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A simulation of atomic force microscope microcantilever in the tapping mode utilizing couple stress theory

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A R T I C L E I N F O

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A B S T R A C T

The nonlinear vibration behavior of a Tapping mode atomic force microscopy (TM-AFM) microcantilever under acoustic excitation force has been modeled and investigated. In dynamic AFM, the tip–surface interactions are strongly nonlinear, rapidly changing and hysteretic. First, the governing differential equation of motion and boundary conditions for dynamic analysis are obtained using the modified couple stress theory. Afterwards, closed-form expressions for nonlinear frequency and effective nonlinear damping ratio are derived utilizing perturbation method. The effect of tip connection position on the vibration behavior of the microcantilever are also analyzed. The results show that nonlinear frequency is size dependent. According to the results, an increase in the equilibrium separation between the tip and the sample surface reduces the overall effect of van der Waals forces on the nonlinear frequency, but its effect on the effective nonlinear damping ratio is negligible. The results also indicate that both the change in the distance between tip and cantilever free end and the reduction of tip radius have significant effects on the accuracy and sensitivity of the TM-AFM in the measurement of surface forces. The hysteretic behavior has been observed in the near resonance frequency response due to softening and hardening of the forced vibration response.

1. Introduction

Tapping mode atomic force microscopy (TM-AFM) which is a type of the dynamic atomic force microscopy (DAFM) reduces sample destruction, in comparison to contact mode, and, as a result, is widely used for surface topography, phase contrast images and also studying compliant materials such as polymers, biomaterials and semiconductors (Jalili and Laxminarayana, 2004, Korayem et al., 2010). In TM-AFM, the tip oscillation amplitude is used as control feedback while the drive frequency is fixed near or at the resonance frequency of the microcantilever. The participation of nonlinear attractive and repulsive interactions lead to the existence of two distinct operating regimes in TM-AFM; attractive and repulsive regimes in terms of the average force (García and San Paulo, 1999).

When a tip scans across a sample surface, it induces a dynamic interaction force between the tip and the surface. So far, many researchers have studied the dynamic responses of the contact mode AFM microcantilevers (Abbasi and Mohammadi, 2010, Chang et al., 2008, Verbiest and Rost, 2016, Huang et al., 2016, Korayem and Ghaderi, 2013). Considering scanning in the tapping mode, the dynamics of the probe become highly nonlinear which can affect the imaging stability and interaction forces. Extracting the nonlinear dynamics of tip-sample interaction forces can lead to open up new possibilities for the nanoscale material property measurements. Hence, investigations on the dynamic behavior of the TM-AFM microcantilever seem to be crucial (Andreaus et al., 2013). Gleyzes et al. (Gleyzes and Boccara, 1991) measured the oscillation amplitude as a function of the excitation frequency for a tip vibrating in the proximity of a sample surface. They observed that for some frequencies two different values of amplitude could be obtained. Fain et al. (Fain et al., 2000) first computed the contact time and the averaged value of the tip surface interaction forces via numerical simulations. Using numerical simulation, García and San Paulo 2000 demonstrated the coexistence of two stable oscillation states in TM-AFM. Raman and his coworkers (Rutzel et al., 2003, Lee et al., 2003) comprehensively studied the nonlinear phenomena of the TM-AFM based on the nonlinear dynamical system theory, computational continuation techniques and detailed experiments on graphite sample. Yagasaki (Yagasaki, 2004) used the averaging method and an extended version of the subharmonic Melnikov method to study the stability and bifurcations of the nonlinear oscillation in the tapping mode AFM.

Applying the virial theorem, San Paulo and García (San Paulo and García, 2001) found that in the steady-state oscillation conditions the average rate at which energy is supplied to the tip must be equal to the average rate at which energy is dissipated by the hydrodynamic and tip-surface interaction forces. By modeling a TMAFM cantilever operated in

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air, the effect of capillary force on the dynamics of TM-AFM has been investigated by Korayem et al. 2011, numerically.

Beams used in MEMS and NEMS, such as AFMs, have the thickness in the order of microns and submicrons. Experimental observations have indicated that the static and dynamic behavior of micro/nanoscale structures are strongly size dependent (Aifantis, 1999, McFarland et al., 2004, McFarland and Colton, 2005, Guo et al., 2005). Hence, size-dependent continuum mechanics models such as higher order continuum theories and nonlocal elasticity theory (Eringen, 1972, Eringen, 1983) should be used. As a higher order continuum theory, the modified couple stress theory was first proposed by Mindlin (Mindlin, 1964) and then elaborated by Yang et al. 2002 in which constitutive equations involve only one additional internal material length scale parameter besides two classical material constants.

Utilizing non-classical beam theories such as the modified couple stress theory, the resonant frequency and sensitivity of AFM microcantilevers were studied by some researchers (Abbasi, 2015, Abbasi and Mohammadi, 2014, Kahrobaiyan et al., 2011) in which the cantilevers operated in the contact mode. Lee and Chang (Lee and Chang, 2011) investigated the flexural sensitivity of a V-shaped cantilever of an AFM using the modified couple stress theory. Utilizing strain gradient theory, Abbasi and his coworker (Abbasi and Afkhami, 2014) analyzed the resonant frequency and sensitivity of a caliper formed atomic force microscope. They (Abbasi and Mohammadi, 2015) also investigated the torsional sensitivity and resonant frequency of an AFM with assembled cantilever probe (ACP) using nonlocal elasticity theory.

