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Dynamic analysis of tapping atomic force microscopy considering various boundary value problems

Rachael McCarty, Ben Carmichael, S. Nima Mahmoodi *

Nonlinear Intelligent Structures Laboratory, Department of Mechanical Engineering, University of Alabama, Tuscaloosa, AL 35487-0276, USA

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ABSTRACT

An accurate understanding of the microcantilever motion and tip-sample force is needed to generate accurate images in Atomic Force Microscopy (AFM). In this paper, different methods to apply the tip-sample force to the dynamic equations of motion and boundary conditions are derived and compared to determine the superior method for dynamic analysis of these systems. Hamilton's principle and the Galerkin method are employed to investigate the vibration of the microcantilever probe used in tapping mode AFM. Three different methods of including contact and excitation force in the equations of motion and boundary conditions are analyzed then compared. The first case considers the contact force at the tip and the inertial force due to tip mass to be a part of the boundary conditions of the microbeam. The second case assumes that the force is a concentrated force that is applied in the equations of motion, and the boundary conditions are the same as for the free end of a microcantilever beam. The third case is a combination where the contact force is included in the equation of motion, but the inertial force due to the tip mass is included in the boundary conditions. For the three cases, the equations of motion, the modal shape functions including the natural frequencies, and the time and frequency response functions are obtained. The numerical results are compared to experimental results obtained from the Bruker Innova AFM. Results show that the first and third methods produce results that accurately match the experimental outcomes. However, since including the forces in the boundary conditions is considerably more complex mathematically, this research indicates including the forces in the equations of motion is preferable unless tip mass is relatively large.

1. Introduction

Atomic Force Microscopy (AFM) was originally invented and used for nano-scale scanning to create a three dimensional image of a physical surface. The scanning process is performed by a microcantilever that contacts or taps the surface. More recently, microcantilever probes have been used extensively for Friction Force Microscopy (FFM), Lateral Force Microscopy (LFM), Piezo-response Force Microscopy (PFM), biosensing, and other applications [1–4]. Most AFMs operate by exciting the microcantilever using a piezoelectric tube actuator at the base of the probe. However, some microcantilevers have a layer of piezoelectric material on one side for actuation purposes. This layer is usually Zinc Oxide (ZnO) [5] or Lead Zirconate Titanate (PZT). The application of the piezoelectric microcantilever is widespread; it has been used for force microscopy, Scanning Near-field Optical Microscopy (SNOM), biosensing, and chemical sensing [6–9]. An accurate understanding of the microcantilever motion and tip-sample force is needed to generate accurate images.

The force between tip and sample consists of two main components: van der Waals force and contact force [10]. Numerical and experimental studies have investigated these nonlinear forces in some detail [11,12]. In non-contact mode, there is only van der Waals force between AFM tip and sample. However, in a tapping contact AFM, both forces are applied to the tip. In this work, only the linear contact force is considered since it is much larger than the van der Waals force.

Dynamics of the microcantilever have been experimentally and analytically studied in some research works. Experimental investigations have been performed in air and liquid on dynamic AFMs and the frequency response of the systems were obtained [13–16]. The nonlinear dynamics of a piezoelectric microcantilever have been studied considering the nonlinearity due to curvature, and piezoelectric material [17,18]. In other works, linear dynamic

* Corresponding author. Tel.: +1 205 348 5056.
E-mail addresses: click003@crimson.ua.edu (R. McCarty), bdcarmichael@crimson.ua.edu (B. Carmichael), NMahmoodi@eng.ua.edu (S.N. Mahmoodi).

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models have been developed for contact AFM probes and numerically solved [19–23]. Some works have conducted numerical studies to determine the number of modes necessary to fully model the complex dynamics of the microcantilever [24,25].

Two methods have been used in research works when including the force at the free end of the microcantilever during dynamic analysis. One method is to consider the force at the end of the beam in the boundary conditions [13,19,20,26–28]. The other method is to consider the force to be a part of the equation of motion using some type of step function, such as the Heaviside or Dirac delta function [17,18,22,24,25,29,30]. Additionally, a hybrid method will be introduced that combines these two methods. In this third method, the contact force will be considered in the equation of motion while the inertial force due to tip mass will be considered in the boundary conditions.

This research work investigates the vibration of dynamic tapping mode AFM for these three different methods of analysis and directly compares the results. For the three different cases, the equations of motion are derived using Hamilton's principle, the modal shape functions including the natural frequency are obtained using separation of variables, and the time response functions are obtained using the Galerkin method. The AFM microcantilever probe and sample is a nonlinear system. However, in this work, the system is linearized by using a spring on the free end to approximate the linear contact force [22,27]. Three linear systems are compared in order to determine the superior method.

