

Quantifying the size-dependent effect of the residual surface stress on the resonant frequencies of silicon nanowires if finite deformation kinematics are considered

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2009 Nanotechnology 20 115701

(<http://iopscience.iop.org/0957-4484/20/11/115701>)

[The Table of Contents](#) and [more related content](#) is available

Download details:

IP Address: 128.138.222.50

The article was downloaded on 25/02/2009 at 13:58

Please note that [terms and conditions apply](#).

Quantifying the size-dependent effect of the residual surface stress on the resonant frequencies of silicon nanowires if finite deformation kinematics are considered

Harold S Park

Department of Mechanical Engineering, University of Colorado, Boulder, CO 80309, USA

E-mail: harold.park@colorado.edu

Received 1 December 2008, in final form 31 December 2008

Published 25 February 2009

Online at stacks.iop.org/Nano/20/115701

Abstract

There are two major objectives to the present work. The first objective is to demonstrate that, in contrast to predictions from linear surface elastic theory, when nonlinear, finite deformation kinematics are considered, the residual surface stress does impact the resonant frequencies of silicon nanowires. The second objective of this work is to delineate, as a function of nanowire size, the relative contributions of both the residual (strain-independent) and the surface elastic (strain-dependent) parts of the surface stress to the nanowire resonant frequencies. Both goals are accomplished by using the recently developed surface Cauchy–Born model, which accounts for nanoscale surface stresses through a nonlinear, finite deformation continuum mechanics model that leads to the solution of a standard finite element eigenvalue problem for the nanowire resonant frequencies. In addition to demonstrating that the residual surface stress does impact the resonant frequencies of silicon nanowires, we further show that there is a strong size dependence to its effect; in particular, we find that consideration of the residual surface stress alone leads to significant errors in predictions of the nanowire resonant frequency, with an increase in error with decreasing nanowire size. Correspondingly, the strain-dependent part of the surface stress is found to have an increasingly important effect on the resonant frequencies of the nanowires with decreasing nanowire size.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Recently, semiconducting nanowires have drawn considerable interest from the scientific community due to their enhanced physical properties [1–3], which emerge due to their large surface area to volume ratio. Nanowires are also important as they will serve as the basic building blocks for future nanoelectromechanical systems (NEMS), which have been proposed for a multitude of cross-disciplinary applications, including chemical and biological sensing, force and pressure sensing, high frequency resonators, and many others [4–8]. Because many of the proposed applications for nanowire-based NEMS, such as resonant mass sensing and high frequency oscillators [6–8] rely on the ability to control and tailor the nanowire resonant frequencies with a high degree of precision,

it is critical to be able to predict and control variations in the nanowire resonant frequencies.

However, the resonant frequencies of nanowires can deviate from those expected from continuum beam theory [9–11] due to the effects of surface stresses [12–14], which act on the nanowire surfaces due to the fact that surface atoms have fewer bonding neighbors, and therefore a lower coordination number [15] than do bulk atoms. In the case of silicon, both experiment [10, 16, 17] and simulation [9, 18] have shown that surface stresses cause silicon nanowires to be elastically softer than bulk silicon.

Within the mechanics and physics communities, researchers have accounted for surface stress effects on the resonant properties of nanowires using linear surface elastic theory, which was developed more than 30 years ago by

Gurtin and Murdoch [19], in which a surface stress tensor is introduced to augment the bulk stress tensor typically utilized in continuum mechanics. Mathematically, the surface stress is decomposed into residual (strain-independent) and surface elastic (strain-dependent) terms [20–22] as

$$\boldsymbol{\tau}(\boldsymbol{\epsilon}) = \boldsymbol{\tau}^0 + \mathbf{S}\boldsymbol{\epsilon}, \quad (1)$$

$$\mathbf{S} = \left. \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{\epsilon}} \right|_{\boldsymbol{\epsilon}=0}, \quad (2)$$

where $\boldsymbol{\tau}^0$ is the residual (strain-independent) part of the surface stress $\boldsymbol{\tau}$, $\mathbf{S}\boldsymbol{\epsilon}$ is the surface elastic (strain-dependent) term and \mathbf{S} is the surface stiffness tensor. Note that (1) is written in terms of the infinitesimal strain tensor $\boldsymbol{\epsilon}$.

Gurtin *et al* [20] were also the first to show that, within the framework of linear elastic beam theory, the beam resonant frequency is independent of the residual surface stress $\boldsymbol{\tau}^0$. This finding has been validated by subsequent researchers, for example by Lu *et al* [21]. In contrast, recent work by Lachut and Sader [22] has shown that previous analytic models of surface stress effects on the resonant frequencies [23] that are based upon one-dimensional models violate Newton's third law. Lachut and Sader have further noted that the effects of the strain-independent part of the surface stress on the resonant frequencies can only be captured by fully three-dimensional models.

