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Nonlinear Dynamical analysis of an AFM tapping mode microcantilever beam

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Abstract. We focus in this paper on the modeling and dynamical analysis of a tapping mode atomic force microscopy (AFM) microcantilever beam. This latter is subjected to a harmonic excitation of its base displacement and to Van der Waals and DMT contact forces at its free end. For AFM design purposes, we derive a mathematical model for accurate description of the AFM microbeam dynamics. We solve the resulting equations of motions and associated boundary conditions using the Galerkin method. We find that using one-mode approximation in tapping mode operating in the neighborhood of the contact region one-mode approximation may lead to erroneous results.

1 Introduction

Successful use of AFMs requires a deeper understanding of nonlinear characteristics and dynamics of the microcantilever system including its interactions with the sample. Several representative models of AFMs exists in literature. The simplest model is the one discussed by Ashhab et al. [1] where they have modeled the cantilever as a single spring mass. For continuous models, dynamic analysis of AFM cantilever microbeams is generally tackled by solving the associated equation of motion using several discretization methods. The Galerkin method is used by Yagasaki [2] to discretize the equation of motion and obtain a single degree of freedom system. Zhao et al. have studied the case of the AFM intermittent contact with soft substrate and they have demonstrated that single-mode analysis lead to erroneous results when used to analyze transient response [3]. In this paper we propose a descent continuous mathematical model of the microcantilever AFM system including the nonlinear interaction with the sample using Van der Waals and DMT forces. Then we solve the obtained equation of motion using a Galerkin approach by taking more than one mode shapes as trial function in the approximation. The obtained time dependent ODEs are solved for limit-cycle solutions using the Finite Difference Method (FDM).

2 Problem Formulation

The considered AFM microbeam shown in Fig. 1 is subjected to intermolecular forces, at its free end, due to the interaction between the AFM probe and the sample surface. At the fixed side of the microbeam it's subjected to a harmonic base excitation (Fig. 1). For the proposed model we neglect the mass of the AFM tip and the effect of the rotary inertia. Using the Hamilton's principle we derive the equations of motion of the system including the interactions between the AFM tip and the sample using classical Van der Waals and DMT forces. In its nondimensional form the equation of motion and the associated boundary conditions are given by

$$w'''' + \ddot{w} + c\dot{w} + \ddot{y} = 0 \tag{1}$$

$$w(0,t) = 0 \qquad w'(0,t) = 0 \qquad w''(1,t) = 0$$
$$w'''(1,t) = \begin{cases} -\dfrac{\Gamma_1}{a_0^2} + \Gamma_2 (a_0 - z)^{3/2} & \text{for } z \leq a_0 \\ -\dfrac{\Gamma_1}{z^2} & \text{for } z > a_0 \end{cases} \tag{2}$$

where

$$z = 1 - w(1,t) - y, \quad \Gamma_1 = \frac{ARL^3}{6EId^3}, \quad \Gamma_2 = \frac{4E^* L^3}{3EI}\sqrt{Rd}$$
$$a_0 = \frac{\hat{a}_0}{d}, \; x = \frac{\hat{x}}{L}, \; t = \frac{\hat{t}}{\tau}, \; w = \frac{\hat{w}(x,t)}{d}, \; y = \frac{\hat{y}}{d} = y_0 \sin(\Omega t)$$

where $d = Z - h$ is the tip-sample approach and $\tau = \sqrt{\dfrac{ML^4}{EI}}$ is a time constant, $M = \rho A_c$ and c is the nondimensional viscous damping coefficient. In the nondimensional form, the dot and prime denote the derivatives with respect to the nondimensional time t and the nondimensional space x, respectively. Table 1 provides the AFM parameters adopted for all simulations presented in the remainder of this paper.

