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Surface elasticity-based modeling and simulation for dynamic and sensing performances of nanomechanical resonators

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Abstract. The dynamic and sensing performances of nanomechanical resonators with their different boundary conditions are studied based on surface elasticity-based modeling and simulation. Specifically, the effect of surface stress is included in Euler-Bernoulli beam model for different boundary conditions. It is shown that the surface effect on the intrinsic elastic property of nanowire is independent of boundary conditions, while these boundary conditions affect the frequency behavior of nanowire resonator. The detection sensitivity of nanowire resonator is remarkably found to depend on the boundary conditions such that double-clamping boundary condition results in the higher mass sensitivity of the resonator in comparison with simple-support or cantilever boundary condition. Furthermore, we show that the frequency shift of nanowire resonator due to mass adsorption is determined by its length, whereas the frequency shift is almost independent of its thickness. This study enables a design principle providing an insight into how the dynamic and sensing performances of nanomechanical resonator is determined and tuned.

Keywords: boundary condition; mass sensing; nanomechanical resonator; surface elasticity

1. Introduction

For a recent decade, nanoscale devices have been highlighted owing to their various applications such as bio/chemical detection (Waggoner and Craighead 2007, Eom *et al*. 2011), water treatment (Falk *et al*. 2010, Azamat 2021), ion transport (Lee *et al*. 2010), and so forth. For instance, nanomechanical resonators have recently received attention due to their notable ability to detect and sense various physical quantities such as quantum state (LaHaye *et al*. 2004, Chan *et al*. 2011, Poot and van der Zant 2012), atomic mass (Yang *et al*. 2006, Gil-Santos *et al*. 2010, Hiebert 2012), (bio)molecular mass (Ilic *et al*. 2004, Ilic *et al*. 2005, Kwon *et al*. 2007, 2009, Lee *et al*. 2008, Hanay *et al*. 2012, Choi *et al*. 2017) and (bio)molecular elastic properties (Gupta *et al*. 2006, Tamayo *et al*. 2006). The ability of resonators to detect and sense these quantities is attributed to their high-frequency dynamic behavior, which originates from the scaling down of a resonator. Specifically, classical Euler-Bernoulli beam theory provides that the frequency (ω) of a resonator is inversely proportional to the square of its length (L), *i.e.* $\omega \propto L^{-2}$ (Meirovitch 1967). As the length of a resonator is scaled down to a few micrometers (~ 1 μm), the frequency of a nanomechanical resonator lies in a range of mega-Hertz (MHz) to giga-Hertz (GHz) (Huang *et al*. 2005, Feng *et al*. 2007). This indicates that nanomechanical resonators are a high-frequency device serving as an actuator. In addition, this high-frequency nanomechanical device has been employed for detecting and sensing a few atoms or molecules (Ilic *et al*. 2005, Yang *et al*. 2006, Hanay *et al*. 2012), because the change of frequency dynamics due to atomic (or molecular) adsorption onto a resonator's surface can be precisely measured. In particular, the atomic (or molecular) adsorption leads to the increase of a resonator's overall mass and, consequently, the decrease of its frequency (Braun *et al*. 2005, Eom *et al*. 2011).

To design and develop a nanomechanical resonator serving as a highly sensitive device for detecting a few atoms or molecules, it is of high importance to quantitatively understand the frequency behavior of nanomechanical resonators and their frequency shift due to atomic (or molecular) adsorption. The atomistic simulation has recently been employed for characterizing the frequency dynamics of nanoscale systems (Eom *et al*. 2011, Eom 2020) such as carbon nanotubes (Zhao *et al*. 2003), graphene (Kim and Park 2009), and metal nanowires (Kim and Park 2008). Although this simulation enables the accurate characterization of the vibration dynamics of nanoscale structures, it is computationally restrictive for studying the frequency dynamics of nanomechanical resonators with their dimensions comparable to those of experimentally developed resonators, which is attributed to the large degrees of freedom for the millions or billions of atoms in the nanomechanical resonators (Eom *et al*. 2011). This has led many researchers to employ a continuum elastic model for studying the vibration dynamics of nanoscale structures. Specifically, the frequency dynamics and frequency shift of nanomechanical resonators in response to mass adsorption have been theoretically characterized based on classical elastic models such as Euler-Bernoulli beam model (Timoshenko and Goodier 1970) and/or von-Karman plate model (Timoshenko 1940). For example, classical Euler-Bernoulli beam model has

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been employed to characterize the frequency dynamics of microcantilever devices and their frequency shift due to molecular adsorption onto the cantilever's surface (Braun *et al*. 2005, Kwon *et al*. 2007). This elastic beam model has been also utilized for analyzing the frequency dynamics of nanowire resonators (Postma *et al*. 2005, Feng *et al*. 2007) and their sensing performances (Dai *et al*. 2009). The elastic plate model has been considered for quantitatively understanding the high-frequency dynamics of graphene resonators (Atalaya *et al*. 2008, Dai *et al*. 2012, Kim *et al*. 2016).

