

Mathematical modeling of nanomachining with atomic force microscope cantilevers

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Abstract. This article theoretically analyzes the cutting depth and material removal rate of an atomic force microscope (AFM) cantilever during nanomachining. An analytical expression for the vibration frequency and displacement of the cantilever has been obtained by using the modified couple stress theory. The theory includes one additional material length scale parameter revealing the micro-scale effect. According to the analysis, the results show that the effect of size-dependent on the vibration behavior of the AFM cantilever is obvious. The maximum displacement of nanomachining with the AFM cantilever represents the cutting depth. The area under the displacement-time curve is related to the material removal rate. When the excitation frequency is closer to the nature frequency of the cantilever, a larger material removal rate is obtained.

1. Introduction

The atomic force microscope (AFM) has become an essential tool for the measurement of surface characteristics of diverse materials on a micro- and nanoscale level since its invention by Binnig et al.[1-4]. In addition, AFM can also be applied to nanolithography. AFM-based nanolithography technique, utilizes the tip of an AFM cantilever, has a very high potential for nanofabrication [5-8]. The nanolithography research can be roughly divided into three categories: (1) local electro-chemical reactions confined by the tip, (2) atomic and molecular manipulations, and (3) direct nanomachining of materials. The direct nanomachining technique for nanostructured materials has a capability to provide the opportunity of quickly fabricating nanodevices for applications in micro/nanoelectromechanical systems.

In the last years, the nanomachining technique has been the interest of many researchers. For example, Voigt et al. [9] utilized a chip cantilever system for material processing tasks on the micro- and nanometer scales by the flexural-torsional resonance mode. Zhu et al. [10] investigated the AFM-based nanometric cutting process of copper using molecular dynamics simulation. Recently, Zhang and Dong [11] utilized AFM to perform a high-rate tunable nanomachining-based nanolithography through controlling of the vibration between the cantilever tip and sample.

In this article, we develop an analytical model based on the modified couple stress theory [12] to analyze the dynamic displacement of AFM-based nanomachining. The theory has been applied to study microbeams and microplates [13-16]. In addition, some researchers utilized the modified couple stress theory to study the vibration behaviors of an AFM cantilever [17-18]. Here the effects of the material length scale parameter on the dynamic response of nanomachining with an AFM cantilever are also investigated.



2. Analysis

An AFM probe is used to machine the specimen and it is considered as a cantilever beam as shown in Figure 1.

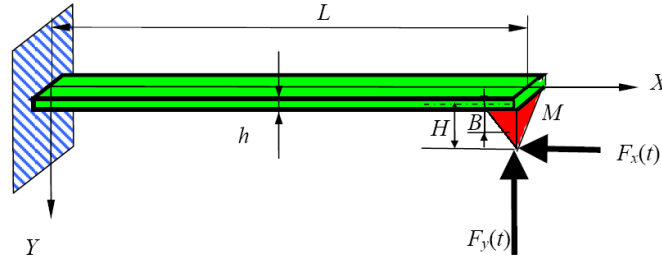


Figure 1. Schematic diagram of nanomachining on a sample by an AFM cantilever.

The probe has the Young's modulus E , shear modulus G , moment of inertia I , density ρ , uniform cross-section A , and length L . When the machining is in progress, the cantilever tip contacts with the specimen and induces a vertical reaction force, $F_y(t)$, and a horizontal reaction force, $F_x(t)$, which are a function of time t . Assuming that the reaction forces are on the tip end, then the product of the horizontal force and the tip length can form the equivalent moment exerted on the cantilever. The cutting system of the AFM cantilever can be modeled as a flexural vibration problem. The motion of the vibration cantilever is a partial differential equation and its transverse displacement is dependent on time t and the spatial coordinate X . The governing equation of transverse vibration based on the Euler-Bernoulli beam theory can be given by [17]

$$(EI + GAl^2) \frac{\partial^4 Y}{\partial X^4} + \rho A \frac{\partial^2 Y}{\partial t^2} = 0 \quad (1)$$

where l is the material length scale parameter which indicates the size-dependent vibration behavior of the microcantilever based on the modified coupled stress and $Y(X, t)$ is the transverse displacement.