The conclusion that the beam resonant frequency is independent of the residual surface stress is obtained as follows. Within two-dimensional linear beam theory, the surface stress $\boldsymbol{\tau}$ can be viewed as a shear stress that acts on the beam surfaces; the surface stress thus contributes to a moment about the nanowire cross section. The moment is subsequently differentiated to obtain the beam equation of motion; because the residual surface stress $\boldsymbol{\tau}^0$ is a constant, it drops out once the differentiation occurs. In contrast, because the surface elastic part of the surface stress is strain-dependent, it does not drop out during the differentiation of the moment. Because it drops out during the differentiation of the moment, the residual surface stress is not found in the beam equation of motion, and therefore does not affect the beam resonant frequency. The mathematics and mechanics underlying the preceding discussion can be found in Gurtin *et al* [20] and Lu *et al* [21].

Having summarized linear surface elastic theory, we address two key questions that motivate the present work: (1) is a nonlinear, finite deformation constitutive theory necessary, and (2) if so, what quantitative differences in the nanowire resonant frequencies would result from linear surface elastic theory and nonlinear, finite deformation model and why? To answer the first question, finite deformation kinematics are necessary because recent studies [9, 18] have shown that silicon nanowires with sub-20 nm cross sections exhibit tensile strains due to surface stresses on the order of 0.1–1%. In contrast, we note that linear elasticity is generally valid for very small strains, i.e. on the order of 0.001% or smaller.

The answer to the second question requires further discussion. One consequence of linear surface elastic theory is that due to equilibrium requirements enforced

between the bulk and surface in deriving the surface elastic formulation [12, 19, 24], the surface stress in the surface elastic formulation is a 2×2 *in-plane* stress tensor, where the out-of-plane stress component must be zero to satisfy the mechanical equilibrium condition. The implication of this 2×2 in-plane surface stress tensor is that surface elastic formulations are unable to capture the surface-stress-driven tensile expansion that silicon nanowires are known to undergo [9, 18, 25]. Furthermore, due to the linear elastic constitutive response that is assumed for both the bulk and surface, the stiffness of both the bulk and surfaces are independent of any surface-stress-induced strain. Because of this, linear surface elastic theory cannot account for changes in the resonant frequency that occur due to changes in bulk or surface stiffness that arise from deformation induced by surface stresses.

We emphasize that the present work represents a substantial theoretical advancement as compared to previous work by Park [9], in which the surface Cauchy–Born (SCB) model was utilized to investigate surface stress effects on the resonant frequencies of silicon nanowires. However, it was not delineated in that work how the residual (strain-independent) and surface elastic (strain-dependent) parts of the surface stress contributed to the resonant frequency shift as compared to the bulk material for silicon nanowires. Because of this, it was also not determined whether the residual surface stress $\boldsymbol{\tau}^0$, in a nonlinear finite deformation formulation, does impact the resonant frequencies of silicon nanowires. Furthermore, it was not delineated how, as a function of nanowire cross sectional size, the residual (strain-independent) and surface elastic (strain-dependent) parts of the surface stress impact the resonant frequencies of silicon nanowires. In the present work, by delineating the size-dependent contributions of both parts of the surface stress as defined in (1), we quantify, for the first time, the errors introduced in modeling the nanowire resonant frequencies that are introduced by neglecting the residual (strain-independent) part of the surface stress $\boldsymbol{\tau}^0$.

Therefore, the purpose of the present work is to demonstrate that when nonlinear, finite deformation kinematics are considered, the residual surface stress does impact the resonant frequencies of silicon nanowires. A related objective is to delineate, as a function of nanowire size, the relative contributions of both the residual (strain-independent) and surface elastic (strain-dependent) parts of the surface stress on the nanowire resonant frequencies. Both goals are accomplished by using the recently developed SCB model [9, 26, 27], which is a nonlinear continuum mechanics model that accounts for nanoscale surface stress effects, to calculate the resonant frequencies of silicon nanowires. We first briefly describe the theory underlying the SCB model, then utilize it to achieve the stated objectives of this paper.

2. Modification to surface Cauchy–Born model to delineate the strain-independent and strain-dependent contributions to the resonant frequencies of silicon nanowires

The standard bulk Cauchy–Born (BCB) model is a multiscale, finite deformation constitutive model that enables the

calculation of continuum stress and stiffness directly from an underlying interatomic potential energy [26, 28–32]. However, because the BCB model does not account for critical nanoscale surface stress effects, the SCB model was recently developed by Park *et al* [26, 33, 34] to capture surface stress effects within the framework of the Cauchy–Born approximation. Because the SCB formulation for silicon was presented in previous works by Park *et al* [9, 26], we give a brief summary of the SCB model here, with a focus on presenting the methodology that is used to delineate the size-dependent contributions of both the strain-independent and strain-dependent parts of the surface stress to the resonant frequencies of silicon nanowires.