In this paper, utilizing a perturbation method and based on the couple stress theory, the nonlinear vibration behavior of an AFM microcanilever in the tapping mode has been analyzed, theoretically. Considering a small distance between the tip and the free end of the cantilever, a discretized dynamic model with Derjaguin-Müller-Toporov (DMT) contact mechanics interaction potential is developed to explore various nonlinear phenomena in TM-AFM.

2. Modeling

2.1. AFM micro cantilever

The geometrical parameters and configuration of a dynamic AFM cantilever in the tapping mode is depicted in Fig. 1. The proposed microcantilever is a small elastic beam with thickness h, width b and length L. It is assumed that the tip is not assembled exactly at the end of the cantilever. Hence, a distance between the tip and the free end of the cantilever is inevitable. L_1 and L_2 are the lengths of the cantilever on the left and right sides of the tip, respectively. The ratio between the cantilever length on the left side of the tip, L_1 and the cantilever length, L is denoted by the tip connection position, which denoted as$C_p = L_1/L$. D is the equilibrium separation between the tip and the sample in the absence of interaction forces and also *z(x,t)* is the instantaneous tip-surface separation.

Indicating the microcantilever transverse deflection relative to a fixed frame attached to the ground by w(x,t) and relative to a non-inertial frame attached to the moving base by $v(x, t)$ and assuming that the base excitation from the piezoelectric actuator towards the sample surface is a simple harmonic base motion with frequency ω and amplitude h_g which defined by $g(t) = h_g\cos(\omega t)$, the following relation can be obtained:

$$z(x, t) = D + w(x, t) = D + v(x, t) + g(t) \tag{1}$$

2.2. Interaction between tip and sample surface

In general, the standard contact models for scanning probe microscopy research are Johnson-Kendall-Roberts (JKR) (Johnson et al., 1971) and Derjaguin-Müller-Toporov (DMT), where both theories are only approximations. The JKR theory can be applied in the case of large tips and soft samples with large adhesion, while the DMT theory is applicable in the case of small tips and stiff samples with small adhesion (Derjaguin et al., 1975, Johnson et al., 1971).

In this study, cantilevers with sharp silicon tips are used to scan the surface of a freshly cleaved highly oriented pyrolytic graphite (HOPG) sample. This falls into the category of small tips and stiff samples with a small adhesion (Palchan et al., 1985). Thus, the DMT contact model is adopted in this work, in which, the tip-sample interaction force in a normal direction can be expressed as (Sadeghpour et al., 2013)

$$F_{ts}(z, \dot{z}) = \begin{cases} -\frac{HR}{6z^2} \ ,z > a_0 \\ -\frac{HR}{6a_0{}^2} + \frac{4}{3}E^*\sqrt{R}\,(a_0 - z)^{3/2} \\ + d_{ts}(a_0 - z)^{1/2}\dot{z} \ , z \le a_0 \end{cases} \tag{2}$$

where H is the Hamaker constant, R the tip radius, a_0 the intermolecular distance at which contact is initiated and d_{ts} is the viscosity of the tip–sample contact in the normal direction. Also, the effective elastic modulus, E^* given by

$$\frac{1}{E^*} = \frac{1 - \nu_t{}^2}{E_t} + \frac{1 - \nu_s{}^2}{E_s} \tag{3}$$

where E_t, E_s, ν_t and ν_s are the elastic modulus and Poisson's ratios of the tip and sample, respectively.

When the distance is more than intermolecular distance $z > a_0$, attractive van der Waals force is assumed between tip apex and sample surface, while for the distance less than intermolecular distance $z < a_0$, repulsive force will be applied.

2.3. Differential equation and boundary conditions

For a typical DAFM microcantilever in the tapping mode, the tip deflections and cross sectional rotations compared to the microcantilever length are very small. Moreover, the microcantilever cross section is relatively uniform along its length and the cross section dimension is approximately small compared to its length. For these reasons, geometric and inertial nonlinearities, shearing deformations and rotational inertia are negligible and one can assume a simple Bernoulli-Euler beam model in the analysis.

Considering the couple stress theory, the potential energy for the

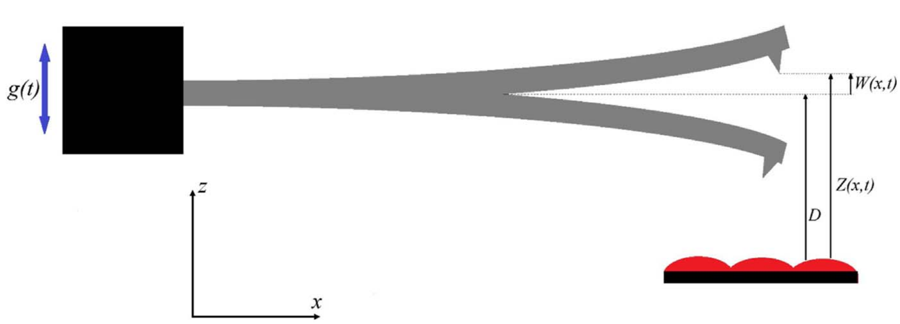

Fig. 1. A schematic of a dynamic AFM microcantilever in the tapping mode. Z(x, t) is the instantaneous tip–sample separation and D is the equilibrium distance between the cantilever and sample.