation, H, R, d_{ts}, a_0, E^*, γ_w and h are Hamaker constant, curvature radius of the probe tip, the moment distance of probe tip and sample surface, interatomic distance, effective elastic modulus, surface energy of liquid-steam and water film thickness, respectively.

At the other hand, as a result of the fluid resistance against the MC oscillation, there are other hydrodynamic forces acting which are calculated based on string of spheres model [16]:

$$F_{hyd}=-\left(3\pi\eta+\frac{3}{4}\pi W_1\sqrt{2\eta\rho_{liq}\omega}\right)\frac{dw}{dt}-\left(\frac{1}{12}\pi\rho_{liq}{W_1}^2+\frac{3}{4}\pi W_1\sqrt{\frac{2\eta\rho_{liq}}{\omega}}\right)\frac{d^2w}{dt^2} \quad (4)$$

In this equation, w is the sphere displacement; η is the fluid's viscosity, ρ_{liq} is the fluid density and ω is the fluid's frequency. Besides the hydrodynamic force, when the MC oscillates in the proximity of the sample surface, the squeeze force exerts on the MC and this can be expressed as equation (5) by taking advantage of solving for Reynolds equation [17].

$$F_{squeeze}=-\frac{\eta {W_1}^3}{h(x)^3}\frac{dw}{dt} \quad (5)$$

2.1 DISCRETIZATION OF THE MC GOVERNING EQUATIONS USING GALERKIN METHOD

Considering the finite element method for discretization of equations of motion, the displacement stemming from deflection and the displacement resulting from slope are $\psi(x,t)=\sum_{i=1}^{4}\bar{N}_i(x).p_i(t)$ and $w(x,t)=\sum_{i=1}^{4}N_i(x).p_i(t)$, respectively, where $N_i(x)$ and $\bar{N}_i(x)$ are the space-dependent shape functions and $p_i(t)$ indicates the parameter's vector of time variations [18]. Inserting $w(x,t)$ and $\psi(x,t)$ in Galerkin equation transforms MC equations of motion into ordinary differential equations by considering the general form for liquid environment:

$$(M+M_{add})\ddot{q}+\left(C+C_{add}+C_{squeeze}\right)\dot{q}+Kq=F_{piezo}+F_{ts} \quad (6)$$

Where, M, C and K are indicative of the mass matrix, damping and stiffness of piezoelectric MC and M_{add}, C_{add}, $C_{squeeze}$ present the effect of liquid environment in form of added mass and damping [15]. The total value of which is calculated by making use of a collection of equations presented here in the form of equation (7):

$$M_{add}=\frac{\rho AL}{L^2+12L}\left(\frac{1}{12}\pi\rho_{liq}{W_1}^2+\frac{3}{4}\pi W_1\sqrt{\frac{2\eta\rho_{liq}}{\omega}}\right)\begin{bmatrix} r_{11} & \ddots & & SYM \\ r_{21} & r_{22} & \ddots & \\ r_{31} & r_{32} & r_{33} & \ddots \\ r_{41} & r_{42} & r_{43} & r_{44}\end{bmatrix}$$

$$C_{add}=\frac{\rho AL}{L^2+12L}(3\pi\eta+\frac{3}{4}\pi W_1\sqrt{2\eta\rho_{liq}\omega})\begin{bmatrix} r_{11} & \ddots & & SYM \\ r_{21} & r_{22} & \ddots & \\ r_{31} & r_{32} & r_{33} & \ddots \\ r_{41} & r_{42} & r_{43} & r_{44}\end{bmatrix} \quad (7)$$

$$C_{squeeze}=\eta.\omega^3\int_0^l \frac{N^T(x).N\ (x)}{(D+l+(L_3-x)Sin(\alpha))^3}dx$$

2.2 VIBRATION RESPONSE OF THE MC

To calculate the frequency response by Laplace transforms we have:

$$L\{q_I(\omega)\}=\frac{L\{F(\mathrm{j}\omega)\}}{-\omega^2.M+K+j\omega C} \quad (8)$$

In addition, the system time response can be calculated according to the Newmark algorithm as Eq. (9).

$$p_{liq}(t+\Delta t)=[\tilde{K}]^{-1}\{F_{eff}(t+\Delta t)\}$$

$$[\tilde{K}]=\frac{4}{\Delta t^2}[M+M_{add}]+\frac{2}{\Delta t}[C+C_{add}+C_{squeeze}]+[K]$$

$$F_{eff}(t+\Delta t)=\{F_{ts}(t+\Delta t)\}+[M+M_{add}](\ddot{p}(t)+\frac{4}{\Delta t}\{\dot{p}(t)\}$$
$$+\frac{4}{\Delta t^2}\{p(t)\})+[C+C_{add}+C_{squeeze}]\left(\{\dot{p}(t)\}+\frac{2}{\Delta t}\{\dot{p}(t)\}\right) \quad (9)$$