3 Mode shapes and natural frequencies

In this section we solve the linearized undamped eigenvalue problem associated to equations (1-2). For that, we

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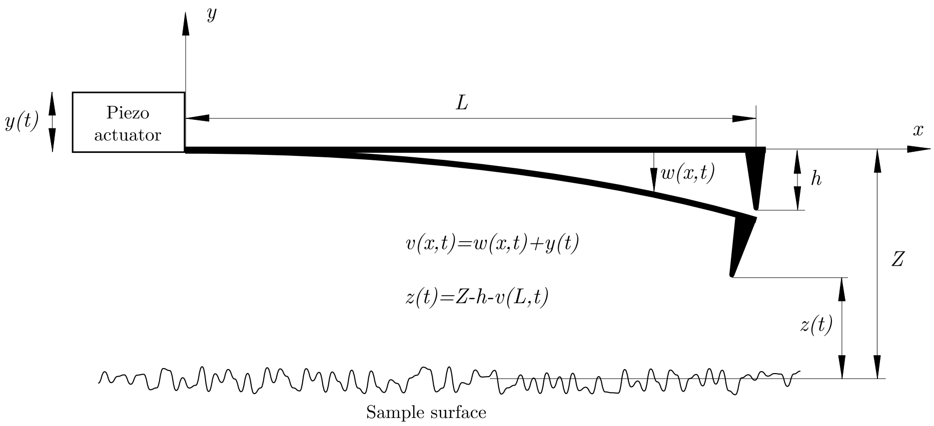

Fig. 1. Model schematic of an AFM tapping mode.

Symbol	Values	Description
R	10×10^{-9}	Tip Radius (m)
A_c	8.09×10^{-11}	Cross section area (m^2)
ρ	2300	Silicon density (kg/m^3)
E	130×10^9	Silicon Young's Modulus (N/m^2)
E^*	10.2×10^9	Sample Young's Modulus (N/m^2)
Q	33.3	Quality factor in air
A	2.96×10^{-19}	Hamaker constant (J)
$\hat{a}_0$	3.8×10^{-10}	Intermolecular distance (m)
h	15.4×10^{-6}	Tip height (m)
b	30×10^{-6}	Beam width (m)
h_b	2.8×10^{-6}	Beam height (m)

Table 1. AFM Parameters [4]

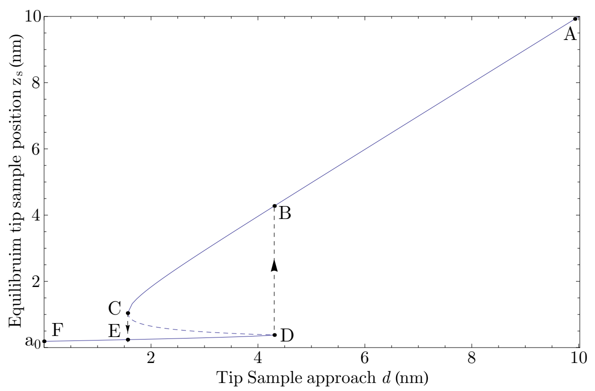

Fig. 2. Equilibrium solutions of the nonlinear static problem.

first solve the static problem by dropping all time dependent terms, which leads to the general analytic solution whose coefficient are determined by solving the nonlinear algebraic system associated to the boundary conditions in equations (2). Fig 2 shows the static tip-sample gap distance z_s versus the tip-sample approach d. The resulting static curve can be divided into two regions; a monostable region formed by the stable branches AB and EF, and a bistable region formed by the stable branches BC and ED and the unstable branch CD. As d decreases away from the sample, z_s decreases until it reaches the bifurcation point C after which it jumps to point E where the tip becomes in close contact with the sample surface. Then, as we move from point F to the bifurcation point D a jump to point B can be experienced.

The next step consists to separate the global deflection $w(x,t)$ into a static part and a dynamic part so that,

$$w(x,t) = w_s(x) + u(x,t) \tag{3}$$

where $w_s(x)$ is the solution of the static problem. The linearized undamped eigenvalue problem associated with equations (1-2) is given by

$$u^{iv} + \ddot{u} = 0 \tag{4}$$

$$u(0,t) = 0, \quad u'(0,t) = 0, \quad u''(1,t) = 0 \tag{5}$$

$$u'''(1,t) = \begin{cases} \frac{3}{2}\Gamma_2(a_0 - 1 + w_s(1))^{1/2}u(1,t) & \text{if } z \le a_0 \\ -2\frac{\Gamma_1}{(1-w_s(1))^3}u(1,t) & \text{if } z > a_0 \end{cases} \tag{6}$$