Experimental results are obtained using the Bruker Innova AFM with an MPP-11123-10 microcantilever. The resonance frequency of the microcantilever is determined using the NanoDrive software package. The point spectroscopy function is used to collect data at increments of 1% of resonance across a range of 90–110% of resonance. This procedure is repeated four times to decrease the effects of statistical bias. The displacement data at each frequency are analyzed to find the maximum amplitude of the tip displacement.

Numerical results are compared to the experimental results. The second method is shown to be simpler than the other methods derivationally, but it yields inaccurate results. The first and third methods produce equally accurate results. Also, the results are very similar to each other. This indicates that either method is equally reliable. However, including the forces in the boundary conditions is considerably more complex mathematically. Therefore, this research indicates that the preferable method is the third method – including contact and excitation forces in the equations of motion and the inertia force due to tip mass in the boundary conditions.

Additionally, most research works neglect the effect of tip mass completely from the equation of motion and boundary conditions [13–30]. In this work, the tip mass is included and its effect on the microbeam dynamics are analyzed. For the first method, tip mass is shown to have a rather large effect on the resulting amplitude. For the third method, tip mass makes practically no difference. These results indicate that if tip mass is large, as in for biosensing applications [31–34], it may be necessary to use the first method, despite its more complex derivation.

2. Methods

The governing equations of motion, natural frequencies, mode shapes, and time response functions for the dynamics of a microcantilever with a spring at the free end are mathematically derived in this section for three cases: (1) the contact force and excitation force at the tip and inertial force due to tip mass are considered to be a part of the boundary conditions of the beam, (2) the contact force and excitation force at the tip and inertial force due to tip mass are considered to be a concentrated force that is applied in the equations of motion, and the boundary conditions are the same as that of a free cantilever beam, and (3) the contact force and excitation force are considered to be a concentrated force that is applied in the equations of motion, and the inertial force due to tip mass is considered to be a part of the boundary conditions of the beam.

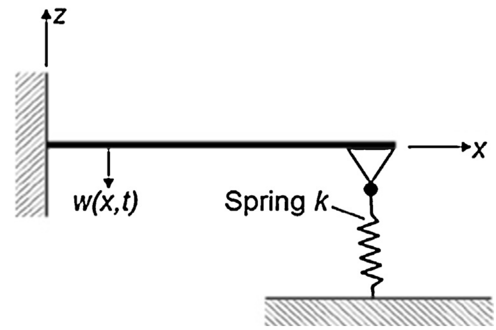

Fig. 1. Microcantilever beam with a spring attached to the free end.

Fig. 1 shows a microcantilever with a spring attached to the free end. The spring represents the elements that produce tip-sample contact force. The bending displacement of the microbeam in the negative z direction at position x along the microbeam and at time t is $w(x, t)$. The coordinate system (x, z) is used to describe the dynamics of the microcantilever, and t denotes time.

2.1. Case 1: forces and tip mass considered in boundary conditions

The first case to be examined, as stated previously, is a system including a spring at the free end where the contact force, excitation force, and inertial force due to tip mass are included in the boundary conditions. The relevant equation from Hamilton's principle is

$$\int_{t_0}^{t_1} (\delta T - \delta U + \delta W) dt = 0, \quad (1)$$

where T is kinetic energy, U is potential energy, and W is the work done by external loads on the microbeam. To derive the equation of motion, expressions for kinetic energy, potential energy, and external work need to be determined. First, the expression for kinetic energy is derived. The kinetic energy will be the combined kinetic energy of the microbeam (T_b) and the tip (T_{tip}).

$$T_b = \int_0^L ½\mathrm{m}_1 \left(\frac{\partial w}{\partial t}\right)^2 dx, \quad (2)$$

$$T_{tip} = ½\mathrm{m}_2 \left(\frac{\partial w_L}{\partial t}\right)^2, \quad (3)$$

where m_1 is the mass per unit length of the beam, m_2 is the tip mass, and L is the length of the microbeam. Also, w_L is the displacement of the microcantilever at the free end and is a function of time.

The potential energy term comes from two sources. U_b is the potential energy due to the strain energy of the microbeam, and U_s is the potential energy due to the spring.

$$U_b = \int_0^L ½\mathrm{EI} \left(\frac{\partial^2 w}{\partial x^2}\right)^2 dx, \quad (4)$$

$$U_S = ½k w_L^2, \quad (5)$$

where E is the elastic modulus of the microbeam, I is the mass moment of inertia of the microbeam, and k is the spring constant.