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VIBRATION OF CANTILEVERS WITH ROUGH SURFACES**

Huiling Duan[1*] **Yahui Xue**[1] **Xin Yi**[1,2]
([1]*State Key Laboratory for Turbulence and Complex System, CAPT, Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing* 100871, *China*)
([2]*Division of Engineering, Brown University, Providence, RI* 02912, *USA*)

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ABSTRACT We study the effect of surface roughness on the resonance frequency of micro-cantilever sensors. The analysis demonstrates that surface roughness can enhance, decrease or even annul the effect of surface stress on the resonance frequency, depending on the surface inclination angle and the Poisson ratio of the coating film on the cantilever.

KEY WORDS surface roughness, surface stress, resonance frequency, micro-cantilevers

I. INTRODUCTION

Micro-cantilevers have been used as physical, chemical and biological sensors, and components in micro-electro-mechanical systems (MEMS) because of their high sensitivity and ease of operation[1–3]. Nowadays, miniaturization of sensors is a major requirement in applications. As the sizes of the cantilevers decrease, not only the surface stress[4–6] but also the surface roughness[7–13] plays an important role in their sensitivities due to the larger surface to volume ratio. Conventionally, the deflections and vibration frequencies of cantilevers are analyzed for planar surfaces. However, real surfaces are rarely smooth. Cantilever bending experiments show that the adsorption-induced surface stress depends on the surface roughness of the cantilever[14–17]. For example, Lavrik et al.[14,15] showed that the cantilever deflection due to molecular adsorption can be enhanced by modifying the surface roughness. Fabre et al.[16] found that the surface stress is related to the surface roughness, which is responsible for differences in hydrogen absorption rates. Godin et al.[18] and Desikan et al.[19] reported that nano-scale surface roughness decreases the adsorption-induced surface stress compared to smooth surfaces. Recently, Weissmüller and Duan[20] found that the sensitivities of cantilevers with rough surfaces are significantly dependent on the topology of the surfaces. The sensitivities can be decreased all the way to zero or even inverted in sign for corrugated surfaces of metals with large Poisson ratios. This implies that deliberate structuring of the surface allows a tuning of magnitude and even sign of the cantilever response. Besides working in a static mode to measure the deflection, micro-cantilever sensors also operate in a dynamic mode to measure the change of the resonance frequency. Duan[21] proposed the design of surface-enhanced cantilever sensors using nano- (micro-) porous films as surface layers, and it

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[*] Corresponding author. E-mail: HLDuan@pku.edu.cn

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was shown that the sensitivities of these novel cantilever sensors for the static deformation and resonance frequencies could be tuned by the porosity, the size of the pores and the structure of the porous films.

In this letter, by means of the Hamilton's equation, we investigate the influence of surface roughness on the resonance frequency of micro-cantilevers with the consideration of surface stress. We demonstrate that surface roughness can enhance, decrease or even annul the effect of surface stress on the change of the resonance frequency of micro-cantilevers, depending on the properties of the surface stress, the inclination angle of the surface roughness and the Poisson ratio of the material.

II. GENERAL THEORY

Consider a cantilever consisting of two layers: the substrate of thickness H and the film (upper layer) of mean thickness $\langle h\rangle \ll H$, as shown in Fig.1. $\langle\cdot\rangle$ denotes the spatial average over all positions and directions. The length and the width of the cantilever are L and T, respectively. It is assumed that the two layers are well bonded. The global coordinate system is defined such that the interface of the film and substrate is the xy-plane, and the z-axial is upward. The origin of the global coordinate system is at the fixed end. The profile (height) of the rough surface $h(\boldsymbol{r})$ is a continuous and differentiable function of the coordinates x and y. The local coordinate system is defined at each point on the rough surface such that the z'-axial is parallel to, and the $x'y'$-plane is perpendicular to, the outer normal ($\hat{\boldsymbol{n}}$), as shown in Fig.1. The Young modulus and the Poisson ratio of the substrate are E_s and ν_s, respectively, and those of the film are E_f and ν_f. Hereinafter the subscripts f and s identify the quantities related to the film and the substrate, respectively.