Consequently, the expression of the mode shape is given by

$$\begin{aligned} \phi_i(x) = & -\frac{\sin\sqrt{\omega_i} + \sinh\sqrt{\omega_i}}{\cos\sqrt{\omega_i} + \cosh\sqrt{\omega_i}}\left(\cos\sqrt{\omega_i}x + \cosh\sqrt{\omega_i}x\right) \\ & + \sin\sqrt{\omega_i}x - \sinh\sqrt{\omega_i}x \end{aligned} \tag{7}$$

here $\phi_i(x)$ and ω_i are the ith mode shape and natural frequency, respectively. The natural frequencies are obtained respectively for the unforced, the contact and the non contact mode by the characteristics equations (8), (9) and (10).

$$1 + \cos\sqrt{\omega}\cosh\sqrt{\omega} = 0 \tag{8}$$

$$\begin{aligned} & \omega^{3/2}(1 + \cos\sqrt{\omega}\cosh\sqrt{\omega}) \\ & + \frac{3\Gamma_2}{2}\sqrt{a_0 - 1 + w_s(1)} \\ & \times\left(\cosh\sqrt{\omega}\sin\sqrt{\omega} - \cos\sqrt{\omega}\sinh\sqrt{\omega}\right) = 0 \end{aligned} \tag{9}$$

$$\begin{aligned} & \omega^{3/2}(1 + \cos\sqrt{\omega}\cosh\sqrt{\omega}) + \frac{2\Gamma_1}{(-1+w_s)^3} \\ & \times(\cosh\sqrt{\omega}\sin\sqrt{\omega} - \cos\sqrt{\omega}\sinh\sqrt{\omega}) = 0 \end{aligned} \tag{10}$$

The variations of the first three natural frequencies, for the unforced and forced cases, with respect to d are displayed in Fig. 3. For the non contact phase, a hardening-type behavior is observed when d decreases. This is due to the increase of the applied forces. In the contact phase, one can point out that there is a softening-type behavior when d decreases. Also, the frequency shifting is more important for the first frequency comparing with the second and the third.

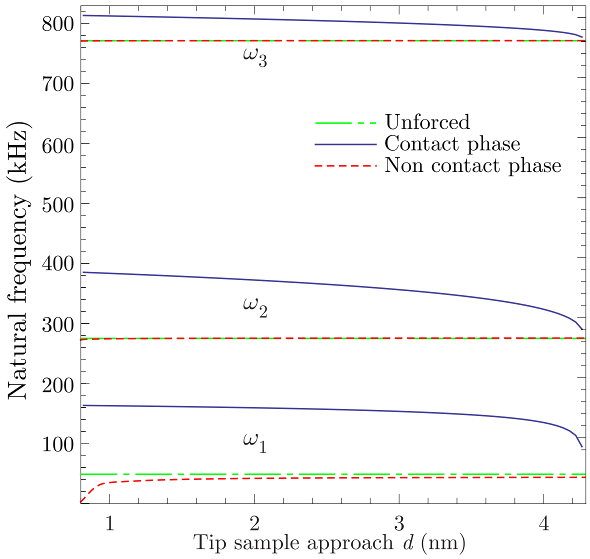

Fig. 3. The first three natural frequencies as function of the tip-sample approach for the free, contact and non contact modes.

4 Nonlinear Dynamic Analysis

The mathematical model, given by equations (1) and (2), consists of one partial differential equation and a set of four boundary conditions. Due to the nonlinear form of the intermolecular force and its switching as the AFM tip passes from the non contact phase to the contact phase or vice versa, the AFM dynamics becomes nonlinear, and thus, an approximate solution must be sought. In particular, we propose the use of the Galerkin method with a set of mode shapes obtained from the eigenvalue problem proposed in the previous section. This is a challenging problem in the sense that the mode shapes change as the AFM probe passes from one operating phase to another. In this paper we limit the test functions used in the discretization process to the unforced mode shapes of the system, which is classically the case when modeling AFM systems [4,2].