Though the classical elastic model (*e.g*. Euler-Bernoulli beam model) is able to capture the high-frequency dynamics of nanomechanical resonators and their sensing performances, this elastic model is unable to accurately depict the dynamic behavior of the resonators due to the scaling down-driven finite size effect such as surface effect (Rayleigh 1890, Shuttleworth 1950, Cammarata 1994, Ibach 1997, Freund and Suresh 2003). Specifically, for a case of nanowire resonator, as the surface-to-volume ratio is remarkably increased, a surface stress produced at the surface of a nanowire becomes to play a critical role on its mechanical deformation and vibration behavior (Jiang *et al*. 2006, Park 2008, Park and Klein 2008, Yun and Park 2009). To understand the effect of surface stress in the mechanical deformation and vibration behaviors of a nanomechanical resonator, a nonlocal elastic model provided by Eringen (1983) has recently been widely employed (Pin *et al*. 2006, Adali 2009, Azandariani *et al*. 2022, Balci 2022, Yi 2022). However, this nonlocal elastic model is unable to provide direct physical insight into the effect of surface stress, since this model requires phenomenological nonlocal parameters that have to be determined by fitting the results to experimental data or atomistic simulation results (Eringen 1983). Besides the nonlocal elastic model, a surface elasticity model has been considered as an alternative approach for studying the surface stress effect (Miller and Shenoy 2000, Sharma *et al*. 2003, Dai *et al*. 2011). In particular, the surface elastic model has allowed for quantitatively studying the mechanical deformation, vibration, and buckling of nanomechanical systems. For instance, the surface elastic model was considered along with Laplace-Young equation for analyzing the deformation and vibration behaviors of nanowires (He and Lilley 2008, Wang and Feng 2009). It should be noted that the Laplace-Young equation used in the previous studies (He and Lilley 2008, Wang and Feng 2009) violates the Newton's third law, by which the frequency dynamics of a nanowire is shown to be unaffected by a constant surface stress (Eom *et al*. 2011). Recently, we studied the frequency behavior and sensing performances of a nanowire resonator by considering an equation of motion for the surface elasticity-based beam model (Dai *et al*. 2011). It is found that strain-dependent surface stress (*i.e*. surface elastic stiffness) makes a critical effect on not only the frequency dynamics of a nanowire resonator but also its frequency shift in response to mass adsorption (Dai *et al*. 2011). In addition, the surface elasticity-based beam model was also considered for studying the frequency response of a nanoscale or microscale cantilever device to atomic mass adsorption (Lu *et al*. 2005). A previous study by Lu *et al*. (2005) showed the important role of surface stress on the frequency response of a cantilever device to atomic mass adsorption.

Despite recent efforts that have been made to quantitatively understand the effect of surface stress in the frequency dynamics and sensing performances of a nanowire resonator, it has not been understood how the effect of surface stress is dependent on boundary conditions. We note that previous studies by He and Lilley (2008) showed a role, which boundary conditions play in the constant surface stress-dependent deformation and frequency behaviors of a nanowire. However, as Laplace-Young equation used in these previous studies by He and Lilley (2008) violates the Newton's third law, these previous studies do not correctly provide insight into how the boundary conditions govern the surface stress effect on the vibration behavior of a nanowire resonator. Moreover, the effect of boundary condition on the sensing performance of nanowire resonator has remained elusive. In this work, we consider a surface elasticity-based Euler-Bernoulli beam model for quantitatively studying the frequency dynamics of a nanowire resonator and its frequency shift due to mass adsorption. We also investigate how the sensing performance of a nanowire resonator is affected by not only boundary conditions but also its size such as length and thickness.

2. Theory and model

2.1 Surface elasticity-based Euler-Bernoulli beam model

As the surface-to-volume ratio of a nanowire resonator increases due to its scaling down to sub-micro-meter, the surface stress plays a crucial role in the mechanical behavior of a resonator. It should be noted that as shown in Fig. 1a, the dimension of a resonator is given by b (width) × h (thickness) × L (length). The surface elasticity states that the surface stress (τ) is given by $\tau = \tau_0 + E_S\varepsilon$ (Rayleigh 1890, Shuttleworth 1950, Freund and Suresh 2003), where τ_0, E_S, and ε represent a constant surface stress, surface elastic stiffness (*i.e*. strain-dependent surface stress), and mechanical strain, respectively. As described earlier (Gurtin and Murdoch 1975, Gurtin *et al*. 1976), Newton's third law demonstrates that the surface stress results in producing a residual stress (σ_R) acting on the cross-sectional area of a resonator. The force equilibrium is written in the form of

$$\int_{-h/2}^{h/2} s_B\,dz + \int_{-h/2}^{h/2} t\cdot d\left(z \pm \frac{h}{2}\right)dz + \int_{-h/2}^{h/2} s_R\,dz = 0 \qquad (1)$$

Here, σ_B is the bending stress given as $\sigma_B = E\kappa z$ with E, κ and z being the elastic modulus of a nanowire, its bending curvature, and a coordinate defined along the direction of a nanowire's thickness, respectively, and $\delta(z)$ is a Dirac delta function. The bending moment acting on a nanowire is given by

$$M = b\int_{-h/2}^{h/2} z s_B\,dz + b\int_{-h/2}^{h/2} z t\cdot d\left(z \pm \frac{h}{2}\right)dz + b\int_{-h/2}^{h/2} z s_R\,dz \qquad (2)$$