As noted in previous expositions on the SCB model for silicon [9, 26], the SCB model is based constructing a surface strain energy density $\gamma(\mathbf{C})$ of a representative surface unit cell, where $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ is the continuum stretch tensor, indicating that the SCB model is a nonlinear, finite deformation model. The surface energy density $\gamma(\mathbf{C})$ is calculated using the T3 parameters of the Tersoff potential [35]; it is further critical to note that the SCB surface energy density $\gamma(\mathbf{C})$ represents the actual surface energy of the surface unit cell, and not the excess in energy as compared to a representative bulk atom, which is how the surface energy is traditionally defined thermodynamically [12]. Once the surface energy density is known, the second surface Piola–Kirchhoff stress $\tilde{\mathbf{S}}(\mathbf{C})$ and the surface stiffness $\tilde{\mathcal{C}}(\mathbf{C})$ can be calculated by taking derivatives of the surface energy density $\gamma(\mathbf{C})$ with respect to the stretch tensor \mathbf{C} (see equations (30) and (31) in Park and Klein [26]).

We now articulate the methodology for separating the effects of the strain-independent and strain-dependent parts of the surface stress on the resonant frequencies of the silicon nanowires. The motivation for the current approach is drawn from equation (1), where the total surface stress $\tau(\epsilon)$ is composed of two parts, the residual (strain-independent) part τ^0 , and the surface elastic (strain-dependent) part $\mathbf{S}\epsilon$. As previously discussed, previous works that have utilized linear surface elastic theory to study surface stress effects on the resonant frequencies of nanowires have found that the residual (strain-independent) part of the surface stress τ^0 does not impact the nanowire resonant frequencies [20, 21].

The purpose of the present work is to investigate whether, if nonlinear, finite deformation kinematics are considered, the residual surface stress τ^0 does in fact impact the resonant frequencies of silicon nanowires, and to quantify the effect of the residual surface stress on the nanowire resonant frequencies with decreasing nanowire size. Therefore, a logical approach to delineating this effect is to subtract the surface elastic part of the surface stress $\mathbf{S}\epsilon$ from the surface stress that is defined in (1), and calculate the resulting nanowire resonant frequencies considering only the residual (strain-independent) surface stress τ^0 .

However, because the SCB model is a nonlinear, finite deformation model, it is not possible to entirely separate or subtract the surface elastic (strain-dependent) part of the surface stress. Therefore, the approximation utilized in the present work, which mirrors that of Park and Klein for metal nanowires [27], is to subtract the *linearized* strain-dependent surface stress such that effects of the strain-independent surface

stress can be studied. This is accomplished by modifying the SCB surface energy density $\gamma(\mathbf{C})$ as

$$\gamma(\mathbf{C}) \rightarrow \beta \left(\gamma(\mathbf{C}) - \frac{1}{2} \alpha \mathbf{E}^T \tilde{\mathcal{C}}_0 \mathbf{E} \right), \quad (3)$$

where $\mathbf{E} = 0.5(\mathbf{F}^T \mathbf{F} - \mathbf{I})$ is the Green strain tensor, α and β are adjustable parameters, and $\tilde{\mathcal{C}}_0$ is the undeformed surface stiffness, i.e. the SCB surface stiffness evaluated at $\mathbf{C} = \mathbf{I}$.

Due to the above modification of the SCB surface energy density, the SCB surface stress and surface stiffness must also be modified, as they are simply strain derivatives of the surface energy density. Upon taking derivatives of the modified surface energy density in (3) to get the modified surface stress and surface stiffness, the surface stress is modified as

$$\tilde{\mathbf{S}}(\mathbf{C}) \rightarrow \beta \tilde{\mathbf{S}}(\mathbf{C}) - \beta \alpha \tilde{\mathcal{C}}_0 \mathbf{E}, \quad (4)$$

while the surface stiffness is modified as

$$\tilde{\mathcal{C}}(\mathbf{C}) \rightarrow \beta \tilde{\mathcal{C}}(\mathbf{C}) - \beta \alpha \tilde{\mathcal{C}}_0. \quad (5)$$

In analyzing (4), it can be seen that the surface stress $\tilde{\mathbf{S}}$ has been modified by subtracting, in a linearized fashion, the strain-dependent part of the surface stress $\tilde{\mathcal{C}}_0 \mathbf{E}$ term. If we compare this $\tilde{\mathcal{C}}_0 \mathbf{E}$ term with the actual surface elastic part of the surface stress $\mathbf{S}\epsilon$, we see that $\tilde{\mathcal{C}}_0 \mathbf{E}$ is essentially the finite deformation analog of the surface elastic (strain-dependent) part of the surface stress $\mathbf{S}\epsilon$ in (1). By subtracting this term from (4), we can achieve our objective, i.e. isolate the effects of the strain-independent surface stress on the resonant frequencies of silicon nanowires if finite deformation kinematics are considered.

