Investigation of piezoelectric microcantilever performance in constant amplitude mode in different work environments

Adel Mohammadi*, Moharam Habibnejad Korayem, and Reza Ghaderi

Robotic Research Laboratory, Center of Excellence in Experimental Solid Mechanics and Dynamics, School of Mechanical Engineering, Iran University of Science and Technology, Tehran, Iran

Received: 29 June 2016 / Accepted: 28 February 2017

Abstract. Vibration frequency and amplitude are major issues in the operation of atomic force microscopes (AFMs), since the slightest variation in amplitude and resonance frequency, changes application type of AFM quickly. Using finite element software does not apply any kind of simplifications on the geometric shape and it has less errors (compared to cases occurred in analytical calculations). In this paper, a novel simulation method based on finite element method software (ABAQUS) is developed for simulation of oscillatory and sensor behaviour of AFM of the piezoelectric microcantilever type in air and water, with different geometrical arrangements. Since the resonance frequency and amplitude are main parameters in the operation of the microscopes, the simulations will be based on these two parameters. The carried out modelling and simulation are done using the quality (Q) factor in air and, also simulation in fluid environment is done by real computational fluid dynamic and according to fluid–structure interaction. Transient and frequency response of the AFMs of single-layer and double-layer (parallel and series) piezoelectric are simulated in different conditions, and energy harvesting of this structures is compared to each other. Simulation results demonstrate the effectiveness of proposed method in reducing vibration and measurement precision in various environments.

Keywords: atomic force microscopes / computational fluid dynamic / fluid–structure interaction / microcantilever / vibration

1 Introduction

Atomic force microscope (AFM) is a tool used for nano-level evaluation, investigation for the structure of materials surface in nanometre scale precision, force measurement between molecules directly in atomic precision and nanometre scale and study of polymeric materials and biomaterials[1–4]. Laser light is widely used in detection of microcantilever (MC) oscillations [5]. The idea of AFMs downsize caused piezoresistive can be used instead of laser light detectors [6,7]. The main disadvantage of this kind of AFMs was low speed of sample imaging. Faster operation, increased accuracy, possibility of downsizing and utilizing multiple parallel microcantilever led to the idea of microcantilever with piezoelectric layer [8–10].

An application of piezoelectric microcantilever attracting many attentions recently is in energy harvesting fields [11–13]. Study of its dynamic behaviour (especially in fluid for specific condition) and prediction of its behaviour is completely necessary. In AFM, when the rate and quality of imaging are relative to microcantilever vibration, then investigation of frequency and amplitude of vibration is of great importance.

Vázquez et al. [14] studied application of AFMs in chemical and biological fields. They analysed the effect of density and various concentrations of water-glycerol mixture on vibrations of cantilever in these environments. They compared the mode shapes and obtained the resonance frequencies in non-viscous liquid by the simulation software. Tung et al. [15] investigated the effects of hydrodynamic forces on oscillating of the MC used in AFM or RF switches. They presented a compact formula of the hydrodynamic forces and vibration amplitude of the microcantilever near the wall surface by advancement of the previous works (using dimensionless parameters) and verified their results by computer simulation. They used ADINA software in their simulations. Baek et al. [16] investigated application of cantilever in ultrasonic energy production and destruction of blood clots leading to brain death. They observed, with vibrations of the MC in liquid near the resonance frequency, ultrasonic energy is produced as well as it can destroy these clots in a split second. They used COSMOL simulation software and
started simulation for the analysis of oscillating behaviour and to verify their calculations. Kiracofe and Roman [17] compared imaging of AFMs in the first and second modes. They proved that use of a higher mode causes resolution of surface imaging and topography increases in this type of microscopes. To do this, the dynamics and dissipative energy of the cantilever when crossing a sample in liquid were examined and showed that resolution increases in the second mode. Salehi-Khojin et al. [18] modelled piezoelectric MC by considering its geometric discontinuity. Unlike previous researches, which modelled the beam continuously, they modelled its discontinuous structure and showed that the previous assumed continuous models do not accurately predict the vibrational behaviour of piezoelectric MC. They compared the obtained relationships with the laboratory data and software simulations in order to obtain mode shapes of piezoelectric MC. Mahmoodi and Jalili [19] investigated non-linear vibrations of piezoelectric MC. Mechanical and electrical connections in piezoelectric material and non-linear geometry of this type of MC cause non-linear parameters in the modelling equations. Computer simulation was used in order to analyse the frequencies and non-linear vibration.