Surface stress $\boldsymbol{\tau}$ exits on the rough surface of the film. For isotropic surfaces, the surface stress can be written as $\boldsymbol{\tau} = \boldsymbol{\tau}_0 + \boldsymbol{\tau}^s$, where $\boldsymbol{\tau}_0 (= \tau_0 \boldsymbol{I})$ is the constant surface stress, and $\boldsymbol{\tau}^s (= 2\mu^s \boldsymbol{\varepsilon}^s + \lambda^s(\mathrm{tr}\boldsymbol{\varepsilon}^s)\boldsymbol{I})$ is the strain-dependent surface stress[5,6]. Here $\boldsymbol{I}$ is the unit tensor in the two-dimensional space, μ^s and λ^s are isotropic surface moduli, and $\mathrm{tr}\boldsymbol{\varepsilon}^s$ denotes the trace of $\boldsymbol{\varepsilon}^s$.

Since $\langle h\rangle \ll H$, we assume that the midplane is at $z = -H/2$. Based on the Bernoulli-Euler assumption, the displacement field can be written as

$$u = u_0(x) - \left(z + \frac{H}{2}\right)\frac{\partial w}{\partial x}, \qquad v = 0, \quad w = w(x) \tag{1}$$

where u, v and w are the displacements in the x-, y- and z-directions, respectively, and $u_0(x)$ is the midplane displacement in the x-direction. Compared to the bending caused by the change of the surface stress, the overall stretching of the cantilever can be neglected, namely, it can be assumed that $u_0(x) = 0$. Then from Eq.(1), the strain components are given by

$$\varepsilon_{xx} = -\left(z + \frac{H}{2}\right)\frac{\partial^2 w}{\partial x^2}, \qquad \varepsilon_{yy} = 0 \tag{2}$$

Based on the Hooke's law, Eq.(2) and the plane stress condition $\sigma_{zz} = 0$, we have $\sigma_{xx} = \hat{E}\varepsilon_{xx}$, where $\hat{E} = E/(1-\nu^2)$. The surface strain $\boldsymbol{\varepsilon}^s$ can be calculated by means of coordinate transformation from the global coordinate system to the local inclined one at $z = h(\boldsymbol{r})$ (see Fig.(1)). Then the surface stress $\boldsymbol{\tau}^s$ can be obtained.

The kinetic energy, U_T, of the cantilever is

$$U_T = \frac{1}{2}\int_V \rho\left[\left(\frac{\partial u}{\partial t}\right)^2 + \left(\frac{\partial w}{\partial t}\right)^2\right]\mathrm{d}V \tag{3}$$

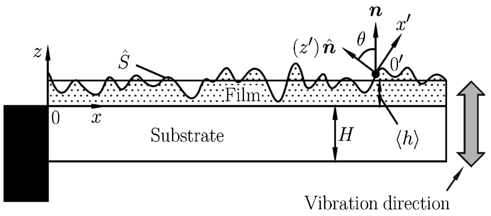

Fig. 1. A micro-cantilever with two layers: the film and substrate. θ denotes the inclination angle between the outer normals of the substrate plane ($\boldsymbol{n}$) and the local inclined surface ($\hat{\boldsymbol{n}}$). See main text for meanings of the remaining variables.

where ρ is density, V the volume of the cantilever, and t time. Here the rotational kinetic energy is ignored. The elastic energy, U_E, coming from the bulk energy and surface energy, is given by

$$U_E = \frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}\mathrm{d}V + \int_{\hat{S}} \tau_0 \varepsilon_{ii}^s \mathrm{d}\hat{S} + \frac{1}{2}\int_{\hat{S}} \tau_{ij}^s \varepsilon_{ij}^s \mathrm{d}\hat{S} \tag{4}$$

where σ_{ij} and ε_{ij} $(i,j=x,y,z)$ are the bulk stress and strain components, τ_{ij}^s and ε_{ij}^s $(i,j=x',y')$are the surface stress and strain components on $\hat{S}$, and $\hat{S}$ denotes the rough surface of the film. Introducing a Lagrangian function $L=U_T-U_E$ into Hamilton's equation $\delta\int_{t_1}^{t_2} L\mathrm{d}t = 0$ leads to the vibration equation for the cantilever

$$\frac{\partial^2}{\partial x^2}\left\{\left\{\frac{\hat{E}_s H^3}{12} + \frac{\hat{E}_f H^3}{3}\left[\left(\eta+\frac{1}{2}\right)^3 - \frac{1}{8}\right] + (2\mu^s+\lambda^s)H^2\left(\eta+\frac{1}{2}\right)^2 \frac{\left[1-\frac{\nu_f}{1-\nu_f}(\nabla h)^2\right]^2}{[1+(\nabla h)^2]^{3/2}}\right\}\right.$$
$$\left.\frac{\partial^2 w}{\partial x^2}\right\} + H(\rho_s+\rho_f\eta)\frac{\partial^2 w}{\partial t^2} = \tau_0 H \frac{\partial^2}{\partial x^2}\left\{\frac{(\eta+\frac{1}{2})}{[1+(\nabla h)^2]^{3/2}}\left[1-\frac{\nu_f}{1-\nu_f}(\nabla h)^2\right]\right\} \tag{5}$$