Table 2 Geometric constants for simulation of the rectangular MC [2]

Parameter	Material	*L*	*W*	*t*	*ρ*	*E*
Unit	–	*(μm)*	*(μm)*	*(μm)*	*(kg/m³)*	*(Gpa)*
Cantilever	Si	375	250	3.5	2330	105
Lower electrode	Au	330	130	0.25	19300	78
Piezoelectric	ZnO	330	130	3.5	6390	104
Upper electrode	Au	330	130	0.25	19300	78
Tip	Si	125	55	3.5	2330	105

Simulations in this paper are examined according to the constants in Table 2 for studying according to piezoelectric MC topography in tapping and non-contact modes taking into account the forces between the sample surface and the probe as the following:

3 PIEZOELECTRIC NON-UNIFORM SIMULATION

As the MC is in a far distance from the surface, no force is exerted on the probe and the force resulted from the piezoelectric voltage is the only effective force in vibrations at the air environment and at the liquid, the cantilever is affected by the hydrodynamic force. In this section, the frequency responses are simulated in the mode of being away from the surface and the results are compared. Table 3 presents the simulation results based on Euler-Bernoulli beam and Timoshenko theories compering experimental results [2] in the air environment:

Table 3 Comparing the frequency response in the air with the experimental result [2] and the Euler- Bernoulli beam theory [19]

Frequency	Euler (kHz)	Timoshenko (kHz)	Experiment (kHz)	Error percentage	
				Euler	Timoshenko
1st	52.377	52.291	52.30	0.14 %	0.017%
2nd	203.414	203.075	203.0	0.20 %	0.03%
3rd	392.375	391.632	382.5	2.5 %	2.3%

As can be seen, the results of modelling using Timoshenko beam theory has a better agreement with the experimental results and the error percentage of the Timoshenko beam to Euler-Bernoulli beam is less in all the three natural frequencies. Figure (2) illustrates the piezoelectric MC frequency response in the water and far from the surface. The first natural frequency including the experimental results [7] and the simulation results are presented in table (4) based on the Euler-Bernoulli [20] and Timoshenko beam theory.
The first natural frequency is 16.36 kHz corresponding to the experimental results and the value obtained based on the Euler-Bernoulli beam theory is 16.39 kHz with an error percentage of 0.18%. As it is observed, with an error level of 0.06%, the results obtained from the

Timoshenko beam theory show an improvement in the results and enhancement in the simulation precision.

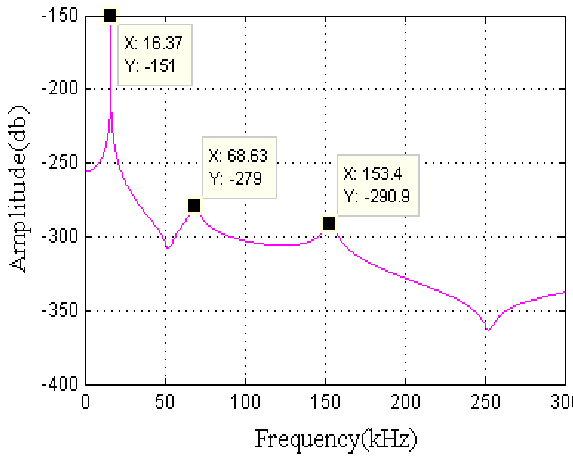

Fig. 2 Frequency response of the piezoelectric MC in the water

Table 4 Comparing the simulation results for the first natural frequency with the experimental results

First natural frequency (kHz)				
Timoshenko		Euler-Bernoulli		experiment
Error	result	Error	result	result
0.06%	16.37	0.18%	16.39	16.36

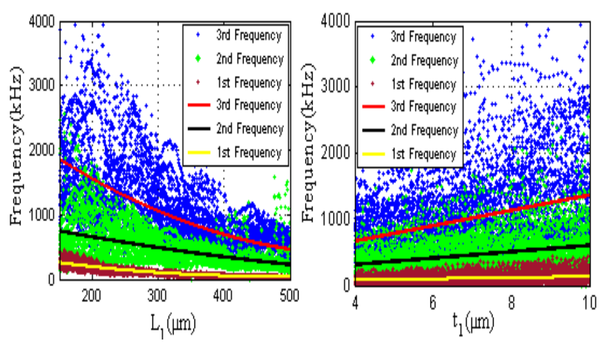

Fig. 3 The effect of the first section length, tip length and the MC thickness on the frequency