In analytical calculations, simplifications are usually done in order to solve the equations or even to obtain equations (simplifications in geometric shape of the sample or even regardless of higher degree equations in obtained equations) which themselves cause getting far from the real environment [20,21]. The laboratory works [22] require high cost and also the lab instruments may not be appropriate. Use of finite element software does not apply any kind of simplifications on the geometric shape and it has less errors (compared to cases occurred in analytical calculations). Qiu et al. [22] experimentally studied the hydrodynamic loading effect on a flexural vibrating microcantilever, which was immersed in six different viscous compressible gases. Their results demonstrated that resonance frequency of all flexural modes mainly depended on the density of the gas, and that it was almost independent from the fluid’s compressibility.

The researches that have been carried out in liquid have been in the form of geometrical simplification (in form of integration of discontinuities of the beam) or in low density and concentration of the fluid and no analysis has been practically done for the piezoelectric MC with real dimensions, floated in the fluid with actual concentration of water in form of fluid–structure interaction (FSI). This was due to that other types of software are not able to converge because of weaknesses in non-linear analysis and the analysis is rapidly diverged. Due to this issue, previous studies, which focus on simulation in the field of FSI are restricted.

In this paper, at the first step, the free vibrations in vacuum and air are analysed to obtain the first three mode shapes. Then the vibrations in the liquid are analysed and effects of different states toward the wall surface and different geometries of piezoelectric MC on resonance frequency and vibration amplitude are evaluated. The impulse response and fast Fourier transform (FFT) ideas are used in order to obtain frequency response that causes increase of accuracy and saving time and money especially in liquid. Finally, vibrational and sensor motions of different piezoelectric MC structures (monolayer, parallel and piecewise) are studied and their simulations are compared with each other.

### 2 Simulation of monolayer piezoelectric microcantilever

The carried out modelling is based on the experimental model which Mahmoodi [23] has used in his researches. Particulars of this microcantilever have been mentioned in Table 1 and its software modelling is shown in Figure 1.

This modelling (Fig. 1) includes real geometry structure, size and property that has been fixed in the end of beam and used merge operator beside of tie interaction between piezoelectric and microcantilever for faster converging. This model has been meshed by three-
2.1 The air environment modelling

In ABAQUS microcantilever modelling in air condition, the effects of air damping are considered and applied in the equivalent damping, by using $Q$ factor. Figure 3 shows frequency response of piezoelectric MC in air which actuated with 0.5 V. Frequency response of this simulation is similar to its experimental sample that Mahmoodi [19] used it in laboratory with same condition. This work has 2.6% error in frequency and 6% error in amplitude in comparison to its experimental sample.

In nanometric distances from the wall, a force is applied on the tip of microcantilever which is modelled by applying a non-linear spring on tip of the microcantilever. Figure 4 symbolically shows the size and changes of interaction force between tip and sample surface in different distances between them. Directions of the arrows show that tip is getting closer (forward) or farther (backward) from the sample surface.

The surface scanning procedure by the needles should be in a way that the surface gets the least damages in order to obtain the highest accuracy. The interaction forces between tip and surface include long-range and short-range forces. Van der Waals, electrostatic and magnetic forces are long-range forces. Among interaction forces, Van der Waals forces are present in all experiments. Van der Waals force is attraction force between polar molecules and is proportional to $r^{-6}$. The short-range forces include adhesive force, elasticity quantum force (due to unwillingness of electron cloud of the molecules to full compliance) and covalent forces.