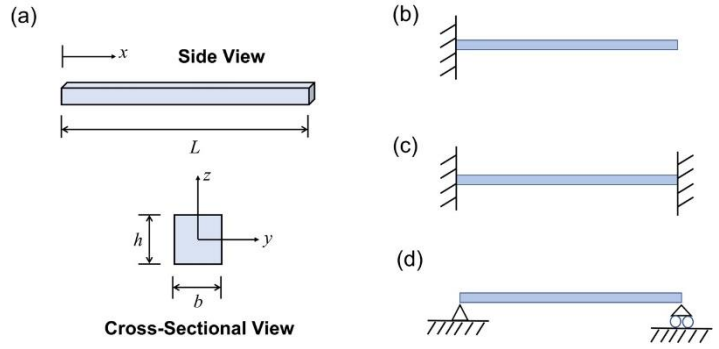


Fig. 1 (a) Schematic illustration of nanowire resonator. (b) Cantilever boundary condition applied to the resonator. (c) Double-clamping boundary condition applied to the resonator. (d) Simple support boundary condition applied to the resonator

Based on Eqs. (1) and (2), the bending moment can be represented in the following form.

$$M = \left(EI + \frac{E_S bh^2}{2} \right) k = \left(EI + \frac{E_S bh^2}{2} \right) \frac{\partial^2 u}{\partial x^2} \tag{3}$$

where I is the cross-sectional moment of inertia for a nanowire resonator, given as $I = bh^3/12$, u is the transverse deflection of a nanowire, and x is a coordinate defined along the longitudinal direction of a nanowire.

2.2 Equation of motion for the vibration of a nanowire

The equation of motion for a vibrating nanowire resonator is given by

$$\frac{\partial^2}{\partial x^2} M(x,t) + \eta \frac{\partial^2}{\partial t^2} u(x,t) = 0 \tag{4}$$

Here, η is a mass per length for a nanowire, and t is the time. With assuming the small deflection amplitude of a nanowire, the transverse deflection $u(x, t)$ can be written as $u(x, t) = \phi(x) \cdot \exp[j\omega t]$, where ω is the frequency of a nanowire, $\phi(x)$ is a (mode) shape function, and j is a unit of a complex number. Based on Eqs. (3) and (4), the equation of motion becomes

$$\frac{d^2}{dx^2} \left[\left(EI + \frac{E_S bh^2}{2} \right) f''(x) \right] - w^2 h \cdot f(x) = 0 \tag{5}$$

Here, a prime indicates a differentiation with respect to a coordinate, *i.e.* $\phi'(x) = d\phi(x)/dx$. The different boundary conditions applied to the resonator are shown in Fig. 1(b) – (d). It should be noted that the shape function $\phi(x)$ satisfies a boundary condition as follows.

Cantilever (CA) boundary condition:

$$f(0) = f'(0) = f''(L) = f'''(L) = 0 \tag{6a}$$

Double-clamping (DC) boundary condition:

$$f(0) = f'(0) = f(L) = f'(L) = 0 \tag{6b}$$

Simple-support (SS) boundary condition:

$$f(0) = f''(0) = f(L) = f''(L) = 0 \tag{6c}$$

By multiplying a shape function into Eq. (5) followed by integration by parts, the equation of motion provides the frequency (ω) of a nanowire resonator in the form of

$$w^2 = \frac{\Lambda + \int_0^L \left(EI + \frac{E_S bh^2}{2} \right) \left[f''(x) \right]^2 dx}{\int_0^L h \left[f(x) \right]^2 dx} \tag{7a}$$

where

$$\Lambda = \left[\left(EI + \frac{E_S bh^2}{2} \right) f'''(x) \cdot f(x) \right]_{x=0}^{x=L} - \left[\left(EI + \frac{E_S bh^2}{2} \right) f''(x) \cdot f'(x) \right]_{x=0}^{x=L} \tag{7b}$$

It should be noted that since the shape function $\phi(x)$ satisfies the boundary condition given by Eq. (6), the parameter Λ becomes zero, *i.e.* $\Lambda = 0$. With introducing a normalized coordinate such as $\xi = x/L$, the frequency (ω) of a nanowire resonator can be measured from a following equation.

$$w^2 = L^{-4} \cdot \frac{\int_0^1 \left(EI + \frac{E_S bh^2}{2} \right) \left[f''(x) \right]^2 d\xi}{\int_0^1 h \left[f(x) \right]^2 d\xi} \tag{8}$$

In order to find the frequency of a nanowire resonator based on Eq. (8), we need to consider a shape function for a given boundary condition such as

CA boundary condition:

$$f(x) = \left[\cos(\lambda x) - \cosh(\lambda x) \right] - B \left[\sin(\lambda x) - \sinh(\lambda x) \right] \tag{9a}$$

DC boundary condition: $f(x) = \sqrt{\frac{2}{3}} \left[1 - \cos(2\pi x) \right]$ (9b)

SS boundary condition: $f(x) = \sin(\pi x)$ (9c)

where λ is a constant that satisfies a transcendental equation such as $\cos\lambda \cdot \cosh\lambda + 1 = 0$, and B is a constant given by $B = (\cos\lambda + \cosh\lambda)/(\sin\lambda + \sinh\lambda)$. For each type of boundary condition, the frequency of a nanowire resonator can be computed from Eqs. (8) and (9).

