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# Three-dimensionally nonlocal tensile nanobars incorporating surface effect: A self-consistent variational and well-posed model

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A naturally discrete nanobar implies that the continuum axiom fails, and the surface-to-volume ratio is very large. The nonlocal theory of elasticity releasing the continuum axiom and the surface theory of elasticity are therefore employed to model tensile nanobars in this work. As commonly believed in the current practice, the axial nonlocal effect is only taken into account to analyze the mechanical behaviors of nanobars, regardless of the three-dimensional inherent atomistic interactions. In this study, a three-dimensional nonlocal constitutive law is developed to model the true nonlocal effect of nanobars, and based on which, a self-consistent variational bar model is proposed. It has been revealed for the first time how both the cross-sectional nonlocal interactions and the axial nonlocality affect the tensile behaviors of nanobars. It is found that the nonlocal influence predicted by the currently axial nonlocal bar model is grossly underestimated. Both the nonlocal cross-sectional and axial interactions become significant when the length-to-height ratio of nanobars is small. If the length-to-height ratio is relatively large (slender bars), the main nonlocal effect stems, however, from the nonlocal cross-sectional effect, rather than the axial nonlocal effect. This work also shows that it is possible to overcome the ill-posed problem of the pure nonlocal integral elasticity by employing both the pure nonlocal integral elasticity and surface elasticity. A well-posed size-dependent governing equation has been established for modeling nanobars under tension, and closed-form solutions are derived for their displacements. Based on the closed-form solutions, the effective elastic modulus is obtained and will be useful for calibrating the physical quantities in the "discrete-continuum" transition region for a span-scale modeling approach. It is shown that the effective elastic modulus may be softening or hardening, depending on the competition between the surface (modulus-hardening) and nonlocal (modulus-softening) effects.

**nonlocal integral elasticity, tensile nanobar, size effect, surface elasticity**

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## 1 Introduction

The increasing development of micro- and nano-electromechanical systems, including nanosensors, nanoactuators, gyroscopes, timing oscillators and accelerometers, requires understanding the mechanical and physical behaviors of their basic structural components. Investigating the mechanics and physics of basic structural components is becoming more and more prevalent in engineering and technological applications.

Components are becoming smaller and faster (higher frequency and extraordinary sensitivity), leading to difficulties in experimentally controlling the precision of the deformation and response of nanostructures, even impossible tasks for measuring or characterizing the response of nanostructures within complex environments. As a result, atomistics (molecular dynamics, density functional theory, and so on), statistical mechanics and continuum mechanics have been frequently used for numerical simulations and predictions of

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the responses of nanoscale structures [1–4]. However, statistical mechanics-based or atomistics-based predictions are generally time-consuming, especially for nanoscale composites.

Continuum mechanics-based methods are hence becoming more and more prevalent in understanding the mechanical behaviors of nano-structural components. Traditional continuum mechanics is usually called the "grand unified theory" for engineering sciences and techniques by adopting Cauchy's stress principle. Cauchy's stress requires, however, the continuum axiom, which cannot be satisfied for nanostructures due to their naturally discrete feature [5]. Generalized continuum mechanics has to be employed for theoretical investigations of nanoscopic structure responses. Unlike Cauchy's stress defined as the force on a unit surface, the atomistic forces are interacted each other by "long-ranged" forces. As a well-accepted kind of the generalized continuum mechanics, the nonlocal theory [6] defines a new concept of stress, which states that the nonlocal stress should be defined as the force crossing a unit surface, rather than on a unit surface as it is defined in the traditional continuum mechanics. With the nonlocal stress definition, the nonlocal theory can account for the effect of "long-ranged" forces and therefore has been frequently employed for predicting the response of nanoscale structures.