According to performance area of the tip, AFM modes are divided into three general categories of the contact mode (almost closer than 5 Å), semi-contact mode (tapping mode, between 4 and 30 Å) and non-contact (between 30 and 150 Å). The operation mode in the present article is of non-contact type. This force is expressed as equation (1), based on the model of Lennard–Jones [25].

$$f_{ts} = \frac{HR}{6\pi^2} \left[ \frac{1}{30}(\frac{\xi}{Z})^8 - \left(\frac{\xi}{Z}\right)^2 \right].$$

In above equation, the forces, respectively, include $f_{ts}$ (the force between needle and surface of the sample), $H$ (Hemker’s constant), $r$ (tip radius of the sample), $\xi$ (atomic size) and $z$ (atomic distance of the sample). This force is modelled by a non-linear spring at the end of microcantilever.

First, by voltage regulation, the free vibration amplitude voltage is set on 2 nm. By changes in the voltage, it is found that with 0.0021 V, it reaches an amplitude of 2.025 nm. Now, we bring the piezoelectric MC to a 3 nm distance from the wall. The non-linear spring in ABAQUS software should be entered into the software in code in keyword part, so that, the non-linear spring is modelled for the software. With-spring mode implies that microcantilever is approaching the wall (in distance of 3 nm) and without-spring mode shows free vibrations away from the sample surface (Fig. 5).

As mentioned earlier, amplitude of 2.025 nm was regulated with change of voltage that after placing the spring (that implies getting close to the sample surface up to a distance of 3 nm), the highest vibration point is 1.62 nm and the lowest point is 1.86 nm that in fact, the vibration amplitude after approaching to the sample surface is averagely 1.74 nm. Results of this simulation show that vibrations of the piezoelectric MC are decreased near the surface up to 0.285 nm (Fig. 5).

2.2 The liquid environment modelling

In liquid modelling usually the equivalent damper is used, whereas in this paper a novel approach based on FSI analysis for simulation of piezoelectric MC in ABAQUS software is developed. Unlike previous modelling, this article has used an actual fluid model instead of damper in this modelling. Since influence of the fluid on microcantilever is non-linear, making it equivalent to the damper or the linear spring causes errors in calculation and reduces accuracy of the simulations. Methodology of this topic will be discussed in details later.

A defect of ABAQUS FSI analysis or other types of finite element software is that it is not able to obtain resonance frequency. So, these types of software were used to be coupled with another computational fluid dynamic (CFD) software or by replacing a damper or an equivalent linear-spring with the fluid, they did not use FSI analysis anymore. But in this article, impulse response and FFT ideas are used in MATLAB to obtain frequency response that causes increase of accuracy and saving time and money especially in liquid. In this idea, by giving a voltage pulse to the piezoelectric, its time response is transferred to MATLAB software and its FFT is calculated. All of the mentioned stages will be presented with pictures in this section. Figure 6 shows CFD and piezoelectric MC models.
used in FSI simulation. For reducing the time and improving the efficiency of solver, smart mesh for fluid is used manually. In the meshing, all model nodes are piezoelectric micro-cantilever model, and fluid in Cartesian space and all elements are in the cubic shape. Fluid model meshing is arranged according to the uniform linear FC3D8 (an 8-node linear fluid brick, number elements: 948, nodes 1335 manually).

In earlier works, fluid was modelled as a spring or damper on structure environment that would cause inaccuracies in the response time of laboratory samples. Whereas in the proposed model in the current study, the fluid environment is modelled in the ABAQUS/CFD, and the effects of fluid on vibration of cantilever by coupling the fluid model with the piezoelectric MC structure model, are investigated. For the simulation of free vibration in the regions far from the
boundaries in the laminar flow, the CFD model is considered for solver. While approaching to the boundaries, the flow changes to turbulent due to reflection of flow, the turbulent flow for the step solver is proposed.