2.3 Frequency response of a nanowire resonator to atomic mass adsorption

In order to quantitatively understand the frequency response of a nanowire resonator to atomic mass adsorption, we consider that a few atoms are locally adsorbed onto the surface of the nanowire at a coordinate $x = a$ (where $0 \le a \le L$). In this work, we assume that the size of an adsorbed atom is much smaller than the thickness of a nanowire resonator. For such an assumption, the frequency response of a nanowire becomes to depend on the mass of adsorbed atoms. We note that as described in a previous study by Gupta *et al*. (2006), when the size of adsorbed atoms (or molecules) becomes comparable to the thickness of a resonator, its frequency response begins to be dependent on not only the mass of adsorbed atoms (or molecules) but also their stiffness.

For atomic (or molecular) adsorption at a coordinate $\xi = \alpha$ (where $\alpha = a/L$), an effective mass per unit length for the atomic mass-adsorbed resonator is given by

$$h_{eff}(x) = \rho A + \Delta m \cdot \delta(x - a) \tag{10}$$

where ρ and A represent the mass density and cross-sectional area of a bare resonator (*i.e*. without any mass adsorption), respectively, Δm is the total mass of adsorbed atoms (or molecules), and $\delta(\xi)$ is a Dirac delta function. From Eqs. (8) and (10), the frequency (ω_{ads}) of the atomic mass-adsorbed resonator as a function of adsorbed mass Δm is given by

$$\omega_{ads}^2(\Delta m, a) = L^{-4} \cdot \frac{\int_0^1 \left(EI + \frac{E_S b h^2}{2} \right) \left[f''(x) \right]^2 dx}{\rho A \int_0^1 \left[f(x) \right]^2 dx + \Delta m \left[f(a) \right]^2} \tag{11}$$

Then, the frequency shift ($\Delta\omega$) due to mass adsorption (Δm) can be computed such as

$$\Delta\omega(\Delta m, a) = \omega_{ads}(\Delta m, a) - \omega_{ads}(0, a) \tag{12}$$

Here, it should be noted that the frequency shift of a resonator due to mass adsorption is a function of not only the amount of adsorbed mass but also the location of mass adsorption.

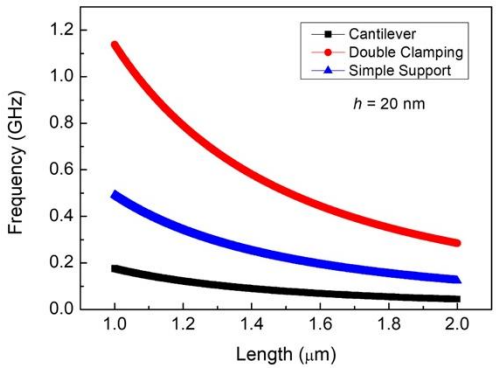
3. Results

3.1 Effect of boundary condition on the frequency dynamics of nanowire resonator

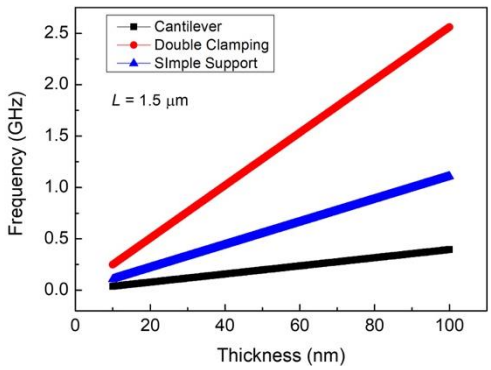
As a silicon nanowire has been extensively employed for developing the nanomechanical resonator (Feng *et al*. 2007, Gil-Santos *et al*. 2010, Postma *et al*. 2005, Verbridge *et al*. 2007), we study the frequency dynamics of a silicon nanowire resonator as a function of its size (*e.g*. length and thickness) and boundary conditions. For silicon nanowire, its elastic modulus E and mass density ρ are given by E = 179 GPa and ρ = 2320 kg/m^3, respectively, based on the material properties of bulk silicon, while the surface elastic stiffness of silicon nanowire is given as E_S = –18.1 N/m based on the atomistic simulation result (Miller and Shenoy 2000). Fig. 2(a) shows the resonant frequency of silicon nanowires (with their thickness of 20 nm) as a function of their length and boundary conditions. It is found that the frequency of silicon nanowires is inversely proportional to the square of their length. This is consistent with Euler-Bernoulli beam theory (Meirovitch 1967), which suggests the frequency (ω) of a nanowire in the form of $\omega = (\theta/L)^2(E_{eff}I/\rho A)^{1/2}$, where θ is a boundary condition-dependent constant, and E_{eff} is the size-dependent effective elastic modulus of a silicon nanowire. Moreover, it is shown that the frequency dynamics of silicon nanowire is significantly dependent on boundary conditions. The resonant frequency of a silicon nanowire is measured in the order of DC > SS > CA. This is congruent with classical Euler-Bernoulli beam theory, which provides that the boundary condition-dependent constant θ is in the order of DC > SS > CA (Meirovitch 1967). As illustrated in Fig. 2(b), the frequency of silicon nanowires depends on their thickness in such a way that their resonant frequency is linearly proportional to their thickness. This result is consistent with the classical Euler-Bernoulli beam theory, which provides the frequency (ω) in the form of $\omega = h(\theta/L)^2(E_{eff}/12\rho)^{1/2}$ with h being the thickness of a nanowire resonator. In addition, the thickness-dependent frequency of silicon nanowire is found to be in the order of DC > SS > CA. The results shown in Fig. 2(a) and (b) clearly suggest the important role of boundary condition on the frequency of a silicon nanowire, which implies that the sensing performance (*i.e*. frequency shift driven by mass adsorption) of the nanowire resonator depends on the boundary condition (for more details, see Section 3.3).