Bars under uni-axial tension are referred to as an one-dimensional (1D) problem in the traditional continuum mechanics. By intuitively following the traditional simplifications for bar-type structures, only the axial (1D) nonlocal effect is taken into account to analyze the mechanical behaviors of nanobars in the current practice, regardless of the three-dimensional (3D) inherent atomistic interactions. For example, the nonlocal differential models incorporating only the axial (1D) nonlocal effect were developed for nanobars and employed to study their axially dynamics behaviors [7–9]. In the framework of the nonlocal integral theory of elasticity, the nonlocal integral models incorporating only the axial (1D) nonlocal effect have been recently established for studying the axial statics and dynamics behaviors of nanobars [10–14].

In fact, these axial (1D) nonlocal analyses cannot account for the dominant nonlocal contribution because of the following reasons.

(1) From the viewpoint of atomistics, the long-ranged interactions between atoms occur in a 3D space, and hence the nonlocal effects are expected to exist in all the three dimensions of any type structure.

(2) The nonlocal theory of elasticity [6] states that the nonlocal stress is predicted by the weighted average of the strain field within the body through nonlocal kernel functions. Thus, the nonlocal influence zone is a 3D domain, and as a result, nonlocality is naturally three-dimensional. Namely, nanobars cannot be simplified as commonly and currently used 1D nonlocal models.

(3) Traditional continuum mechanics breaks down firstly at the smallest dimension among all feature sizes of bars as they become from macro-scale to the nanoscale [15]. Thus, the axial nonlocal effect becomes dominant if and only if the axial length of a bar is far larger than its cross-sectional feature size. For the case of bars with large length-to-height ratios (slender bars), the nonlocal effect attributed to the cross-sectional direction becomes significant and is likely to be dominant for the nonlocal size contribution.

(4) These intuitively developed 1D nonlocal bar models suffer from a lack of an 1D physical justification needed for nonlocal problems. Actually, the implied hypothesis for the currently 1D nonlocal bar models [10–14] is that bar's length is far smaller than its cross-sectional feature size (under such case, it implies that both the surface and cross-sectionally nonlocal effects can be neglected).

(5) The stress profile within the cross-section of a nanobar predicted by the 1D nonlocal bar models [10, 12, 14] is basically local instead of nonlocal.

All these manifest that the nonlocal effect must be taken into account in all the three dimensions of bars, and therefore we will model the nanobars using a 3D nonlocal constitutive law, instead of the 1D nonlocal model as it is commonly believed in the current practice. It is found in this study that the nonlocal influence predicted by the currently axial (1D) nonlocal bar model is grossly underestimated. More importantly, for slender nanobars whose length-to-height ratio is relatively large, the dominant nonlocal effect stems from the cross-sectional direction rather than the commonly believed axial direction.

Furthermore, the frequently-employed differential-type constitutive relation making use of the Helmholtz's differential operator, as originally suggested by ref. [16] for non-boundary-value problems (dispersion of waves, screw dislocations), was used to develop the nonlocal differential models for nanobars [7–9, 17], nanabeams [18–23], nanoplates [24, 25] and nanoshells [26, 27], regardless of the fact that their sizes are finite and should be referred to as boundary value problems. Thus, these nonlocal differential models are inconsistent variational formulations. In this study, a 3D nonlocal constitutive law is developed to model the true nonlocal effect of nanobars, and based on which, a self-consistent variational bar model is proposed.

The surface-to-volume ratio of bars becomes very large when they are down to nanoscale, and as a result, the surface effect becomes significant and has to be taken into consideration. A theoretical framework for surface elasticity was proposed in the seminal work [28], known as Gurtin-Murdoch theory, which states that the material properties in the bulk and surface are different and the free surface layer can be viewed and treated as a zero thickness film. The Gurtin-Murdoch theory has been widely employed or modified for both elastostatics and elastodynamics of nanostructures [29–33]. Nanobars (nanorods) have also been modeled by using the 1D nonlocal elasticity as well as the Gurtin-Murdoch surface model [34]. Recently, both the 1D nonlocal elasticity and the Gurtin-Murdoch surface model were employed to study the elastodynamics of defected nanorods or nanowires systems [35–37]. This work also shows that it is possible to overcome the ill-posed problem of the pure nonlocal integral elasticity by employing both the pure nonlocal integral elasticity and surface elasticity. Thus, a self-consistent variational and well-posed governing equation can be established for modeling tensile nanobars.