Now, we give to the piezoelectric a voltage pulse that its transient response is in form of Figure 7.

By transferring this test’s impulse response to MATLAB and calculating FFT, a frequency of 16 635 Hz is obtained. Figure 8 shows the FFT obtained from impulse test response.

Comparing this simulation with Vázquez’s experimental data [1], it was found that there is an error in frequency of 1.3% (frequency of 16 635 Hz compared to experimental data of 16 400 Hz [1]). Figure 9 is obtained by stimulating the model with frequency of 16 635 Hz. We conclude from Figure 9 that, simulation in amplitude of 3.6% has some errors (0.81 nm compared to the experimental data of 0.84 nm [1]).

As observed in Figure 9, increase of amplitude and ultimately its balance on 0.003 s (without reduction of vibration amplitude) implies authenticity of the collection’s stimulation in resonance frequency.

One of the important issues in simulation of piezoelectric MC forced vibrations near the wall surface inside the liquid is to consider the flows returned from the wall and their effects on vibrations of the collection which need a correct fluid model with wall boundary conditions. In order to verify the correct boundary conditions of the wall and to ensure about presence of the flows returned from the wall and their effects on microcantilever vibrations, first the microcantilever is simulated a micrometer away from the wall surface. In this distance, attraction (or repulsion) non-linear forces do not affect the vibrations of microcantilever and the only effective factors of changes of vibration amplitude are the flows returned from the wall. Effects of the return flows on vibration amplitude are expected to be more in closer distances and the disturbance effects of these flows on the vibrations are gradually reduced by getting farther from the wall. As observed in Figure 10, in a distance of 20 and 30 μm from the vibration disturbance until reaching the balance amplitude, there is disturbance in the variations that are reduced by getting farther from the wall and also the amplitude is gradually increased. Figure 11 shows diagram of tip distance from the wall and vibration amplitude of the MC.

Figures 10 and 11 indicate presence of the return flows (caused by fluid model despite the wall boundary condition) very well that ensures us about considering and observing the effects of fluid flows in evaluation of the vibrations near the wall surface in liquid. After being ensured about model’s validity, in terms of having wall boundary conditions, we take it to a 3 nm distance from the wall in which the water is intensely turbulent and should be considered in the fluid model status. Also, like the simulation in air, in this environment and distance the non-linear attractions are entered into the microcantilever’s tip. This force is modelled with the non-linear spring again.

To do so, the amplitude is raised to nm by changing the amplitude voltage again and then by bringing it to the sample surface, its changes are observed. The amplitude reaches up to 2.031 nm by a voltage of 0.009 V that, by approaching the surface we put the non-linear spring on tip of the microcantilever and also, the meshing type is changed too because of divergence. Figure 12 shows changes of the model type and fluid meshing (free element-FC3D4). It should be considered that in determination of boundary conditions of this model the underlying plate of the wall model has been introduced and Figure 13 shows a comparison of the free vibration mode with microcantilever vibration in a 3 nm distance from the wall.

Decrease of vibration near the wall is obviously observed in Figure 13. The highest point in vibration near the wall is 1.4 nm and the lowest point is 1.67 nm; thus, the
vibration amplitude in the 3 nm distance from the wall has been obtained 1.535 nm (24% vibration decrease compared to free vibrations).

3 Simulation of other structures of piezoelectric microcantilever

Existence of issues like application of various types of microcantilever mode shape or the energy harvesting issue in energy production that has attracted lots of attentions recently have led to investigations in other structures of microcantilever. We will examine vibrations of the dual-layer piezoelectric MC and the piecewise piezoelectric MC and efficiency of these two structures in producing the output voltage.