3.2 Role of boundary condition on the size-dependent elastic properties of nanowire

Now, we investigate how the boundary condition affects the size-dependent elastic properties of silicon nanowires. As reported in previous studies by Miller and Shenoy (2000) and Park *et al*. (2009), the size-dependent elastic properties of metal nanowires are attributed to the surface stress, which originates from the imbalance between the atomic bond coordination of bulk and surface atoms for a nanowire. For a recent decade, force probe-based experimental studies (Wu *et al*. 2005, Agrawal *et al*. 2008, McDowell *et al*. 2008a, Zhu *et al*. 2009) and atomistic simulation-based studies (Park and Klein 2007, Agrawal *et al*. 2008, McDowell *et al*. 2008b) have confirmed that the surface stress results in the size-dependent elastic modulus of metal nanowires. Despite these previous experimental and computational studies, the role of boundary condition in the surface stress-driven size-dependent elastic properties of nanowires has remained elusive. Here, we measured the size-dependent effective elastic modulus (E_{eff}) of a silicon nanowire based on a classical Euler-Bernoulli beam theory, which suggests the effective elastic modulus in the form of $E_{eff} = 12(\rho/h^2)(L/\theta)^4\omega^2$ with ω being the frequency of the nanowire. As shown in Fig. 3, the effective elastic modulus of silicon nanowires depends on their thickness in such a



(a)



(b)

Fig. 2 (a) Frequency of silicon nanowire resonators (with their thickness of 20 nm) with respect to their length and boundary conditions. (b) Frequency of silicon nanowires (with their length of 1.5 μm) as a function of their thickness and boundary condition

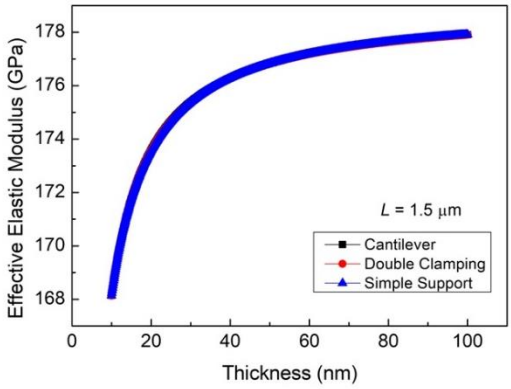


Fig. 3 Effective elastic modulus of a silicon nanowire (with its length of 1.5 μm) as a function of its thickness with different boundary conditions

way that as their thickness decreases, so does their effective elastic modulus. This scaling down-driven decrease of elastic modulus for a silicon nanowire is attributed to a negative surface elastic stiffness, which is consistent with previous results (Lee and Rudd 2007, Zhu *et al.* 2009). More interestingly, it is found that the size-dependent effective elastic modulus of a silicon nanowire is independent of boundary conditions. This result is in contrast to the previous findings of He and Lilley (2008), who showed that the size-dependent elastic modulus of metal nanowires is critically governed by boundary conditions. The discrepancy between our results and previous results (He and Lilley 2008) is ascribed to the fact that the Laplace-Young equation used in previous studies by He and Lilley (2008) violates the Newton's third law. Specifically, He and Lilley (2008) did not consider the residual stress produced as a reaction against the surface stress in the Laplace-Young equation.

In order to theoretically understand the silicon nanowire's size-dependent elastic modulus and its independence of boundary condition, we revisit a theoretical model given by Eq. (8). Specifically, based on Eq. (8), the resonant frequency of a silicon nanowire can be written as

$$w = \left(\frac{q}{L}\right)^2 \sqrt{\frac{EI}{rA}\left(1+\frac{E_S b h^2}{2EI}\right)} \tag{13a}$$

where θ is a boundary condition-dependent constant given as

$$q = \left[\int_0^1 \left[f''(x)\right]^2 dx \Big/ \int_0^1 \left[f(x)\right]^2 dx\right]^{\frac{1}{4}} \tag{13b}$$

Based on the Euler-Bernoulli beam theory providing the resonant frequency in the form of $\omega = (\theta/L)^2(E_{eff}I/\rho A)^{1/2}$, the effective elastic modulus (E_{eff}) of a silicon nanowire can be represented in the following form

$$\frac{E_{eff}}{E} = 1 + 6\left(\frac{E_S}{E}\right) h^{-1} \tag{14}$$

The Eq. (14) clearly demonstrates that the effective elastic modulus of a silicon nanowire is only dependent on the thickness of the nanowire, which is consistent with the simulation result (Fig. 3).