It is now appropriate to discuss the two parameters α and β . As shown in previous works using the SCB model for silicon [9, 26], silicon nanowires tend to expand and develop a tensile strain at equilibrium due to the effects of surface stresses. Because both the SCB model and the BCB model, which is used for the nanowire bulk, are nonlinear, finite deformation constitutive models, any deformation that is caused by the surface stresses changes the stiffness of both the SCB and BCB models, which then results in a change in resonant frequency due to the change in stiffness.

Therefore, to eliminate any differences in nanowire resonant frequency that might arise between the modified SCB model in (3)–(5) and the non-modified SCB model [9, 26] due to differences in bulk stiffness, we picked α and β for each nanowire geometry such that the tensile strain that is caused by the surface stresses through the modified SCB model in (3)–(5) matches that of the non-modified SCB model [9, 26]. To accomplish this, we chose $\alpha = 0.7$, and solved for β , where β varied between 0.84 and 0.93 depending on the nanowire geometry; the value for α could not be increased due to numerical instabilities, which indicates that we were not able to remove the entire contribution of the strain-independent surface stress. Furthermore, because the modified SCB surface stress in (4) and the non-modified SCB surface stress are equivalent at equilibrium, we can ascribe any changes in resonant frequency between the two SCB models mainly to differences in the modified SCB surface stiffness in (5) as

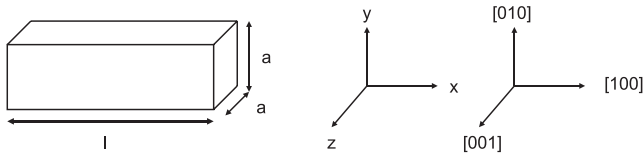


Figure 1. Nanowire geometry considered for numerical examples.

Table 1. Summary of nanowire geometries considered: constant length and constant aspect ratio (CAR). All dimensions are in nm.

Constant length	Constant aspect ratio
240 × 12 × 12	96 × 12 × 12
240 × 18 × 18	144 × 18 × 18
240 × 24 × 24	192 × 24 × 24
240 × 30 × 30	240 × 30 × 30

compared to the non-modified SCB surface stiffness. Because of this fact, we refer from here on to the modified SCB model described in (3)–(5) as the ‘stiffness modified’ SCB model [27].

3. Numerical examples

All numerical examples were performed on three-dimensional, single crystal silicon nanowires of length l that have a square cross section of width a as illustrated in figure 1. Two different parametric studies are conducted in this work, which consider nanowires with constant length and constant aspect ratio (CAR); the geometries are summarized in table 1.

All wires had a $\langle 100 \rangle$ longitudinal orientation with unreconstructed $\{100\}$ transverse surfaces, and had either fixed/free boundary conditions, where the left ($-x$) surface of the wire was fixed while the right ($+x$) surface of the wire was free, or fixed/fixed boundary conditions, where both the left ($-x$) and right ($+x$) surfaces of the wire were fixed. All FE simulations were performed using the stated boundary conditions without external loading, and utilized regular meshes of 8-node hexahedral elements.

Both the stiffness modified SCB nanowires and non-modified SCB nanowires were first relaxed to a minimum energy configuration to account for deformation induced by surface stresses; we emphasize that using the parameters α and β in (3)–(5), both the stiffness modified SCB nanowires and non-modified SCB nanowires had the same surface-stress-induced tensile strain at equilibrium. We further emphasize that previous works [9, 26] have demonstrated the ability of the SCB model to accurately capture surface-stress-induced strain and deformation that occurs in silicon nanowires as compared to benchmark atomistic calculations. Once the minimum energy configuration for either boundary condition is known, a standard eigenvalue problem of the form

$$(\mathbf{K} - \omega^2 \mathbf{M})\mathbf{u} = 0, \quad (6)$$

where \mathbf{M} is the mass matrix and \mathbf{K} is the stiffness matrix of the discretized FE equations, is solved using the FE stiffness matrix from the equilibrated (deformed) nanowire

