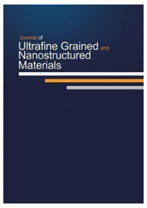

Journal of Ultrafine Grained and Nanostructured Materials
https://jufgnsm.ut.ac.ir
Vol. 50, No.2, December 2017, pp. 117-123
Print ISSN: 2423-6845   Online ISSN: 2423-6837
DOI: 10.22059/JUFGNSM.2017.02.06

Effects of Fluid Environment Properties on the Nonlinear Vibrations of AFM Piezoelectric Microcantilevers

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Recieved: 10 June 2017;   Accepted: 24 November 2017

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ABSTRACT

Nowadays, atomic-force microscopy plays a significant role in nanoscience and nanotechnology, and is widely used for direct measurement at atomic scale and scanning the sample surfaces. In tapping mode, the microcantilever of atomic-force microscope is excited at resonance frequency. Therefore, it is important to study its resonance. Moreover, atomic-force microscopes can be operated in fluid environments such as their applications in chemical and biological sensors. Additionally, piezoelectric microcantilevers are used to enhance atomic-force microscope scanning. Motivated by these considerations, presented herein is a finite element investigation into the nonlinear vibration behavior of piezoelectric microcantilever of atomic-force microscopes in fluid environment. For this purpose, a 3D finite element model coupled with a computational fluid dynamics model is introduced based upon a fluid-solid interaction analysis. First, the reliability of present fluid-solid interaction analysis is revealed by comparison with experimental data available in the literature. Then, numerical results are presented to study the influences of fluid dynamic viscosity and density on the resonance frequency, resonance amplitude and time response of piezoelectric microcantilever. It was shown that increasing the fluid density and dynamic viscosity results in the decrease of resonance frequency. For example, for density equal to 1000 kg/m^3, increasing the viscosity of fluid environment from 0.1 to 1, 10 and 20 mPa.s leads to decrease of resonance frequency about 3%, 29% and 42%, respectively. Also, the resonance amplitude of microcantilever increases as the density increases, while increasing dynamic viscosity has a decreasing effect on the resonance amplitude.

Keywords: *Piezoelectric microcantilever; Atomic-force microscopy; Nonlinear vibration; Fluid-solid interaction analysis.*

How to cite this article:
Ahmadi M, Ansari R, Darvizeh M, Rouhi H. Effects of fluid environment properties on the nonlinear vibrations of AFM piezoelectric microcantilevers . J Ultrafine Grained Nanostruct Mater, 2017; 50(2):117-123.

1. Introduction

Since the invention of the atomic-force microscopy (AFM) [1], the field of scanning probe microscopy (SPM) has been revolutionized by interatomic forces for imaging topography on the order of fractions of a nanometer. Also, the capabilities of AFM (force measurement, imaging and manipulation) have accelerated the development of nanoscience and nanotechnology. AFM can be efficiently used to scan surfaces at nanoscale and it is able to provide images with high resolution [2-5]. This advantageous tool has wide-ranging applications in different disciplines such as medicine, solid-state physics, molecular engineering, surface chemistry, molecular biology and cell biology [6-14].

AFM has a microcantilever (MC) with a probe to scan the sample surface. MC's tip radius of curvature is on the order of nanometers. As the probe (MC's tip) approaches the sample surface, MC is deflected due to tip-sample forces including van der Waals (vdW) forces, mechanical contact force, Casimir forces, electrostatic forces, etc.

Previous results have proved that utilizing piezoelectric MCs in AFM improves the performance of AFM resulting in better sensing and faster scanning [15-19]. Piezoelectric MCs also make energy consumption about a quarter. Moreover, they can be used as actuator or sensor owing to their good sensitivity.

Depending on the application, AFM can work in several modes. Generally, the imaging modes of AFM can be classified into two main categories: static or contact modes and dynamic or non-contact or tapping modes. In tapping modes, the MC is vibrated at resonance frequencies [20-24]. Accordingly, studying the vibrational response of AFM's MC is among the important research topics [25-31].