In summary, our results provide that while the boundary conditions affect the frequency of a silicon nanowire, they do not make any effect on the surface stress-induced size-dependent elastic modulus of a silicon nanowire.

3.3 Effect of boundary condition on the sensing performance of silicon nanowire resonator

In order to understand the sensing performance of a nanowire resonator, we consider the frequency shift of a silicon nanowire resonator with its dimension of L = 1.5 μm and $b = h$ = 20 nm in response to the mass adsorption of Δm = 1 zg (where 1 zg = 10^{-21} g). Here, the frequency shift of a silicon nanowire resonator was computed from Eq. (12) with setting Δm = 1 zg. Then, the frequency shift ($\Delta\omega$) of a silicon nanowire in response to the adsorbed mass of 1 zg becomes to be a function of a value α (*i.e.* the location of mass adsorption). Fig. 4 depicts the frequency shift of a silicon nanowire with respect to the location of mass adsorption (*i.e.* α) and boundary condition. It is shown that the frequency shift due to mass adsorption reaches a maximum at α = 0.5 for DC and SS boundary conditions, while it is maximized at α = 1 for CA boundary condition.

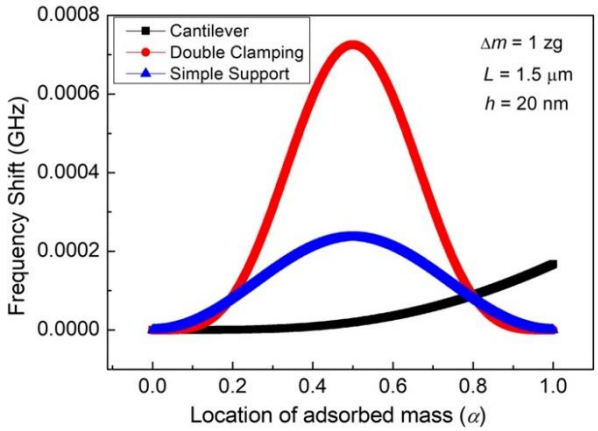


Fig. 4 Frequency shift of a silicon nanowire resonator (with its dimension of L = 1.5 μm and $b = h$ = 20 nm) in response to the mass adsorption of 1 zg with respect to the location of mass adsorption and boundary conditions

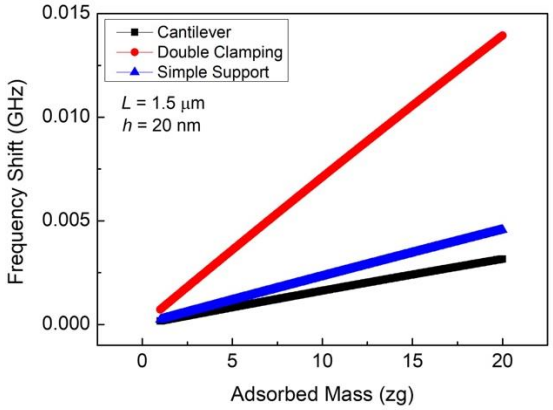


Fig. 5 Frequency shift of silicon nanowire resonator (with its dimension of L = 1.5 μm and $b = h$ = 20 nm) in response to mass adsorption as a function of the amount of adsorbed mass

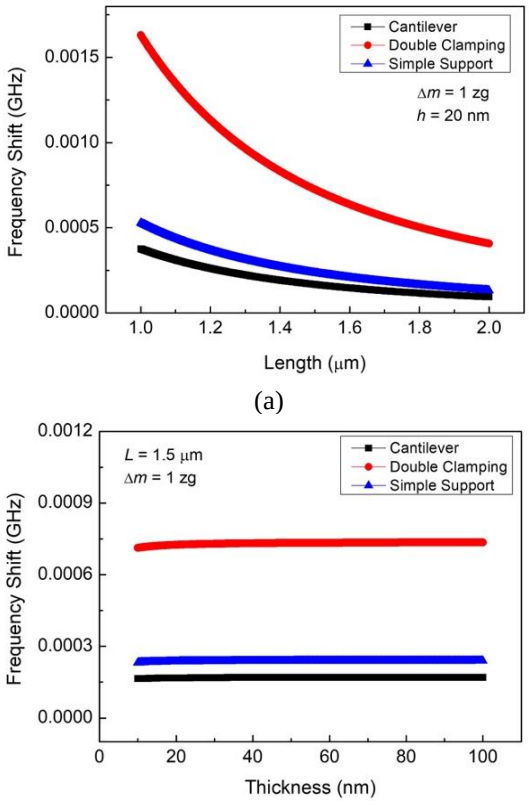


Fig. 6 (a) Frequency shift of a silicon nanowire resonator (with its thickness of 20 nm) in response to the adsorbed mass of 1 zg as a function of the resonator's length. (b) Frequency shift due to the adsorbed mass of 1 zg with respect to the resonator's thickness