Using equation (3), the equation of motion and associated boundary condition describing the AFM dynamics are given by

$$u^{iv} + \ddot{u} + c\dot{u} - \Omega^2 y_0 \sin(\Omega t) = 0 \tag{11}$$

$$u(0,t) = 0, \quad u'(0,t) = 0, \quad u''(1,t) = 0$$

$$w_s'''(1) + u'''(1,t) = \begin{cases} -\dfrac{\Gamma_1}{a_0^2} + \Gamma_2 (a_0 - z)^{3/2} & \text{for } z \le a_0 \\ -\dfrac{\Gamma_1}{z^2} & \text{for } z > a_0 \end{cases} \tag{12}$$

Using the Galerkin method to approximate the dynamic component u, that is

$$u(x,t) \simeq \sum_{i=1}^{N} \phi_i(x) q_i(t) \tag{13}$$

where $q_i(t)$ is the i^{th} time-dependent modal amplitude. The first four nondimensional frequencies are given by $\omega_1 = 3.51602$, $\omega_2 = 22.0345$, $\omega_3 = 61.6972$ and $\omega_4 = 120.902$.

Next, we present frequency-response of the AFM microcantilever beam in tapping mode. In order to investigate the frequency-response curves, we search for limit-cycle solutions of the discretized equation of motion using the Galerkin procedure and the FDM. The stability of the obtained periodic solution is examined using Floquet theory. We consider the case where the tip-sample approach is d = 90 nm, the tip is initially located far from the sample surface and thus the Van der Waals forces have a secondary influence.

For a fixed tip-sample approach d and amplitude of the base excitation y_0 we calculate the tip amplitude as we increase (or we decrease) the excitation frequency. Here the number of time steps in the FDM is held fixed at 200. Then we use Floquet theory to ascertain the stability of the resulting periodic solution. Fig. 5 displays the frequency-response curve when d = 90 nm, $y_0 = 0.0209$ and using one mode approximation. During a frequency forward sweep, the Floquet multipliers of each calculated periodic solution lie within the unit circle. Then reaching the point SN1, where one of the Floquet multipliers leaves the unit circle through +1, characterizes a saddle node at SN1 in the lower branch. Similarly, a saddle node at SN3 is identified in the upper branch in Fig. 5. During a frequency reverse sweep, we identify two saddle nodes at SN4 and SN2. It is important to notice that, in Fig. 5, the initial softening-type behavior (prior to a_0) is transformed into a hardening-type behavior when the tip reaches the sample surface.

In order to validate the proposed reduced-order model using one mode shape of the unforced system in the Galerkin procedure, we compare the frequency-response curve obtained in Fig. 5 to published results in references [4] and [2]. Fig. 4 shows good agreement between the proposed model and those already published.

In Fig. 6, we compare periodic solutions for different number of mode shapes. Similar to the case of a single mode approximation, we find four saddle nodes at SN1, SN2, SN3, and SN4. However, the location of the saddle node at point SN4 changes as we increase the number of mode shapes. It should be noted that the convergence of the Galerkin method is satisfactory one mode approximation in the lower branches (corresponding to the non contact mode). On the other hand, Fig. 5 shows that using one mode is not sufficient to capture the dynamics of the AFM microbeam in the upper branches (corresponding to the tapping mode). In addition, we observe that using three modes leads to acceptable approximated solution of the nonlinear problem and that the contribution of the fourth mode in the periodic solutions is not significant.

5 Conclusion

In this paper, we developed a mathematical model of a tapping mode AFM microbeam subjected to base excitation and intermolecular forces. The resulting dynamical model consists of one partial differential equation subject to a set of four boundary conditions.We derived analytical solutions for the static and eigenvalues problems and noticed that the intermolecular forces significantly change these solutions when the AFM microbeam operates within or in the neighborhood of the contact region. We derived closed-form solutions of the eigenvalues and mode shapes, and we showed that the fundamental frequency and corresponding mode shape are affected by changing the tip sample approach in the contact region. We also observed that increasing the tip sample separation tends to soften