3.1 SENSITIVITY ANALYSIS

Sensitivity analysis is performing studies so as to define how it is possible to change a value of a parameter and then evaluate the effect it may exert on the model's output parameters. Efast method has been used to analyse sensitivity in the present study that is a variance-based method and it can take the interactive effects of the parameters into consideration [21]. In liquid environment, the first three natural frequencies of the MC have undergone sensitivity analysis and the effect rate of nine geometrical parameters of the beam has been investigated including, the first part length (L_1), the middle part length of the cantilever ($L_2 - L_1$), tip length ($L_3 - L_2$), thickness and width of the piezoelectric layer, cantilever and electrodes. Figure (3) illustrates the effects of the first length part of the MC, and the MC thickness as two influential factors affecting the natural frequency in the water.

As it is observed, with the increase in length, the frequency is reduced that in the first vibration mode, the curve variations gradient is higher for the first part and in the higher vibration modes, the tip curve gradient is increased. Also, since the MC's stiffness increases in line with the increase in its thickness, the natural frequency is also increased and the results are indicative of the higher natural frequencies' sensitivities to MC thickness changes. In Fig. 4, the results obtained from sensitivity analysis using Efast method for the first mode in the air environment have been shown. The results are indicative of the frequency sensitivity percentage of each geometrical parameter.

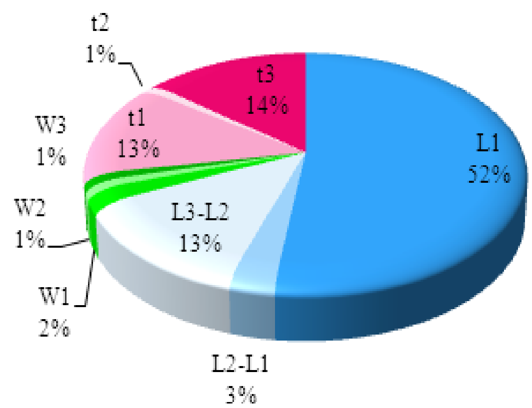

Fig. 4 Sensitivity percentage of the first natural frequency to the MC geometric parameters in the air by using Efast method

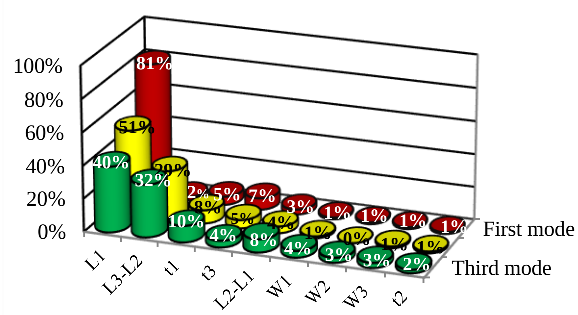

Fig. 5 Sensitivity percentage of the first three natural frequencies to the MC geometric parameters in the water by using Efast method

Also Fig. 5 shows the sensitivity analysis results regarding the first three natural frequencies of the MC in the water environment. As it is observed, the most effective parameter is the MC's first length part; and the layers' width as well as the electrodes' thickness do not have a considerable effect on frequency in the both environment.
Furthermore, it is observed that in higher vibration modes, the effect of the first length part is reduced and the effects of the other two parts of the length are increased. Comparing the results obtained herein with the results attained for the sensitivity analysis in air, it can be seen that the length effect in respect to air is higher regarding the three vibration modes [15].

5 CONCLUSION

The study and prediction of the piezoelectric MCs' vibration behaviour entail precise modelling thereof. To do so, the piezoelectric MC has been modelled based on Timoshenko's beam theory and through applying Hamilton's principle in the form of a four layer MC. To analyse the system's performance, frequency response has been investigated based on finite element method in the air and water environment by considering the effect of the tip-sample and environmental forces. To validate the results, the frequency response subject to different work environments has been compared with the experimental results.
The results indicate that the simulation results highly match the experimental results and this is reflective of a reduction in the error percentage by 0.12% in water in comparison to Euler-Bernoulli theory. In the air, it is shown that modelling based on the Timoshenko beam theory, by considering the effects caused by shearing, have led to the improvement of the results too. Also the reduction in the frequency in the water because of the environmental forces is clearly shown. The results obtained from sensitivity analysis also illustrate that most effective parameters on the natural frequency is the length and the least effective one is the width of the layers. In the first frequency, the length of the first part of the MC is the most effective parameter and in higher frequencies, the maximum effect belongs to the tip length.

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