This suggests that DC and SS boundary conditions result in the maximum frequency shift due to mass adsorption occurring at $x = L/2$ (*i.e.* at a distance of half-length from a one-end), while CA boundary condition leads to the maximum frequency shift for mass adsorption at $x = L$ (*i.e.* at a distance of length L from a fixed end). The behaviour of frequency shift due to mass adsorption with dependence on α for different boundary conditions can be theoretically understood with using Eqs. (9), (11), and (12). In particular, the frequency shift due to mass adsorption becomes to maximize when a shape function $\phi(\xi)$ reaches a maximum value. By setting $d\phi(\xi)/d\xi = 0$, the value of α for maximal frequency shift is found to be $\alpha = 0.5$ for DC and SS boundary conditions, and $\alpha = 1$ for CA boundary condition. The magnitude of maximum frequency shift due to mass adsorption is measured in the order of DC > SS > CA. This behaviour of frequency shift due to mass adsorption with respect to boundary conditions is comparable to that of the frequency of a bare resonator (*i.e.* without mass adsorption) as described in Fig. 2. Specifically, as the frequency of a bare resonator is measured in the order of DC > SS > CA (*i.e.* Fig. 2), the frequency shift due to mass adsorption is estimated in the same order, *i.e.* DC > SS > CA (*i.e.* Fig. 4). This clearly shows that boundary conditions affect not only the frequency dynamics of a nanowire resonator but also its frequency shift in response to mass adsorption.

Now, we numerically investigate the mass sensitivity of a silicon nanowire resonator with its dimension of L = 1.5 μm and $b = h$ = 20 nm. Here, the mass sensitivity is defined as $S = \Delta\omega/\Delta m$. For the adsorbed mass of 1 to 20 zg, as shown in Fig. 5, the frequency shift due to mass adsorption is linearly proportional to the amount of adsorbed mass. In other words, the mass sensitivity (S) of a nanowire resonator is a constant for the case of adsorption of a few atoms (with their total mass up to 20 zg). More remarkably, the mass sensitivity of a nanowire resonator is critically dependent on the boundary condition. The mass sensitivity was measured as $S_{DC} = 6.97 \times 10^{-4}$ GHz/zg for DC boundary condition, $S_{SS} = 2.28 \times 10^{-4}$ GHz/zg for SS boundary condition, and $S_{CA} = 1.58 \times 10^{-4}$ GHz/zg for CA boundary condition, respectively. This illustrates that the mass sensitivity of a nanowire resonator is significantly determined by boundary conditions. For highly sensitive mass detection, the DC boundary condition is preferable in comparison with other boundary conditions. In particular, the mass sensitivity of a nanowire resonator is evaluated in the order of DC > SS > CA, as similar to the case of

frequency.

As the frequency dynamics of a nanowire resonator is determined by its dimension such as length and thickness, we scrutinize the sensing performance of a nanowire resonator with respect to its dimension. Fig. 6a shows the frequency shift due to the adsorbed mass of 1 zg (for a resonator with its dimension of $b = h = 20$ nm) as a function of the resonator's length. As expected, the DC boundary condition leads to the higher frequency shift due to the adsorbed mass of 1 zg in comparison with other boundary conditions. Interestingly, it is shown that the frequency shift due to the adsorbed mass is inversely proportional to the square of the resonator's length. This is attributed to the fact that the frequency shift due to the adsorbed mass is linearly proportional to the frequency of a bare resonator (Braun *et al*. 2005, Kwon *et al*. 2007), which is inversely proportional to the square of a resonator's length.

Furthermore, we study how the thickness of a resonator affects its frequency shift due to mass adsorption. As shown in Fig. 6b, it is remarkably found that the frequency shift due to the adsorbed mass of 1 zg is almost independent of the resonator's thickness. Specifically, the frequency shift due to the adsorbed mass of 1 zg is measured as $\Delta\omega_{DC}$ = 7.12 MHz for DC boundary condition, $\Delta\omega_{SS}$ = 2.31 MHz for SS boundary condition, and $\Delta\omega_{CA}$ = 1.64 MHz for CA boundary condition, respectively. Though the frequency shift due to mass adsorption is independent of the resonator's thickness, the frequency shift is governed by boundary conditions in such a way that the DC boundary condition results in the higher frequency shift in comparison with other boundary conditions. Our results shown in Fig. 6 suggest that the frequency response of a nanowire resonator to mass adsorption is determined by its length, while its thickness does not play any role in the frequency shift due to the mass adsorption.