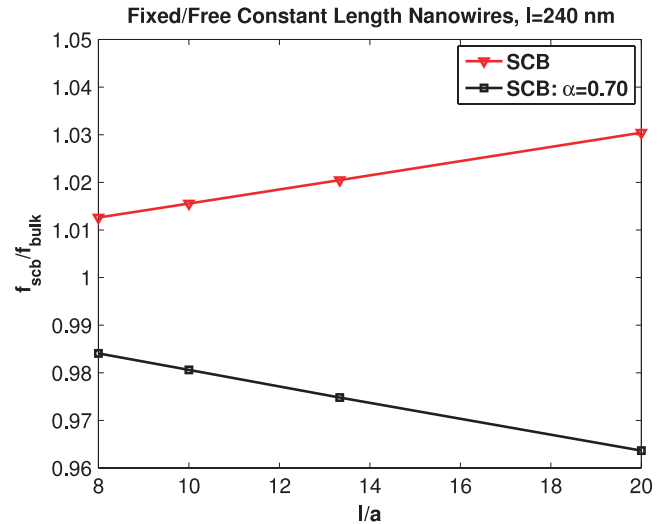


Figure 2. Effect of subtracting the strain-dependent surface stress and stiffness on the resonant frequencies of fixed/free constant length nanowires.

configuration to find the resonant frequencies $f = \sqrt{\omega^2}$. Resonant frequencies were also found using the standard BCB model (without surface stresses) on the same geometries for comparison to quantify how surface stresses change the resonant frequencies as compared to the bulk material for a given geometry and boundary condition; all calculations were performed using the Sandia-developed simulation code Tahoe [36].

4. Numerical results and discussion

We can now present numerical simulations that enable us to delineate the effects of the strain-independent and strain-dependent parts of the surface stress on the resonant frequencies of silicon nanowires if finite deformation kinematics are considered. We compare in this section resonant frequency results calculated using the non-modified SCB model ($\alpha = 0$, $\beta = 1$) and those calculated using the stiffness modified SCB model described in equations (3)–(5). In both cases, the SCB resonant frequencies are normalized by those obtained using the BCB model, i.e. neglecting surface stress effects, to quantify how surface stress effects impact the resonant frequencies of nanowires as compared to the corresponding bulk material for different geometries and sizes.

We first discuss the results for constant length nanowires as shown in figures 2 and 3. Because the stiffness modified SCB results are found by subtracting the strain-dependent part of the surface stress and stiffness as shown in equations (4) and (5), the difference between the SCB curve and the SCB ($\alpha = 0.7$) curves can be interpreted to be the resonant frequency shift caused by subtracting the strain-dependent part of the surface stress and stiffness. As discussed earlier, we were not able to subtract the entire contribution of the strain-dependent surface stress; therefore, the actual resonant frequencies due to the strain-independent surface stress alone

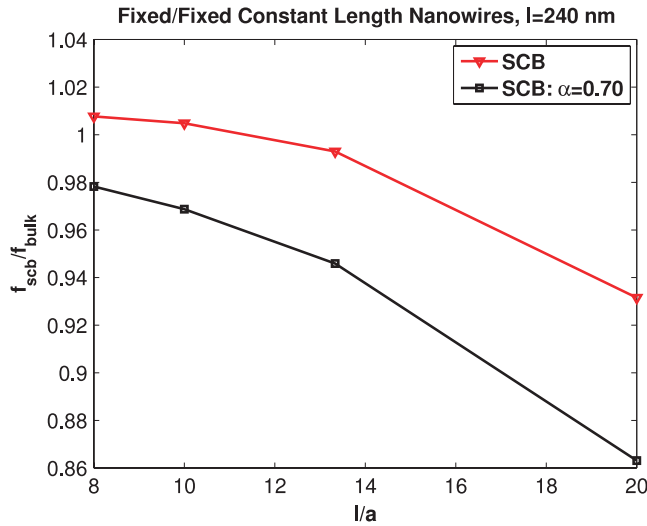


Figure 3. Effect of subtracting the strain-dependent surface stress and stiffness on the resonant frequencies of fixed/fixed constant length nanowires.

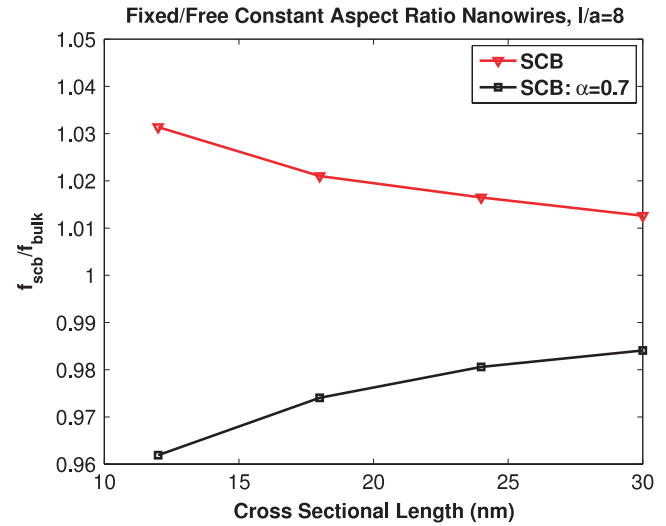


Figure 4. Effect of subtracting the strain-dependent surface stress and stiffness on the resonant frequencies of fixed/free constant aspect ratio nanowires.

are likely to be further reduced as compared to the SCB ($\alpha = 0.7$) curves in figures 2 and 3.