This paper is planned as follows. In Sect. 2, we give the statement of tensile problem to be studied. Then, Sect. 3 suggests a 3D nonlocal constitutive law and correspondingly proposes a self-consistent variational and well-posed model for bars under tension. Next, in Sect. 4, the closed-form solution for displacements is derived. Based on the closed-form solution of displacements, the effective modulus is achieved in Sect. 5, and the size-dependent effects are explored in detail. Finally, Sect. 6 draws some conclusions.

## 2 Statement of problem

We consider an isotropic and homogeneous nanobar of length $L$ and of uniform rectangular cross-section $A$ (with width $2w$ and height $2h$), as plotted in Figure 1. The nanobar is assumed to be clamped at $x_1 = 0$ and subjected to a tensile load $P$ at the free end where $x_1 = L$. As illustratively shown in Figure 1, a surface layer of zero thickness is assumed to be on the bulk of the nanobars. The bulk is assumed to satisfy the nonlocal theory of elasticity [6], while the free surface layer is governed by the surface theory of elasticity developed in ref. [28].

For the sake of simplification, the displacement field at a reference point $\boldsymbol{x}$ of nanobar under tension is commonly

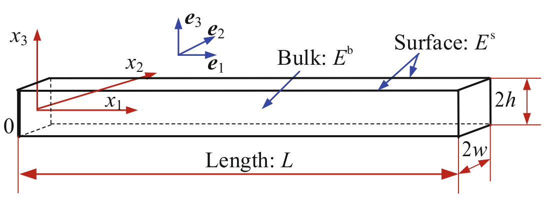


**Figure 1** (Color online) Schematic illustration of a nanoscale bar and its coordinate.

assumed to take the form

$$\boldsymbol{u} = u(x_1)\boldsymbol{e}_1. \tag{1}$$

Here $x_1$ denotes the axial direction, and $\boldsymbol{e}_i$ $(i = 1, 2, 3)$, are the unit basis vectors, as shown in Figure 1. The gradient of the displacement field, $\nabla\boldsymbol{u}$, can be obtained as

$$\nabla\boldsymbol{u} = \frac{\mathrm{d}u}{\mathrm{d}x_1}\boldsymbol{e}_1 \otimes \boldsymbol{e}_1.$$

Here $\otimes$ denotes the tensor product. Thus, the strain tensor $\boldsymbol{\varepsilon}$ in the bulk of the nanobar can be given by

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}}\right) = \varepsilon_{11}(x_1)\boldsymbol{e}_1 \otimes \boldsymbol{e}_1, \tag{2}$$

where the nonzero strain component is

$$\varepsilon_{11}(x_1) = \frac{\mathrm{d}u}{\mathrm{d}x_1}. \tag{3}$$

### 2.1 Surface elasticity theory

Let us simply recall the Gurtin-Murdoch surface theory of elasticity. For infinitesimal deformations, the in-plane components $\sigma^{\mathrm{s}}_{\alpha\beta}$ and out-of-plane components $\sigma^{\mathrm{s}}_{n\alpha}$ of the zero-thickness surface layer have the following stress-strain relation [28]:

$$\begin{aligned}\sigma^{\mathrm{s}}_{\alpha\beta} =&\sigma_0\delta_{\alpha\beta} + (\mu^{\mathrm{s}} - \sigma_0)(u_{\alpha,\beta} + u_{\beta,\alpha}) + (\lambda^{\mathrm{s}} \\ &+ \sigma_0)\varepsilon_{\gamma\gamma}\delta_{\alpha\beta} + \sigma_0 u_{\alpha,\beta}, \\ \sigma^{\mathrm{s}}_{n\alpha} =&\sigma_0 u_{n,\alpha},\end{aligned} \tag{4}$$