3.1 Dual-layer piezoelectric microcantilever

This model includes two piezoelectrics which are placed in parallel on each other. For examining this type of structure, we stimulate only one of them respectively and study its time response. Figure 14 shows this model.

First, with a voltage of 0.008 V the upper piezoelectric plate (at this second the lower plate is neutral) and then the lower plate (at this second the upper plate is neutral) are stimulated. Figure 15 shows the time response of these two stimulations in resonance frequency of the collection.

As observed in Figure 15, in an equal voltage, the dual layer piezoelectric MC has 28% decrease in vibration amplitude by stimulating the lower plate compared to the vibrations from stimulating the upper plate.

In study of the vibrations near the surface, like monolayer piezoelectric MC, in this section the non-linear spring should be entered into the bottom of the microcantilever (instead of non-linear attraction) in code. Figure 16 shows the vibrations within a distance of 3 nm. Like the free vibrations, first the upper plate and in the next stage the lower plate is stimulated. For a better comparison, first the amplitude voltage change should be raised to 2 nm and in the next stage, the nanometre spring which shows proximity to the 3 nm distance from the surface is placed.

Considering Figure 16, amplitude in a voltage of 0.007 V reaches to amplitude of 1.9 nm by stimulating the top layer. But after approaching the surface (placing the spring), the amplitude reaches to 1.469 nm (average of the highest vibration point of 1.58 nm with the lowest point of 1.358 nm); namely, the amplitude is reduced about 23% and stimulation of the bottom layer in proximity of the amplitude surface reaches to 1.535 nm (that the average highest point in vibration near the surface reaches to 1.42 nm and the lower point reaches to 1.65 nm, the amplitude decreases to 29%).

Another important application of piezoelectric MC structures is the great attention they have attracted to themselves in field of applying these structures in energy harvest ground. Figure 17 shows the output voltage obtained from piezoelectric compared to the input voltage in different modes of stimulation.

As observed in Figure 17, the obtained output voltage is 45.392 times more than the input voltage in stimulation mode of the upper piezoelectric layer and 15.66 times in stimulation mode of the lower layer (stimulation voltage). In fact, it is concluded that in a specified voltage, efficiency of electrical power generation in stimulation of the upper layer of dual-layer piezoelectric is 2.9 times more than stimulation of the lower layer of the dual-layer piezoelectric MC.

3.2 Piecewise piezoelectric microcantilever

Microcantilever of this section has also two piezoelectrics but unlike the previous section in which the piezoelectrics were placed on each other in parallel, in this structure these
two piezoelectrics are placed along the microcantilever in a row (series). Figure 18 shows software modelling of this structure type. Figure 19 presents software simulation of this structure with a voltage of 0.007 V. In simulation of this model, initially the first piezoelectric layer (while the second layer is neutral) and in next stage, unlike the previous one, the second piezoelectric layer is stimulated (in this stage the first piezoelectric is neutral).

According to Figure 19, the vibration amplitude in stimulation mode of the second piezoelectric is 0.3 nm. As it can be observed, in the same voltage, stimulation of the first piezoelectric (the one connected to the fixed support) has a significant amplitude increase compared to stimulation of the second piezoelectric (the free piezoelectric not attached to the fixed support). In fact, in the second mode (stimulation of the second piezoelectric) compared to the first mode (stimulation of the first piezoelectric) we observe a 90% reduction in vibration amplitude.

The same as the structure of piezoelectric MC, output current of the voltage is measured by stimulation in different modes. Figure 20 shows the output voltage compared to the input voltage (actuated voltage) for different stimulation modes of piecewise piezoelectric MC.

As it can be observed in Figure 20, the obtained voltage output in stimulation mode of the first piezoelectric layer is 208.47 and in stimulation mode of the second one it is 68.232 times more than the input voltage (stimulation voltage). In fact it is concluded that in a specified voltage, efficiency of electrical power generation in stimulation of the first piezoelectric is three times more than stimulation of the second piezoelectric. Comparing Figure 20 with Figure 17, it can be observed that in a specified voltage, the highest voltage that can be obtained from piecewise piezoelectric MC is 4.6 times more than the voltage that can be received from dual-layer piezoelectric.