4. Discussion

In this study, we have considered the effect of adsorbed mass in the resonant frequency shift of a silicon nanowire resonator, while there might be other effects (*e.g*. adsorbate stiffness, or intermolecular interactions between adsorbed atoms or molecules) that determine the frequency shift of a resonator due to atomic (or molecular) adsorption. For example, as described in previous studies (Eom *et al*. 2007, Zheng *et al*. 2009), when biomolecules (*e.g*. DNA) are adsorbed onto the nanomechanical resonator, the intermolecular interactions between biomolecules may play a role on the dynamic response of nanomechanical resonator. The surface stress driven by biomolecular interactions is estimated in the order of <0.01 N/m (Lu *et al*. 2005, Wu *et al*. 2005), which is much smaller than the surface elastic stiffness (*i.e*. E_S = –18.1 N/m) of a silicon nanowire. This implies that the surface stress induced by biomolecular interactions can be ignored in comparison with strain-dependent surface stress (*i.e*. surface elastic stiffness) of a silicon nanowire for understanding the frequency response of silicon nanowire resonator to the atomic (or molecular) adsorption. As the purpose of this study is to understand how the size of a nanowire resonator affects its frequency dynamics and response to molecular adsorption, we neglect the biomolecular interaction-driven surface stress that is much smaller than the strain-dependent surface stress of silicon nanowire. In addition, as reported in previous studies (Tamayo *et al*. 2006, Gupta *et al*. 2006), the elastic stiffness (*i.e*. elastic modulus) of adsorbed (bio)molecules affects the resonance behavior of nanomechanical resonator. However, in this work, the elastic modulus of a silicon nanowire is larger by four orders of magnitude than that of biological molecules (*e.g*. proteins and DNA), which implies that the elastic properties of adsorbed biomolecules can be neglected for the resonant frequency shift of a silicon nanowire resonator due to (bio)molecular adsorption. Specifically, the elastic modulus of protein molecules is measured in the order of 0.1 GPa (Yoon *et al*. 2009), while the elastic modulus of a silicon nanowire is given as 179 GPa. This indicates that the frequency response of nanomechanical resonator to (bio)molecular adsorption may not be affected by the elastic properties of adsorbed (bio)molecules. Overall, though there might be the effect of adsorbate intermolecular interactions or adsorbate stiffness in the frequency behavior of a nanomechanical resonator, as described in this work, these effects may be neglected for silicon nanowire resonator-based detection.

In addition, in order to gain a detailed insight into the mass sensitivity of a silicon nanowire resonator, we revisit a theoretical model which provides the frequency of the mass-adsorbed resonator, *i.e*. Eq. (11). In particular, based on Taylor's series expansion of Eq. (11), the frequency of mass-adsorbed resonator is given as

$$\omega_{ads} \approx \omega - \frac{1}{2}L^{-2}\cdot\frac{\Delta m\left[\phi(\alpha)\right]^2}{\rho A\int_0^1\left[\phi(\xi)\right]^2 d\xi}\cdot\left[\frac{\left(EI+\frac{E_S bh^2}{2}\right)\int_0^1\left[\phi''(\xi)\right]^2 d\xi}{\rho A\int_0^1\left[\phi(\xi)\right]^2 d\xi}\right]^{\frac{1}{2}} \quad (15)$$

Consequently, the mass sensitivity of the resonator can be written as

$$S \equiv \frac{\Delta\omega}{\Delta m} = -\frac{1}{2}\left(\frac{\theta}{L}\right)^2\frac{\left[f(a)\right]^2}{\rho A\int_0^1\left[f(x)\right]^2 dx}\sqrt{\frac{EI+E_S bh^2/2}{\rho A}} \quad (16)$$

where a parameter θ is a boundary condition-dependent constant given by Eq. (13.b). As illustrated in Eq. (16), the mass sensitivity is governed by not only the size of the resonator, *i.e*. length (L), width (b) and thickness (h), and the location of mass adsorption (*i.e*. α) but also the boundary condition related to the mode shape function $\phi(\xi)$ (or boundary condition-dependent constant θ). We note that the mass sensitivity is proportional to θ^2, and that as the boundary condition-dependent constant θ is in the order of DC > SS > CA, the mass sensitivity (S) of the resonator is in the order of DC > SS > CA, which is consistent with the simulation result (*i.e*. Fig. 5). More importantly, as described in Eq. (16), the mass sensitivity of the resonator is strongly affected by its length in such a way that the mass

sensitivity is inversely proportional to the square of the length. This is consistent with simulation result shown in Fig. 6(a). The result clearly suggests that the mass sensitivity of the resonator can be improved by the scaling down of the resonator (*i.e*. the decrease of the resonator's length).

5. Conclusions

In this work, we study how the boundary conditions make an effect on the frequency dynamics and sensing performances of a silicon nanowire resonator by using a surface elasticity-based modeling and simulations. We developed a theoretical model based on the surface elasticity coupled to Euler-Bernoulli beam model for quantitatively characterizing the frequency dynamics of a nanowire resonator and its frequency response to mass adsorption. We show that while the boundary conditions affect the frequency dynamics of a nanowire resonator, its size-dependent elastic modulus due to the surface stress is independent of the boundary conditions. This suggests that the size-dependent elastic modulus of a nanowire is an intrinsic property that does not depend on the boundary conditions. We found that the DC boundary condition leads to the higher detection sensitivity of a nanowire resonator in comparison with the case of other boundary conditions. Interestingly, the frequency shift of a nanowire resonator in response to mass adsorption is governed by its length, but the frequency shift is independent of its thickness. Our results highlight that the sensing performance of a nanowire resonator is determined by its length and boundary conditions. Our study provides a design principle showing how the frequency dynamics and sensing performances of a nanowire resonator can be determined and/or tuned. Moreover, our model can be further extended for studying the mechanical behaviors (*e.g*. deformation, vibration, bucking, etc.) of nanoscale structures and systems, in which the effect of surface stress becomes to play a dominant role.

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