where the superscript s denotes surface, $\sigma_0$ is the residual (initial) surface stress, $\delta_{\alpha\beta}$ is the Kronecker delta, and $\lambda^{\mathrm{s}}$ and $\mu^{\mathrm{s}}$ are the surface Lamé constants. In this study, we only consider the case where the residual surface stress equals zero ($\sigma_0 = 0$). Thus, the nonzero surface stress $\sigma^{\mathrm{s}}_{11}$ can be expressed as

$$\sigma^{\mathrm{s}}_{11} = E^{\mathrm{s}}\frac{\mathrm{d}u}{\mathrm{d}x_1}, \tag{5}$$

where $E^{\mathrm{s}} = \lambda^{\mathrm{s}} + 2\mu^{\mathrm{s}}$.

### 2.2 3D nonlocal integral elasticity

When structures or materials are down to nanoscale, they cannot be treated as continuum due to the naturally discrete nanostructures made of atoms. This leads to a simple fact that the continuum assumption, which plays a foundational role in modeling structures using the classical continuum mechanics, fails at the nanoscale. The nonlocal theory of elasticity, as one of the well-accepted generalized elasticity theories, can release the continuum assumption by defining a new concept of stress field. Unlike Cauchy's stress defined as the force acting on a unit area, the nonlocal stress can be viewed as "long-ranged" forces crossing a plane with unit area and hence allows for the interactions between atoms.

In the context of the nonlocal theory of elasticity [6], the nonlocal stress tensor should be considered as a response of all strains in the neighboring domain of interest and can be defined as

$$\sigma_{ij}^{\mathrm{b}}(\boldsymbol{x}) = \int_V \mathcal{K}(\|\boldsymbol{x}-\boldsymbol{x}'\|, \tau)C_{ijkl}\varepsilon_{kl}(\boldsymbol{x}')\mathrm{d}V(\boldsymbol{x}'), \quad (6)$$

where $\boldsymbol{x}$ and $\boldsymbol{x}'$ are the reference point and its neighboring point, respectively. $C_{ijkl}$ is the fourth-order elasticity tensor. The kernel function, $\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}', \tau)$, is called the nonlocal attenuation function used to weight all the strains within the domain of interest. Thus, $\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}', \tau)$ can be viewed as a weighting function. One of the broadly concerned problems is that classical (local) mechanics can be recovered from the nonlocal theory of elasticity if the small size effect is negligible (the size is large enough). Thus, the normalization condition is often employed to address this problem.

$$\int_{V_{\mathrm{inf}}} \mathcal{K}(\|\boldsymbol{x}-\boldsymbol{x}'\|, \tau)\mathrm{d}V(\boldsymbol{x}') = 1. \quad (7)$$

This means that the integral of the kernel function over an infinite volume $V_{\mathrm{inf}}$ should be 1. It shall be noted that when considering a finite material within a vacuum environment, the vacuum part may be thought to as a "virtual medium" with zero value of material properties [38], and then the previous normalization (7) can also be suitable. It can be easily checked that the local and nonlocal stress tensor can be identical to each other when considering a constant strain tensor. The intrinsic characteristic length $\tau$ is used to control the shape of the weighting function and allows the nonlocal constitutive equation to capture the 3D "long-ranged" interaction forces between atoms. The intrinsic length is only decomposed as $\tau = e_0 a$, where $a$ is a material internal characteristic length (e.g., crystal constant), and $e_0$ is an unknown dimensionless constant to be calibrated by use of atomistics simulations or experimental work.

In the case of homogeneous and isotropic bars, the nonzero stress can be obtained as

$$\sigma_{11}^{\mathrm{b}}(\boldsymbol{x}) = E^{\mathrm{b}} \int_V \mathcal{K}(\|\boldsymbol{x}-\boldsymbol{x}'\|, \tau)\varepsilon_{11}(\boldsymbol{x}')\mathrm{d}V(\boldsymbol{x}'). \quad (8)$$