4 The sensor mode of piezoelectric microcantilever

In recent decades, application and performance of the sensor mode have been highly considered. Displacement of the piezoelectrics causes voltage generation in them. This property causes them to be used as sensors in addition to being used as stimulating factors. This characteristic has a wide application in minimizing and accelerating AFMs and other components in field of MEMS. Figure 21 is an example of vibration detection by piezoelectric, applied in AFMs.

As it can be observed in Figure 21, there are similarities between the time response of the free vibrations and the output voltage (obtained from last connection point of piezoelectric to the fulcrum). Another advantage of sensor mode which is important in field of energy and MEMS is changes of output voltage based on variations of the amplitude in different modes and structures of piezoelectric MC. Figure 22 shows changes of output voltage of piezoelectric in different modes and structures.

As it can be observed in Figure 22, in the same amplitudes, the highest output voltage belongs to dual-layer piezoelectric MC and the lowest output voltage belongs to mono-layer piezoelectric MC. Amount of the output voltage in a fixed amplitude for dual-layer piezoelectric MC is 2.6 times more than the piecewise piezoelectric MC and 40 times more than the monolayer piezoelectric MC.
5 Conclusion

The main objective of this paper was to perform a dynamic and sensor analysis of piezoelectric MC in different conditions. Modelling of the piezoelectric MC was conducted by real dimensions and geometries of laboratory sample that air effects on model oscillator were applied by Q factor and equivalent damping and liquid effects were applied by real water CFD modelling and FSI analysis. The CFD modelling including laminar flow in the free vibration and turbulent flow in forced vibration has been meshed by FC3D8 elements. The frequency response was obtained by steady-state dynamic, direct analysis in ABAQUS step in the air environment and impulse test and FFT in the liquid environment. Dynamic analysis was simulated by dynamic implicit step by applying AC voltage with resonance frequency to the piezoelectric layer in the both environments. In the sensor mode of piezoelectric MC, a node of the piezoelectric producing the most voltage by oscillation (fixed nodes of the end of beam) was investigated. The obtained results in this paper are respectively expressed as follows:

- resonance frequency of 57 000 Hz in the air for the first mode,
- 14% reduction in vibration amplitude near the surface in air environment,
resonance frequency of 16,635 Hz in liquid environment for the first mode,
- 24% decrease in vibration amplitude near the surface in liquid environment,
- 28% increase in vibration amplitude by stimulation of the upper layer in piezoelectric MC with two parallel layers,
- 23% decrease in vibration amplitude near the surface for the dual-layer piezoelectric MC with top layer actuated,
– 29% decrease in vibration amplitude near the surface for the dual-layer piezoelectric MC with bottom layer actuated,
– the output voltage stimulation of upper layer of dual-layer piezoelectric in similar voltage is 3 times more than stimulation of the lower piezoelectric layer in dual-layer piezoelectric MC,
– 91% decrease in vibration amplitude by stimulation of the second piezoelectric plate in the piecewise piezoelectric MC,
– the output voltage in the first piezoelectric stimulation mode is 3 times more than stimulation of the second piezoelectric layer for piecewise piezoelectric MC in a similar input voltage,
– the maximum received output voltage in piecewise piezoelectric is 4.6 times more than the maximum output voltage of the dual-layer piezoelectric MC in similar stimulation voltage.
– having the maximum output voltage in dual-layer piezoelectric MC compared to other structures in equal stimulation amplitudes.

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Cite this article as: A. Mohammadi, M.H. Korayem, R. Ghaderi, Investigation of piezoelectric microcantilever performance in constant amplitude mode in different work environments, Mechanics & Industry 18, 504 (2017)