where $\eta = h/H \ll 1$, and ρ_s and ρ_f are the densities of the substrate and the film, respectively. As shown in Eq.(5), the constant surface stress τ_0 does not influence the resonance frequency, but only affects the equilibrium position of vibration. If the surface of the film is smooth ($\nabla h = 0$), the terms on the right side of Eq.(5) vanish, and τ_0 does not influence the vibration.

Complications arise when we try to find the exact solution of Eq.(5). Since $\eta \ll 1$, we neglect the term η and its higher order terms in Eq.(5). Moreover, we assume that the derivative of $(\nabla h)^2$ with respect to x is very small. Therefore, we replace $(\nabla h)^2$ with its mean value g^2 where $g(=\sqrt{\langle(\nabla h)^2\rangle})$ is the average surface slops. Then Eq.(5) can be reduced to the following equation:

$$\frac{\hat{E}^* H^3}{12}\frac{\partial^4 w}{\partial x^4} + \rho_s H \frac{\partial^2 w}{\partial t^2} = 0 \tag{6}$$

where

$$\hat{E}^* = \left[1 + \frac{3(2\mu^s+\lambda^s)}{\hat{E}_s H(1+g^2)^{3/2}}\left(1-\frac{\nu_f}{1-\nu_f}g^2\right)^2\right]\hat{E}_s \tag{7}$$

The solution to Eq.(6) gives the fundamental resonance frequency $\tilde{f}$ of the micro-cantilever with the influence of the surface stress and surface roughness. The frequency shift $\Delta f_r = \tilde{f} - f_0$ is

$$\frac{\Delta f_r}{f_0} \approx \frac{3(2\mu^s+\lambda^s)}{2\hat{E}_s H(1+g^2)^{3/2}}\left(1-\frac{\nu_f}{1-\nu_f}g^2\right)^2 \tag{8}$$

where f_0 denotes the classical fundamental resonance frequency of the micro-cantilever without the surface stress and surface roughness. Equation (8) shows that $\Delta f_r/f_0$ is a function of the thickness and elastic modulus of the substrate, the surface moduli, the Poisson ratio of the film ν_f, and the average surface slope g. If there is no roughness ($g=0$), Eq.(8) reduces to

$$\frac{\Delta f_s}{f_0} \approx \frac{3(2\mu^s+\lambda^s)}{2\hat{E}_s H} \tag{9}$$

where Δf_s is the resonance frequency shift only due to the effect of surface stress. From Eqs.(8) and (9), we obtain

$$\frac{\Delta f_r}{\Delta f_s} \approx (1+g^2)^{-3/2}\left(1-\frac{\nu_f}{1-\nu_f}g^2\right)^2 \tag{10}$$

In the case of slight roughness ($g \ll 1$), Eq.(10) shows that the surface roughness weakens the influence of the surface stress on the frequency shift ($\Delta f_r/\Delta f_s < 1$). If Δf_s for a flat surface is larger than Δf_r, then the roughness is always slight, which can be treated as a perturbed state of the flat surface. For strong roughness, $\Delta f_r/\Delta f_s$, depending on $\nu_f$and g, can be bigger, smaller than 1, or even equal to 0 when $g=\sqrt{(1-\nu_f)/\nu_f}$, which means the surface roughness can enhance, decrease or annul the effect of surface stress on the resonance frequency.

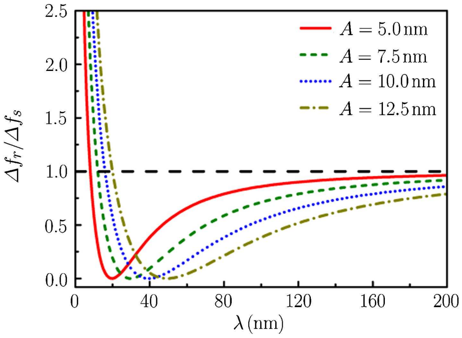

Fig. 2. Ratio $\Delta f_r/\Delta f_s$ as a function of the wavelength λ for a rough surface $h(\boldsymbol{r}) = \langle h \rangle + A \sin\left(\frac{2\pi x}{\lambda_1}\right) \sin\left(\frac{2\pi y}{\lambda_2}\right)$, ($\nu_f = 0.44$).