To agree with the 3D constitutive relations, the elastic (tensile) modulus $E^{\mathrm{b}}$ (or equivalent Young's modulus from the 1D viewpoint) for the bulk has the following relation:

$$E^{\mathrm{b}} = \frac{Y(1-\nu)}{(1+\nu)(1-2\nu)} = \lambda^{\mathrm{b}} + 2\mu^{\mathrm{b}},$$

where $Y$ is called Young's modulus from the 3D viewpoint, $\nu$ is Poisson ratio, and $\lambda^{\mathrm{b}}$, $\mu^{\mathrm{b}}$ are Lamé constants. At this junction, one can recall that the displacement field in eq. (1) only considers the case with a neglectable Poisson ratio effect ($\nu = 0$). Thus, for the case where the Poisson ratio effect must be taken into consideration, the displacement field should be modified accordingly and the proposed methodology is also helpful for developing a 3D size-dependent model by following a similar thread. Because the aim of this paper is to establish a self-consistent variational and well-posed model and meanwhile show the importance of 3D nonlocal effect, we just consider the commonly adopted displacement field (1) for the sake of both comparison and simplification.

In the classical bar theory, the bar problem has been long known as a 1D problem. In current practice, by intuitively following the 1D simplification, the nonlocal stress in eq. (8), originally defined as 3D "long-ranged" interaction forces between atoms, is simplified as

$$\sigma_{11}^{\mathrm{b}}(\boldsymbol{x}) = E^{\mathrm{b}} \int_0^L \mathcal{K}(\|\boldsymbol{x}-\boldsymbol{x}'\|, \tau)\varepsilon_{11}(\boldsymbol{x}')\mathrm{d}V(\boldsymbol{x}'), \quad (9)$$

which implies that the stress contribution in the axial (length) direction is only taken into consideration and normalization (7) has been employed to neglect the stress contribution in the radius (or cross-sectional) direction. It has to be emphasized that the nonlocal stress (9) in the cross-sectional direction is local rather than nonlocal. This will be failed at most of the cases due to the confirmed fact that classical local mechanics breaks down firstly at the shortest size among all dimensions in nanostructures [15]. It was recently pointed out by ref. [38] that the simplification is and only if the length of a bar-type structure is far smaller than its height or width (cross-sectional feature size).

Figure 2 gives a schematic illustration of 1 and 3D nonlocal bars. As illustratively shown in Figure 2(a), the 1D nonlocal model (9) requires that the micro-structural characteristic occurring in the axial direction. Nanomaterials can only be few in number to fulfill this rigorous requirement; for example, these nanomaterials (exemplified by carbynes [39] where only one atom exists in theories radius direction) are naturally pure 1D structures. Of course, some quasi-1D nanostructures may satisfy the rigorous requirement; for instance, single-walled nanotubes, whose thicknesses are assessed by use of equivalent "thickness" techniques, may also be successfully modeled by the 1D nonlocal model (9).

For most of materials, they possess characteristic microstructures in all the three directions, as illustratively shown in Figure 2(b), and the classical continuum mechanics will fail at first if they are down from macro-scale to nanoscale where their smallest length (among width, thickness and length) is comparable to their intrinsic nonlocal parameter (although the nonlocal kernel function may work in infinite domain, the

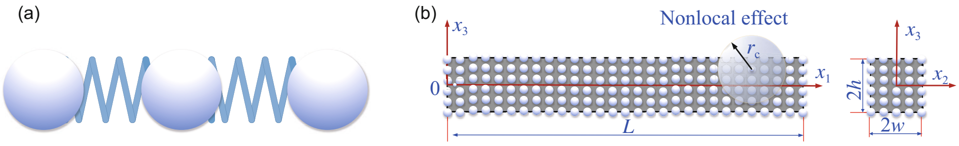


**Figure 2** (Color online) Schematic illustration of 1D and 3D bars. (a) 1D bar; (b) 3D bar.

cut-off radius $r_c$ is commonly adopted in atomistics simulations to save computational cost but keep engineering accuracy). Regarding this fact, the 1D nonlocal model (9) may also be reasonable when considering a short and thick nanobar [38] where its thickness and width are far larger than its length which is comparable to its intrinsic nonlocal parameter. Otherwise, the 3D nonlocal model (8) has to be employed for general nanostructures to seek for a more realistic and rational study.