Figures 2 and 3 demonstrate two key facts. First, they clearly demonstrate that the residual surface stress does, in contrast to predictions that arise from linear surface elastic theory [20, 21], impact the resonant frequencies of silicon nanowires. Second, figures 2 and 3 also demonstrate that the effect of the residual surface stress on the resonant frequency is boundary condition dependent. For example, for the fixed/free constant length nanowires in figure 2, a slight increase in resonant frequency is observed for the SCB model for increasing aspect ratio l/a , or decreasing cross sectional size. However, when the strain-dependent surface stress is subtracted in the stiffness modified SCB model, the resonant frequency is observed to decrease with increasing aspect ratio l/a . This result strongly indicates that consideration of the residual surface stress alone would lead to incorrect predictions and trends regarding surface stress effects on the resonant frequencies of nanowires with decreasing size.

In contrast, for the fixed/fixed constant length nanowires in figure 3, the overall trend that is predicted by considering the residual surface stress alone through the stiffness modified SCB model, i.e. that of an increase in resonant frequency with increasing aspect ratio, matches the SCB solution. However, it is important to note that the difference between the stiffness modified SCB resonant frequency and the SCB resonant frequency is always larger than the difference between the SCB resonant frequency and the bulk resonant frequency for all aspect ratios considered. For example, when $l/a = 8$, the difference between the SCB and bulk resonant frequency is about 1.015%, while the difference between the stiffness modified SCB and bulk resonant frequency is about 2%. When $l/a = 20$, the difference between the SCB and bulk resonant frequency is about 7%; however, the difference between the stiffness modified SCB and the bulk resonant frequency is nearly 14%.

We also discuss the recent predictions of resonant frequency shift due solely to the strain-independent surface stress by Lachut and Sader [22]. In that work, an expression was derived for the resonant frequency shift of a fixed/free beam due to the strain-independent surface stress within the context of linear elastic beam theory; we simplify that expression (equation (4) in Lachut and Sader [22]) to account for the fact that the nanowire cross sections considered in the present work are square, and arrive at

$$\frac{\Delta\omega}{\omega_0} = -0.042 \frac{\nu(1-\nu)\sigma_s}{Eh}, \quad (7)$$

where $\Delta\omega$ is the shift in resonant frequency, ν is Poisson's ratio, σ_s is the strain-independent surface stress, E is the Young's modulus and h is the nanowire length. Importantly, (7) indicates that the shift in resonant frequency due to the strain-independent surface stress should be dependent only on the nanowire length h . In looking at both the fixed/free constant length case in figure 2 and the fixed/fixed constant length case in figure 3, it is clear that the resonant frequency is not constant as is predicted by (7). Instead, when only the strain-independent surface stress is considered by utilizing the stiffness modified SCB model, the resonant frequencies are predicted, for both boundary conditions, to decrease with increasing aspect ratio l/a .

We now quantify how the residual surface stress impacts the resonant frequencies of nanowires as a function of size. To do so, we discuss the results for nanowires with a constant aspect ratio of $l/a = 8$; as shown in table 1, the cross sectional length a was increased from 12 to 30 nm to investigate the size effect. The results for the CAR nanowires, for both boundary conditions, are shown in figures 4 and 5.

In both figures, it is clear that consideration of the residual surface stress alone would lead again to incorrect predictions of the nanowire resonant frequencies, with an increase in error for decreasing nanowire size. For the SCB model for both

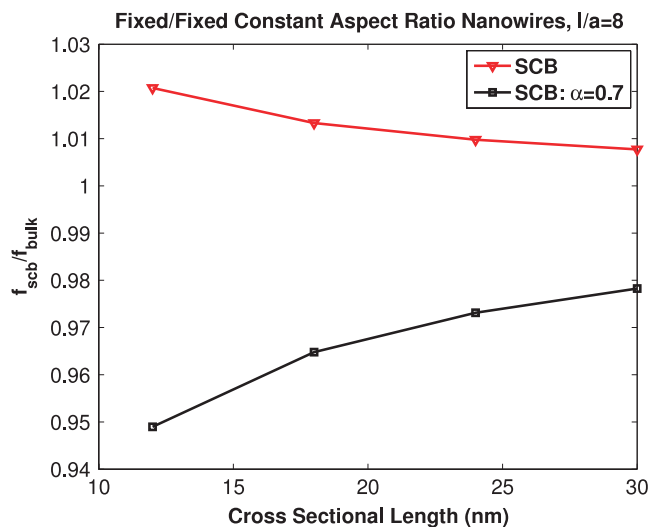


Figure 5. Effect of subtracting the strain-dependent surface stress and stiffness on the resonant frequencies of fixed/fixed constant aspect ratio nanowires.

boundary conditions and all nanowire sizes, a small increase in resonant frequency as compared to the bulk material is predicted. However, for the stiffness modified SCB model, there are two key differences. First, the resonant frequencies predicted by the stiffness modified SCB model are smaller, and not larger than the bulk resonant frequencies. Second, a decrease in resonant frequency for the stiffness modified SCB model is observed for decreasing nanowire size, in contrast with the full SCB results.