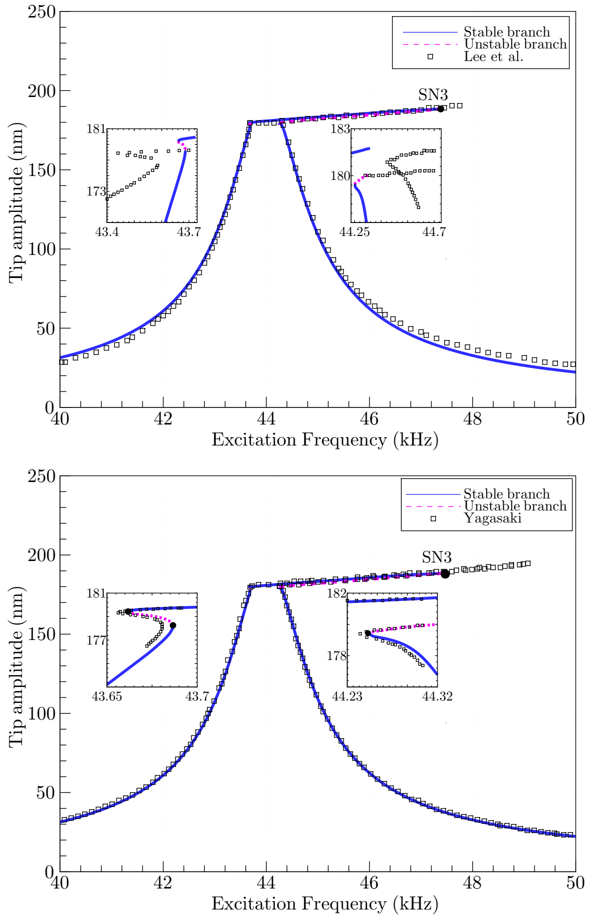

Fig. 4. Validation of the frequency-response curve for $N = 1$, $d =$ 90 nm and $y_0 = 0.0209$

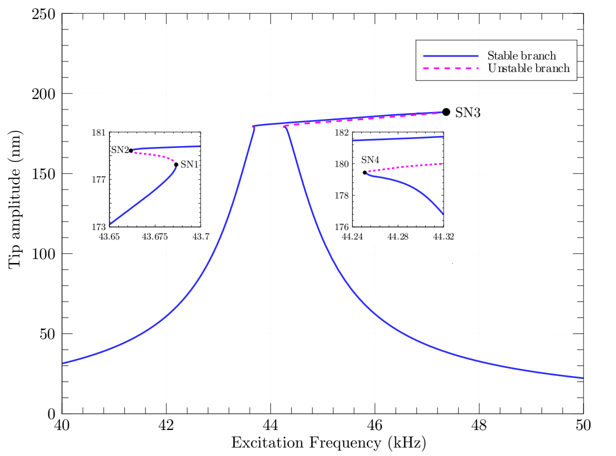

Fig. 5. Frequency-response curve using one mode approximation where $d = 90$ nm and $y_0 = 0.0209$

and harden the microbeam in the contact and non contact regions, respectively.

Due to the nonlinear form of the intermolecular forces, we provided approximation of the solution to the dynamical problem using the Galerkin method. We adopted the mode shapes of the unforced microbeam in the Galerkin approximation. We addressed issues related to the type and number of the mode shapes used in the Galerkin approximation. We studied the time and frequency-responses of the AFM microbeam subject to the intermolecular forces

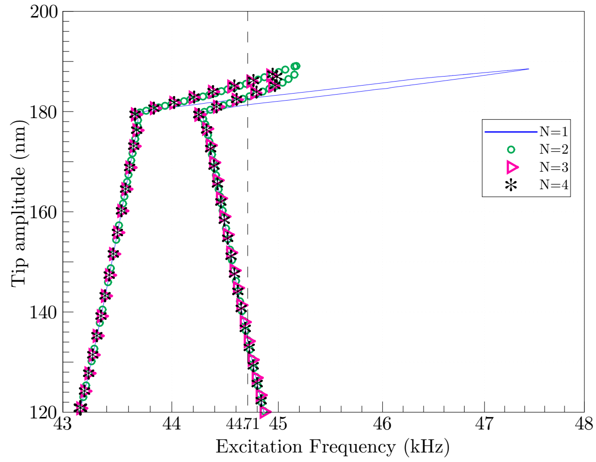

Fig. 6. Frequency-response curve using one to four modes approximations where $d = 90$ nm and $y_0 = 0.0209$

and base excitation. We thoroughly examined the effects of region switching and nonlinear form of the intermolecular force on the AFM microbeam performance.

We concluded that using one-mode approximation in tapping mode away from the contact region was sufficient to yield precise simulations. However, operating in the neighborhood of the contact region, one-mode approximation may not lead to accurate results.

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