AFM can be used in both air and liquid environments [32-34]. For example, one can mention the potential applications of piezoelectric MCs in the field of chemical or biological sensors. In this regard, there are a number of papers on the behaviors of MCs in air and liquid environments [35-40]. Among them, the following ones can be cited. Song and Bhushan [25] employed the finite element method (FEM) in order to study the tapping mode in AFM and transient response in air and liquid phases. They added additional mass and hydrodynamic damping to consider hydrodynamic effects. Bonaccurso et al. [35] performed experimental tests on AFM working in Newtonian and non-Newtonian liquids. Rankl et al. [38] investigated the frequency response of a magnetically driven AFM microcantilever close to a sample surface in liquids. Using laser Doppler vibrometry, Vazquez et al. [40] studied the density and viscosity effects of different water and glycerol mixtures on the vibration behavior of a commercial piezoelectric MC probe.

A literature review shows that there is lack of a detailed parametric investigation into the effects of density and viscosity of fluid on the vibrational behavior of AFM in the liquid environment. Considering the application of AFM in different liquid environments, the influences of those parameters on the nonlinear vibration behavior of piezoelectric AFM were studied in the present paper based on FEM. A three-dimensional finite element model coupled with a computational fluid dynamics (CFD) model was proposed in the context of a fluid-solid interaction (FSI) analysis. In the first step, the results were validated using the experimental results of Vazquez et al. [40]. In the next step, the effects of variation of dynamic viscosity (at a fixed density) and variation of density (at a fixed dynamic viscosity) on the vibration characteristics of AFM were analyzed. It should be remarked that such a parametric study cannot be performed experimentally, and the results of present simulation study might be helpful to design AFM operating in liquid environments.

2. Finite element modeling

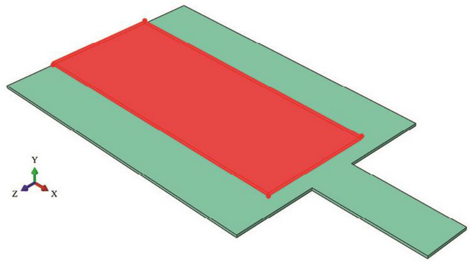
An AFM microcantilever with piezoelectric layer tied to its top surface is considered. The DMASP microcantilever made by Bruker Corporation is chosen for the simulation whose properties are listed in Table 1. In this table, h, b, l, E and ρ denote thickness, width, length, elastic modulus and density, respectively. The beam section and piezoelectric layer are made from silicon and ZnO materials.

The 3D finite element model of microcantilever is shown in Fig. 1. The cantilever is meshed by 20-node quadratic brick elements, and the piezoelectric layer is meshed by 20-node quadratic piezoelectric brick elements. Also, in order to model the fluid by CFD, a cube with the microcantilever cut out of the

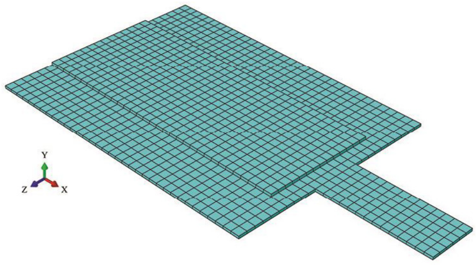
Table 1- Properties of piezoelectric MC [41]

	h (μm)	b (μm)	l (μm)	E (Gpa)	ρ (kg/m^3)
Microcantilever base	3.0	250	350	180	2330
Piezoelectric layer	3.4	130	330	130	6390
Tip	3.0	55	137	180	2330

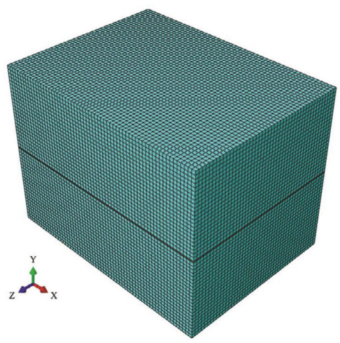
middle is considered and meshed with 8-node linear fluid brick elements (Fig. 1). Both FEM and CFD parts of the FSI simulations are performed using the ABAQUS software through a co-simulation considering the geometrically nonlinear effects. A dynamic implicit solver and a flow solver are employed in the FEM and CFD parts, respectively. The connection between the fluid part and the solid part is made using a fluid-structure co-simulation boundary in ABAQUS. The FSI simulations are performed using an arbitrary Lagrangian-Eulerian (ALE) methodology for the fluid flow, and some portion of the fluid domain is deformed consistent with a boundary motion.