It is clear from figures 4 and 5 that the strain-dependent surface stress becomes increasingly important with decreasing nanowire size. This occurs because as the nanowire size decreases, the surface area to volume ratio increases; this is critical because subtraction of the strain-dependent surface stress, as in (4) leads to a corresponding reduction in surface stiffness, as in (5). As the surface area to volume ratio increases with decreasing nanowire cross sectional size, subtraction of the strain-dependent surface stress leads to a corresponding reduction in surface stiffness, which increasingly reduces the overall nanowire stiffness with decreasing size. We note that this effect also was observed in figure 2 for the fixed/free constant length nanowires; there, an increase in nanowire aspect ratio l/a also corresponds to a decrease in nanowire cross sectional size. Because of the decrease in size, subtracting the strain-dependent surface stress as is done for the stiffness modified SCB model leads to an overall decrease in nanowire elastic stiffness, thus leading to the observed reduction in resonant frequencies for the stiffness modified SCB model with decreasing nanowire size.

5. Conclusions

The key findings of this work are summarized as follows: (1) We have demonstrated using the recently developed surface Cauchy–Born model that if nonlinear, finite deformation kinematics are considered, then unlike the results obtained using

linear surface elastic theory, the residual (strain-independent) surface stress does impact the resonant frequencies of silicon nanowires. (2) Consideration of the residual surface stress alone leads to significant errors in predictions of the nanowire resonant frequencies, with the error increasing with decreasing nanowire size. (3) The surface elastic (strain-dependent) part of the surface stress has an increasingly large effect on the nanowire resonant frequencies with decreasing nanowire size; this is because the surface stiffness, and its difference from the bulk stiffness, has an increasingly important effect on the overall elastic stiffness of the nanowire with decreasing size. (4) The present results strongly indicate that knowledge of the state of strain is not sufficient to predict the resonant frequencies, and thus the elastic properties of the nanowires. This was demonstrated by considering two different SCB models, the SCB model and the stiffness modified SCB model, both of which lead to equivalent states of deformation due to surface stresses, but which generate significantly different predictions in the nanowire resonant frequencies. (5) Nonlinear, finite deformation kinematics appear to be essential in describing surface stress effects on the elastic properties, and therefore the resonant frequencies of nanowires due to the ability to capture changes in both bulk and surface elastic stiffness that arise from deformation induced by surface stresses.

Acknowledgment

HSP gratefully acknowledges NSF grant number CMMI-0750395 in support of this research.

References

- [1] Canham L T 1990 Silicon quantum wire array fabricated by electrochemical and chemical dissolution of wafers *Appl. Phys. Lett.* **57** 1046–8
- [2] Li D, Wu Y, Kim P, Shi L, Yang P and Majumdar A 2003 Thermal conductivity of individual silicon nanowires *Appl. Phys. Lett.* **83** 2934–6
- [3] Wong E W, Sheehan P E and Lieber C M 1997 Nanobeam mechanics: elasticity, strength, and toughness of nanorods and nanotubes *Science* **277** 1971–5
- [4] Cleland A N and Roukes M L 1996 Fabrication of high frequency nanometer scale mechanical resonators from bulk Si crystals *Appl. Phys. Lett.* **69** 2653–5
- [5] Huang X M H, Zorman C A, Mehregany M and Roukes M L 2003 Nanodevice motion at microwave frequencies *Nature* **42** 496
- [6] Craighead H G 2000 Nanoelectromechanical systems *Science* **290** 1532–5
- [7] Lavrik N V, Sepaniak M J and Datskos P G 2004 Cantilever transducers as a platform for chemical and biological sensors *Rev. Sci. Instrum.* **75** 2229–53
- [8] Ekinci K L and Roukes M L 2005 Nanoelectromechanical systems *Rev. Sci. Instrum.* **76** 061101
- [9] Park H S 2008 Surface stress effects on the resonant properties of silicon nanowires *J. Appl. Phys.* **103** 123504
- [10] Li X, Ono T, Wang Y and Esashi M 2003 Ultrathin single-crystalline-silicon cantilever resonators: fabrication technology and significant specimen size effect on Young's modulus *Appl. Phys. Lett.* **83** 3081–3