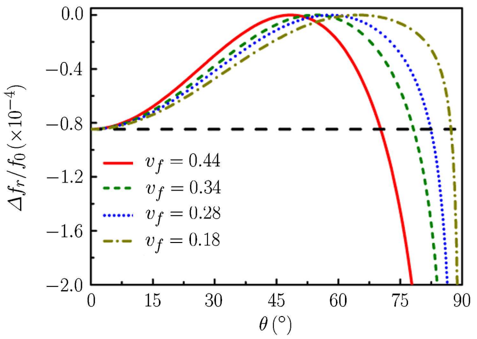

Fig. 3. Cantilever sensitivity $\Delta f_r/f_0$ for a rough surface covered by pyramidal hillocks versus the inclination angle θ.

III. NUMERICAL RESULT

Noting that a general continuous and smooth surface profile can be depicted by a Fourier series of trigonometric functions, we consider a representative surface profile $h(\boldsymbol{r}) = \langle h \rangle + A \sin\left(\frac{2\pi x}{\lambda_1}\right) \sin\left(\frac{2\pi y}{\lambda_2}\right)$, where A is the amplitude of the rough surface, and λ_1 and λ_2 are the spatial wavelengths along the x- and y-axes, respectively. The ratio $\Delta f_r/\Delta f_s$ as a function of the wavelength, $\lambda(\equiv \lambda_1 = \lambda_2)$, of the rough surface is shown in Fig.2, for four amplitudes, 5.0 nm, 7.5 nm, 10.0 nm and 12.5 nm. For a particular A, a smaller λ corresponds to stronger roughness. Figure 2 shows that, for a small λ (strong roughness), the surface roughness enhances the effect of surface stress on the frequency shift as indicated by Eq.(10). As λ increases, the ratio $\Delta f_r/\Delta f_s$ drops off quickly. Then $\Delta f_r/\Delta f_s$ reaches the minimum value 0, where the surface roughness annuls the effect of the surface stress on the shift of the resonance frequency. This phenomenon, which means that the dynamic response of the cantilever is dramatically affected by the surface roughness, may have profound implications for the design and analysis of the sensitivities of micro-cantilever sensors. For a large wavelength, $\Delta f_r/\Delta f_s$ increases as λ increases, but is always smaller than 1. When $\lambda \to \infty$, Δf_r reduces to the case of a smooth surface Δf_s ($\Delta f_r/\Delta f_s \to 1$).

To estimate the effect of topology of the surface roughness on the frequency shift, we consider a silicon substrate covered completely by pyramidal hillocks with an identical inclination angle θ[20]. Figure 3 shows the cantilever sensitivity $\Delta f_r/f_0$ as a function of θ for different Poisson ratios $\nu_f = 0.44$ (Au), 0.34 (Cu), 0.28 [Si(100)], 0.18 [Si(111)][22]. Since θ is uniform, we have $g = \tan\theta$. The parameters of the substrate are $H = 1$ μm, $E_s = 130$ GPa and $\nu_s = 0.28$. The surface moduli are chosen as the ones of gold film $\lambda^s = -2.70738$ N/m and $\mu^s = -2.62728$ N/m[23]. As θ increases approximately to 45° for the case $\nu_f = 0.44$, Δf_r vanishes, which means that surface roughness annuls the effect of the surface stress entirely. When θ becomes large (about 75° for $\nu_f = 0.44$, strong roughness), the surface roughness starts to enhance the effect of surface stress on the shift of the resonance frequency. For strong roughness, the frequency shift will be enhanced as θ increases.

IV. CONCLUSION

In summary, we show that the resonance frequency of micro-cantilevers is affected by the surface roughness, besides the conventional factors such as the surface and bulk elasticity of the material. The effect of the surface roughness on the resonance frequency depends on the profile of the surface roughness including the wavelength, amplitude, the inclination angle, and the Poisson ratio of the material. It is shown that depending on the surface inclination angle and the Poisson ratio, the surface roughness can enhance, decrease or even annul the effect of the surface stress on the resonance frequency. As real surfaces often have various roughness, this effect may have profound implications for the design and analysis of the sensitivities of micro-cantilever sensors when they operate in a dynamic mode.

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