(a)



(b)



(c)

Fig. 1- (a) 3D finite element model of AFM piezoelectric microcantilever, (b) meshed instance of piezoelectric microcantilever, (c) meshed instance of fluid environment.

As it was mentioned earlier, in order to model the fluid by CFD, a box with the microcantilever cut out of the middle is considered. The size of the liquid box is considered as 600 $\mu m \times 600\ \mu m \times 800\ \mu m$ arranged along the MC length. The liquid in CFD is modeled as an incompressible Newtonian laminar fluid whose equations in integral form for an arbitrary control volume is given by

$$\frac{d}{dt}\int_V \rho\mathbf{v}\, dV + \int_S \rho\mathbf{v}\otimes(\mathbf{v}-\mathbf{v_m}).\mathbf{n}\, dS = -\int_V \nabla P\, dV + \int_S \boldsymbol{\tau}.\mathbf{n}\, dS + \int_V \mathbf{f}\, dV \quad \text{(eq. 1)}$$

where V, **n**, ρ, p, **v**,$\mathbf{v_m}$, **f** and τ epresent arbitrary control volume with surface area , outward normal to , the fluid density, the pressure, the velocity vector, the velocity of moving mesh and the viscous shear stress, respectively.

The end side of piezoelectric MC is fixed, and no slip boundary conditions with no initial velocity is considered for the walls of fluid part. With coupling FEM and CFD through surface to surface interaction, the FSI simulation is performed to study the nonlinear vibration of AFM microcantilever in the fluid environment. A pulse voltage is applied to piezoelectric layer, and the resonance frequency of MC is derived by FFT (Fast Fourier Transport) from its time response. Then, the AFM is excited by applying a harmonic voltage (with the obtained resonance frequency from FFT) to piezoelectric layer, and consequently, the time response and

Table 2- Resonance frequencies of piezoelectric microcantilever in water and glycerol mixtures

% Volume percentage of glycerol	Resonance frequency	Error as compared to experiment [40]
0	16.940 KHz	3.5 %
10	16.507 KHz	3.2 %
20	15.997 KHz	0.8 %
30	15.289 KHz	1.1 %
40	14.304 KHz	3.3 %

resonance amplitude are obtained.

3. Validation

Firstly, to verify the validity of the model, the resonance frequencies of MC in water and glycerol mixture with various volume percentages of glycerol are calculated and compared to those reported in [40]. Table 2 indicates the results of this validation study. As compared to the experimental data, the average value of error is about 2.38%. This reveals the accuracy and validity of present FSI analysis.

4. Effects of fluid properties

In this section, the influences of fluid properties including dynamic viscosity and density on the nonlinear vibrations of AFM microcantilever are studied. The results are generated assuming 0.5 volt excitation (the voltage of excitation is usually selected within the range of 0-1 volt [26, 40, 42-44]).

First, the effects of dynamic viscosity are highlighted. Fig. 2 shows the effect of dynamic viscosity on the resonance frequency of piezoelectric MC. In this figure, the resonance

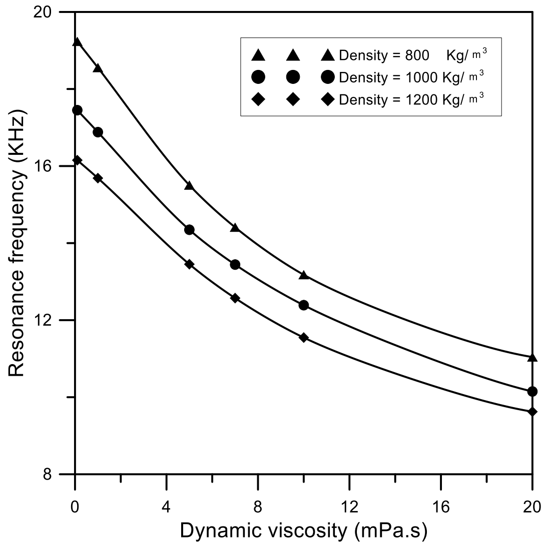


Fig. 2- Effect of dynamic viscosity on resonance frequency.