The corresponding boundary conditions for nanomachining by the AFM cantilever are [19]

$$Y(0, t) = 0 \quad (2)$$

$$\frac{\partial Y(0, t)}{\partial X} = 0 \quad (3)$$

$$(EI + GAl^2) \frac{\partial^2 Y(L, t)}{\partial X^2} = -HF_x(t) - MB^2 \frac{\partial^3 Y(L, t)}{\partial X \partial t^2} \quad (4)$$

$$(EI + GAl^2) \frac{\partial^3 Y(L, t)}{\partial X^3} = F_y(t) + M \frac{\partial^2 Y(L, t)}{\partial t^2} \quad (5)$$

where H and M is the height and mass of the tip, respectively. B is the distance between the lower edge of the cantilever and centroid of the tip. The $F_y(t)$ and $F_x(t)$ are a function of time t and denote the vertical and horizontal cutting force on the sample under the normal and lateral direction, respectively.

The relationship between F_x and F_y can be expressed as $F_x = \frac{2 \cot \theta}{\pi} F_y$ which is obtained from a geometrical relation for a cone shape cantilever tip and θ is a half-conic angle.

The vertical cutting force is assumed to be as follows:

$$F_y(t) = P \sin(\Omega t) \quad (6)$$

where Ω is the excitation frequency of the cutting force, and P is a constant force.

In order to simplify the manipulation, the following dimensionless variables are introduced

$$x = \frac{X}{L}, \quad v = \frac{Y}{L}, \quad \delta = \frac{B}{L}, \quad m = \frac{M}{\rho AL}, \quad \tau = \frac{t}{\sqrt{\rho AL^4 / EI}},$$

$$\Lambda = \frac{\Omega}{\sqrt{EI/\rho AL^4}}, \quad \eta = \frac{GAl^2}{EI} = \frac{12G}{E(h/l)^2} \quad (7)$$

where v is the dimensionless transverse displacement of the cantilever. τ is the dimensionless time. m and δ are the dimensionless mass and centroid of the tip, respectively. Λ is the dimensionless excitation frequency in the transverse direction of the cantilever. η is the dimensionless additional flexural rigidity based on the modified coupled stress theory. Meanwhile, h/l is the ratio of the cantilever thickness to material length scale parameter. Accordingly, the dimensionless vertical and horizontal cutting forces are expressed as follows:

$$F_y(\tau) = f_y \sin(\Lambda \tau) \text{ and } F_x(\tau) = f_x \sin(\Lambda \tau) \quad (8)$$

where $f_y = \frac{PL^2}{EI}$ and $f_x = \frac{2 \cot \theta PL^2}{\pi EI}$ denote the dimensionless constants and are relevant to cutting force in the vertical and horizontal directions, respectively. In addition, the transverse displacement can be separated into the dimensionless spatial variable $y(x)$ and the dimensionless time and it is

$$v = y(x) \sin(\Lambda \tau) \quad (9)$$

Substituting the harmonic solution given by Eq. (6) into Eqs.(1)-(5) and using the parameters given by Eqs. (8) and (9), the governing equation and boundary conditions can be simplified to the following dimensionless equations:

$$(1 + \eta) \frac{d^4 y}{dx^4} + \Lambda^2 y = 0, \quad (10)$$

$$y(0) = \frac{dy(0)}{dx} = 0 \quad (11)$$

$$(1 + \eta) \frac{d^2 y(1)}{dx^2} = -f_x \frac{H}{L} + \Lambda^2 m \delta^2 \frac{dy(1)}{dx} \quad (12)$$

$$(1 + \eta) \frac{\partial^3 y(1, \tau)}{\partial x^3} = f_y - \Lambda^2 m y(1) \quad (13)$$