The integral-type constitutive law (9) cannot be solved easily, even for the intuitive 1D simplification. As a result, the weighting function is chosen from the viewpoint of easy implement and therefore often treated as the Green's function of a differential operator, $\mathcal{D}_{\boldsymbol{x}}\mathcal{K}(\boldsymbol{x},\boldsymbol{x}',\tau)=\delta(\boldsymbol{x}-\boldsymbol{x}')$ where $\mathcal{D}_{\boldsymbol{x}}$ is a differential operator and $\delta(\boldsymbol{x}-\boldsymbol{x}')$ is the Dirac delta function. For example, when choosing the Helmholtz's differential operator $\mathcal{D}_{\boldsymbol{x}}=1-(e_0a)^2\nabla^2$, the frequently-employed differential-type constitutive relation of eq. (9) can be recovered as

$$\left(1-(e_0a)^2\nabla^2\right)\sigma^{\mathrm{b}}_{11}=E^{\mathrm{b}}\varepsilon_{11}, \tag{10}$$

in which the 1D Laplacian operator is denoted as $\nabla^2=\partial^2/\partial x^2$. However, caution must be drawn for the considerable differences in the boundary value problems modeled by using the integral- and differential-type constitutive laws [12, 40], although the two kind constitutive laws can predict the same results for non-boundary-value problems, such as dispersion of waves.

### 2.3 On compatibility condition between surface and bulk

This study will solve the problem how the cross-sectional interaction effect (stems from the naturally 3D nonlocality and the surface elasticity) affects the statics of bars with manometer feature size. To this end, the surface stresses and 3D weighting functions are simultaneously employed.

The compatibility condition between the surfaces stress tensor and the bulk stress tensor must take the form

$$\boldsymbol{n}\cdot\boldsymbol{\sigma}^{\mathrm{b}}=\nabla_{\mathrm{s}}\cdot\boldsymbol{\sigma}^{\mathrm{s}}\quad\text{or}\quad\sigma^{\mathrm{b}}_{ji}n_j=\sigma^{\mathrm{s}}_{i\alpha,\alpha}. \tag{11}$$

Note that $\nabla_{\mathrm{s}}$ is the surface nabla operator, and subscript $\alpha=x_1,t$ where $t$ is the tangent direction of the considered surface point. Vector $\boldsymbol{n}$ denotes the unit vector of the normal to the surface.

It can be checked that the bar problem of interest can always fulfill the previous compatibility condition for the displacement field (1) considered herein. Next, the importance of the cross-sectional effect on the statics of bars will be revealed.

## 3 Elastostatics for bar problem

### 3.1 Choice of 3D weighting function

The requirements, which a 3D weighting function $\mathcal{K}(\boldsymbol{x},\boldsymbol{x}',\tau)$ should fulfill, have been summarized in some references, see refs. [6, 15, 41, 42]. Generally speaking, the 3D weighting function must decay as the spatial distance increases and should be degraded into a Dirac delta function to make sure that the classical mechanics can be recovered in the limit case where the long-ranged interaction effect is ignorable.

Various 1D forms of kernel (weighting) functions are employed and discussed for modeling nanobars (nanorods) [12, 43]. In this study, we use the 3D form of the bi-exponential function, which can be expressed as

$$\begin{aligned}&\mathcal{K}(\|\boldsymbol{x}-\boldsymbol{x}'\|,\tau)=\xi_1\delta(\boldsymbol{x}-\boldsymbol{x}')\\&+\frac{\xi_2}{(2\tau)^3}\exp\left(-\frac{|x_1-x_1'|+|x_2-x_2'|+|x_3-x_3'|}{\tau}\right),\end{aligned} \tag{12}$$

where the weighting coefficients $\xi_1$ and $\xi_2$ have the relation: $\xi_1+\xi_2=1$. Note that its 1D weighting function in the axial direction is $\mathcal{K}_1(|x_1-x_1'|,\tau)$, and can be assumed to be the combination of the bi-exponential function [16, 44] and the delta function:

$$\mathcal{K}_1(|x_1-x_1'|,\tau)=\xi_1\delta(x_1-x_1')+\xi_2\frac{1}{2\tau}\exp\left(-\frac{|x_1-x_1'|}{\tau}\right). \tag{13}$$