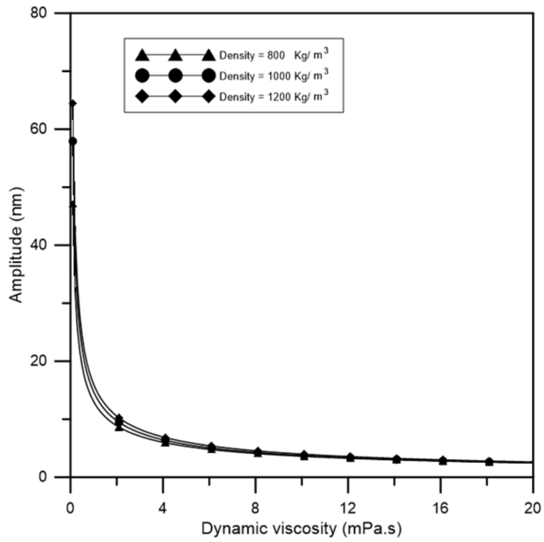


Fig. 3- Effect of dynamic viscosity on resonance amplitude.

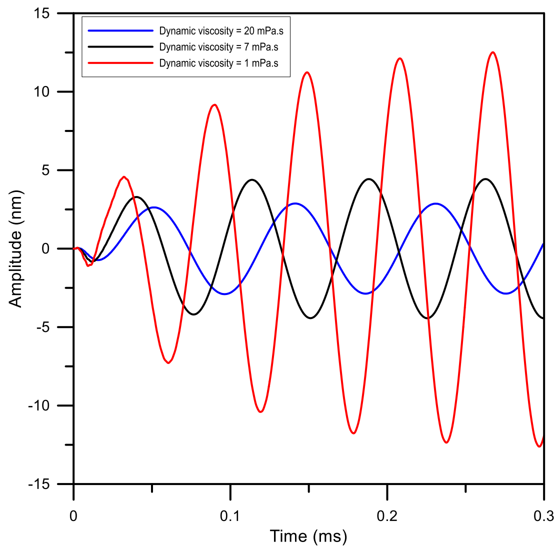


Fig. 4- Time responses for density equal to 1000 Kg/m3 and three values of dynamic viscosity.

frequency is plotted versus dynamic viscosity ranging from 0.1 to 20 mPa.s for three values of density including 800, 1000 and 1200 kg/m^3. It is observed that the resonance frequency decreases as the dynamic viscosity increases. For example, for density equal to 1000 kg/m^3, increasing the viscosity of fluid environment from 0.1 mPa.s to 1 mPa.s, 10 mPa.s and 20 mPa.s leads to nonlinear decrease of the resonance frequency from 17.450 KHz to 16.880 KHz, 12.389 KHz and 10.148 KHz, respectively. Furthermore, at a given dynamic viscosity, increasing fluid density has a decreasing effect on the resonance frequency.

Fig. 3 depicts the variations of resonance amplitude against dynamic viscosity for various values of density. This figure shows that the resonance amplitude nonlinearly decreases with increasing fluid dynamic viscosity. For instance, considering density equal to 1000 kg/m^3, the resonance amplitude of AFM microcantilever changes from 64.50 nm to 12.81 nm, 3.82 nm and 2.85 nm, respectively, as the viscosity changes from 0.1 mPa.s to 1 mPa.s, 10 mPa.s and 20 mPa.s. Also, at a given dynamic viscosity, the resonance

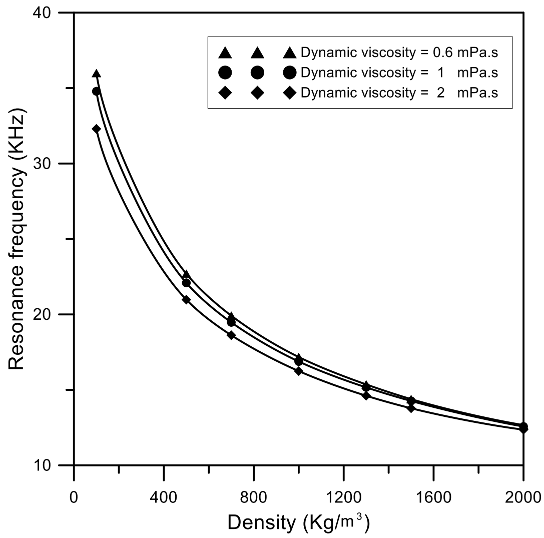


Fig. 5- Effect of density on resonance frequency.