- [11] Chen C Q, Shi Y, Zhang Y S, Zhu J and Yan Y J 2006 Size dependence of the young's modulus of ZnO nanowires *Phys. Rev. Lett.* **96** 075505
- [12] Cammarata R C 1994 Surface and interface stress effects in thin films *Prog. Surf. Sci.* **46** 1–38
- [13] Diao J, Gall K and Dunn M L 2003 Surface-stress-induced phase transformation in metal nanowires *Nat. Mater.* **2** 656–60
- [14] Park H S, Gall K and Zimmerman J A 2005 Shape memory and pseudoelasticity in metal nanowires *Phys. Rev. Lett.* **95** 255504
- [15] Sun C Q, Tay B K, Zeng X T, Li S, Chen T P, Zhou J, Bai H L and Jiang E Y 2002 Bond-order–bond-length–bond-strength (bond-OLS) correlation mechanism for the shape-and-size dependence of a nanosolid *J. Phys.: Condens. Matter* **14** 7781–95
- [16] Kizuka T, Takatani Y, Asaka K and Yoshizaki R 2005 Measurements of the atomistic mechanics of single crystalline silicon wires of nanometer width *Phys. Rev. B* **72** 035333
- [17] Han X, Zheng K, Zhang Y F, Zhang X, Zhang Z and Wang Z L 2007 Low-temperature *in situ* large-strain plasticity of silicon nanowires *Adv. Mater.* **19** 2112–8
- [18] Lee B and Rudd R E 2007 First-principles calculation of mechanical properties of Si (100) nanowires and comparison to nanomechanical theory *Phys. Rev. B* **75** 195328
- [19] Gurtin M E and Murdoch A 1975 A continuum theory of elastic material surfaces *Arch. Ration. Mech. Anal.* **57** 291–323
- [20] Gurtin M E, Markenscoff X and Thurston R N 1976 Effects of surface stress on the natural frequency of thin crystals *Appl. Phys. Lett.* **29** 529–30
- [21] Lu P, Lee H P, Lu C and O'Shea S J 2005 Surface stress effects on the resonance properties of cantilever sensors *Phys. Rev. B* **72** 085405
- [22] Lachut M J and Sader J E 2007 Effect of surface stress on the stiffness of cantilever plates *Phys. Rev. Lett.* **99** 206102
- [23] McFarland A W, Poggi M A, Doyle M J, Bottomley L A and Colton J S 2005 Influence of surface stress on the resonance behavior of microcantilevers *Appl. Phys. Lett.* **87** 053505
- [24] He J and Lilley C M 2008 Surface effect on the elastic behavior of static bending nanowires *Nano Lett.* **8** 1798–802
- [25] Balamane H, Halicioglu T and Tiller W A 1992 Comparative study of silicon empirical interatomic potentials *Phys. Rev. B* **46** 2250–79
- [26] Park H S and Klein P A 2008 A surface Cauchy–Born model for silicon nanostructures *Comput. Methods Appl. Mech. Eng.* **197** 3249–60
- [27] Park H S and Klein P A 2008 Surface stress effects on the resonant properties of metal nanowires: the importance of finite deformation kinematics and the impact of the residual surface stress *J. Mech. Phys. Solids* **56** 3144–66
- [28] Tadmor E, Ortiz M and Phillips R 1996 Quasicontinuum analysis of defects in solids *Phil. Mag. A* **73** 1529–63
- [29] Arroyo M and Belytschko T 2002 An atomistic-based finite deformation membrane for single layer crystalline films *J. Mech. Phys. Solids* **50** 1941–77
- [30] Zhang P, Huang Y, Geubelle P H, Klein P A and Hwang K C 2002 The elastic modulus of single-wall carbon nanotubes: a continuum analysis incorporating interatomic potentials *Int. J. Solids Struct.* **39** 3893–906
- [31] Tang Z, Zhao H, Li G and Aluru N R 2006 Finite-temperature quasicontinuum method for multiscale analysis of silicon nanostructures *Phys. Rev. B* **74** 064110
- [32] Tadmor E B, Smith G S, Bernstein N and Kaxiras E 1999 Mixed finite element and atomistic formulation for complex crystals *Phys. Rev. B* **59** 235–45
- [33] Park H S, Klein P A and Wagner G J 2006 A surface Cauchy–Born model for nanoscale materials *Int. J. Numer. Methods Eng.* **68** 1072–95
- [34] Park H S and Klein P A 2007 Surface Cauchy–Born analysis of surface stress effects on metallic nanowires *Phys. Rev. B* **75** 085408
- [35] Tersoff J 1989 Modeling solid-state chemistry: interatomic potentials for multicomponent systems *Phys. Rev. B* **39** 5566–8
- [36] 2008 Tahoe <http://tahoe.ca.sandia.gov>