The solutions of $y(x)$ can be expressed as the following form:

$$y(x) = Q_1 \sin(\gamma x) + Q_2 \cos(\gamma x) + Q_3 \sinh(\gamma x) + Q_4 \cosh(\gamma x) \quad (14)$$

where $Q_1 \dots Q_4$ are arbitrary constants. γ is the wave number and it is

$$\gamma^4 = \frac{\Lambda^2}{1 + \eta}. \quad (15)$$

Substituting Eq. (14) into Eqs. (11)-(13), the constants $Q_1 \dots Q_4$ can be solved and expressed as follows:

$$Q_1 = \frac{f_y \phi_1 + f_x \psi_1}{2(1 + \eta) \gamma^3 \Delta(\gamma)} \quad (16)$$

$$Q_2 = \frac{f_y \phi_2 + f_x \psi_2}{2(1 + \eta) \gamma^3 \Delta(\gamma)} \quad (17)$$

$$Q_3 = -Q_1, \quad Q_4 = -Q_2 \quad (18)$$

where

$$\Delta(\gamma) = m^2 \delta^2 \gamma^4 (\cosh \gamma \cos \gamma - 1) + m \gamma [(\delta^2 \gamma^2 + 1) \cosh \gamma \sin \gamma \quad (19)$$

$$+ (\delta^2 \gamma^2 - 1) \sinh \gamma \cos \gamma] - (1 + \cosh \gamma \cos \gamma)$$

$$\phi_1 = \cosh \gamma + \cos \gamma - m \delta^2 \gamma^3 (\sinh \gamma + \sin \gamma) \quad (20)$$

$$\psi_1 = \frac{H}{L} \gamma [m \gamma (\cosh \gamma - \cos \gamma) + \sinh \gamma - \sin \gamma] \quad (21)$$

$$\phi_2 = m \delta^2 \gamma^3 (\cosh \gamma - \cos \gamma) - (\sinh \gamma + \sin \gamma) \quad (22)$$

$$\psi_2 = -\frac{H}{L} \gamma [\cosh \gamma + \cos \gamma + m\gamma(\sinh \gamma - \sin \gamma)] \quad (23)$$

If we set $\Delta(\gamma) = 0$ given in Eq.(19), the characteristic equation of free vibration for the AFM cantilever can be obtained. And then the wave number of free vibration γ_n will be solved. In addition, using the relationship between the wave number and frequency given by Eq. (15), the dimensionless free vibration frequency ω_n based on the modified couple stress theory can be determined by

$$\omega_n = \gamma_n^2 \sqrt{1 + \eta}. \quad (24)$$

While the dimensionless excitation frequency Λ can be set as follows:

$$\Lambda = r\omega_n \quad (25)$$

where r is the frequency ratio.

In addition, the displacement of nanomachining with the AFM cantilever can be determined from Eqs. (14), (24), and (25).

3. Results and discussion

The cutting force in the vertical direction is assumed to be as follows:

$$F_y(\tau) = f_y \left(\sin r\omega_n \tau + \frac{1}{3} \sin 3r\omega_n \tau + \frac{1}{5} \sin 5r\omega_n \tau \right) \quad (26)$$

The following material properties and geometrical parameters are used [5,19]: $L = 300 \mu\text{m}$, $E = 170 \text{ GPa}$, $G = 66.4 \text{ GPa}$, $I = 33.3 \times 10^{-24} \text{ m}^4$, $A = 10^{-10} \text{ m}^2$, $H = 10 \mu\text{m}$, $\rho = 2300 \text{ kg/m}^3$, $M = 2 \times 10^{-13} \text{ kg}$, $B = 2.5 \mu\text{m}$, $P = 10^{-8} \text{ nN}$, $f_y = 0.16 \times 10^{-3}$. In addition, the excitation frequency cannot be the same with the natural frequency of the cantilever.