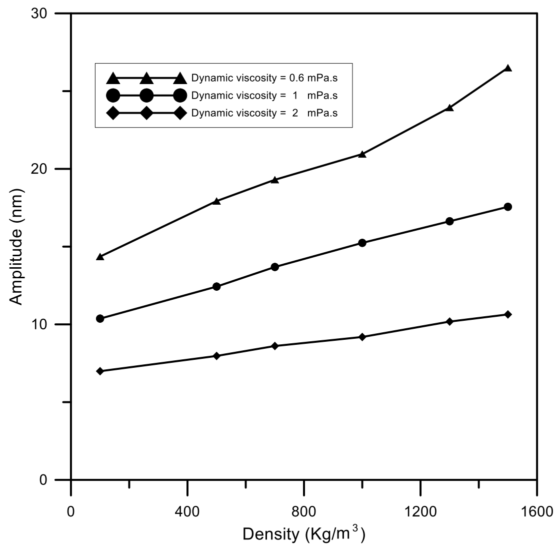


Fig. 6- Effect of density on resonance amplitude.

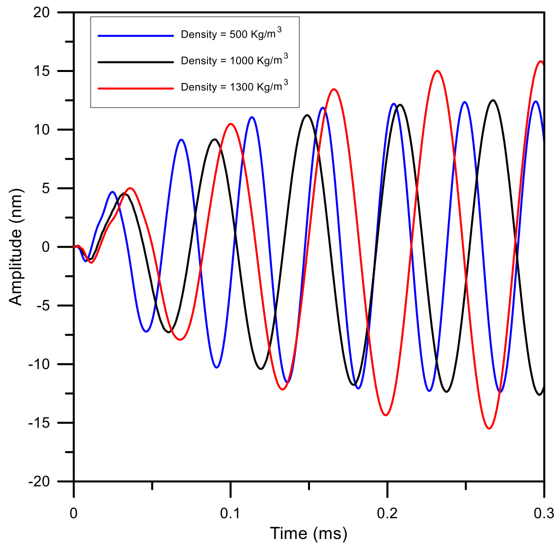


Fig. 7- Time responses for dynamic viscosity equal to 1 mPa.s and three values of density.

amplitude gets larger with the increase of fluid density.

Fig. 4 provides a comparison between the time responses of MC for three values of dynamic viscosity including 1 mPa.s, 7 mPa.s and 20 mPa.s. In all of these figures, the density of fluid is taken to be 1000 kg/m^3. The time required to reach the steady state decreases with increasing the fluid viscosity.

Now, the effects of fluid density are studied. In Figs. 5 and 6, the variations of resonance frequency and resonance amplitude with density are shown for dynamic viscosity of 0.6 mPa.s, 1 mPa.s and 2 mPa.s. According to Fig. 5, the resonance frequency nonlinearly decreases with increasing fluid density. Moreover, Fig. 6 indicates that increasing the density leads to the linear increase of resonance amplitude. Increasing the density of fluid environment from 100 kg/m^3 to 500 kg/m^3, 1000 kg/m^3 and 1500 kg/m^3 with no change in the viscosity of 1 mPa.s leads to the decrease of the resonance frequency from 34.786 KHz to 22.092 KHz, 16.880 KHz and 14.263 KHz, respectively. Moreover, the amplitude increases from 10.37 nm to 12.43 nm, 15.24 nm and 17.56 nm, respectively.

Finally, some examples of time responses for different values of fluid density are presented in Fig. 7. This figure indicates the time responses for three values of density including 500, 1000 and 1300, Kg/m^3. In these figures, the dynamic viscosity is assumed as 1 mPa.s.

5. Conclusions

Since AFM can be operated in liquid environments, the effects of liquid properties on the resonance characteristics of AFM microcantilevers were studied in this work. To this end, a 3D finite element model coupled with a computational fluid dynamics model was developed based on FSI simulations. It was considered that the MC has a piezoelectric layer attached on its top surface. It was shown that the results generated from the present finite element method are in excellent agreement with experimental data. Selected results were also given to investigate the effects of fluid dynamic viscosity and density on the resonance frequency and resonance amplitude of piezoelectric MC. It was concluded that increasing the fluid density and dynamic viscosity leads to the decrease of resonance frequency. Also, it was revealed that the resonance amplitude gets larger as the density increases, whereas increasing dynamic viscosity has a decreasing effect on the resonance amplitude.

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