Figure 2 shows the comparison of dimensionless dynamic displacement of the free end of an AFM cantilever obtained by the modified couple stress theory with $H/L = 1/30$ and $h/l = 4$ for various frequency ratios r during nanomachining. The frequency ratio is defined as the ratio of the excitation frequency to the natural frequency of mode 1 of the cantilever.

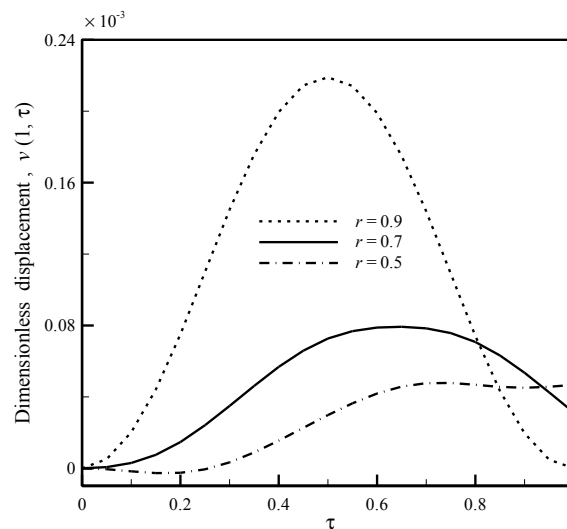


Figure 2. The dimensionless dynamic displacement of the free end of an AFM cantilever obtained by the couple stress theory with $H/L = 1/30$ and $h/l = 4$ for various frequency ratios r .

For different frequency ratios, the different displacements of the AFM cantilever are obtained. As expected, a larger vibration displacement is obtained as the r value is closer to 1. A larger displacement indicates a larger cutting depth. In addition, the figure can be used to predict peak displacement. A higher peak displacement indicates a larger cutting depth. The area under the curve is related to the material removal rate. A larger material removal rate is obtained when the value of r increases.

Figure 3 illustrates the dynamic displacement of the free end of an AFM cantilever obtained by the modified couple stress theory with $H/L = 1/30$ and $r = 0.9$ for various ratios of microcantilever thickness to material length scale parameter h/l . It is noted that for the case of $h/l = \infty$, it implies the result obtained based on the classical beam theory. It can be seen that the displacement increases with increasing the value of h/l . This is because the effect of material length scale parameter on the displacement becomes small when the value of h/l increases. The phenomena show size-dependent vibration behavior of the cantilever.

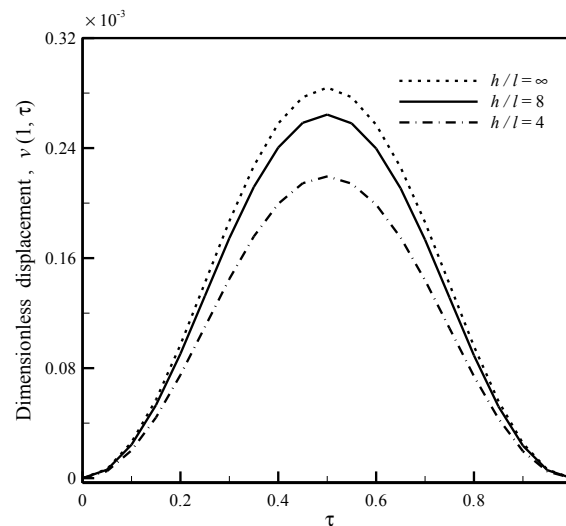


Figure 3. The dynamic displacement of the free end of an AFM cantilever obtained by the modified couple stress theory with $H/L = 1/30$ and $r = 0.9$ for various ratios of microcantilever thickness to material length scale parameter h/l .

4. Conclusions

According to the analysis, the displacement increased with increasing the ratio of the microcantilever thickness to material length scale parameter. The size-dependent vibration behavior of the AFM cantilever was obvious. The displacement of the AFM cantilever is related to the cutting depth. A large material removal rate is obtained when the excitation frequency was close to the natural frequency of the cantilever.

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