The classical mechanics can be recovered by simply setting $\xi_2=0$ in eq. (13). This is also known as the two-phase nonlocal model which has been firstly suggested in ref. [45] and is recently used due to the fact that the boundary value problem can be relatively easy to be controlled [12, 40, 46–48]. Furthermore, the governing equations based on the two-phase nonlocal model can overcome the ill-posed problem of the pure nonlocal model based only on the bi-exponential function ($\xi_2 = 1$). For the present two-phase 3D nonlocal weighting function, as it will be revealed later, the ill-posedness when $\xi_2 = 1$ can also be overcome if the surface energy effect is taken into account.

Using constitutive eq. (8) with the 3D weighting function (12), the nonlocal (bulk) stress $\sigma^{\rm b}_{11}$ can be expressed by

$$\sigma^{\rm b}_{11}(\boldsymbol{x}) = E^{\rm b}\xi_1\varepsilon_{11}(x_1) + \frac{E^{\rm b}\xi_2}{8\tau^3} \times \int_{-w}^{w}\int_{-h}^{h}\int_{0}^{L} \exp\left(-\frac{|x_1-x_1'|+|x_2-x_2'|+|x_3-x_3'|}{\tau}\right) \times \varepsilon_{11}(x_1'){\rm d}x'_1{\rm d}x'_2{\rm d}x'_3. \quad (14)$$

After making some integral manipulations, we have

$$\sigma^{\rm b}_{11}(\boldsymbol{x}) = E^{\rm b}\xi_1\varepsilon_{11}(x_1) + \frac{\xi_2 E_{\rm 2D}(x_2,x_3)}{2\tau} \times \int_0^L \exp\left(-\frac{|x_1-x_1'|}{\tau}\right)\varepsilon_{11}(x'){\rm d}x_1', \quad (15)$$

where the 2D distributed modulus $E_{\rm 2D}$ taking the cross-sectional nonlocal effect into account is expressed as

$$E_{\rm 2D}(x_2,x_3) = \frac{E^{\rm b}}{4\tau^2}\int_{-w}^{w}\int_{-h}^{h}\exp\left(-\frac{|x_2-x'_2|+|x_3-x'_3|}{\tau}\right){\rm d}x'_2{\rm d}x'_3.$$

The previous integration furnishes to yield

$$E_{\rm 2D}(x_2,x_3) = E^{\rm b}\left(1-\frac{1}{2}e^{-\frac{x_2+w}{\tau}}-\frac{1}{2}e^{\frac{x_2-w}{\tau}}\right) \times \left(1-\frac{1}{2}e^{-\frac{x_3+h}{\tau}}-\frac{1}{2}e^{\frac{x_3-h}{\tau}}\right). \quad (16)$$

As seen, the 2D distributed modulus $E_{\rm 2D}$ is not only dependent on the intrinsic length but dependent also on the position at the cross-section of bars.

Figure 3 shows the effects of the intrinsic length and the cross-sectional position on the 2D distributed modulus $E_{\rm 2D}$. Unlike the 1D nonlocal model assuming that $E_{\rm 2D}$ is a constant and equals the classical modulus $E^{\rm b}$, the 2D distributed modulus $E_{\rm 2D}$ is actually not a constant through the cross-section, as plotted in Figure 4. Clearly, the size-dependent ("modulus-softening") effect is more significant when the position is closer to the free surfaces, especially near two free surfaces (the upper left corner in Figure 4). Also, from Figure 3, we can observe a significant size-dependent effect when $\tau = 0.5w$, but a negligible size-dependent effect when $w = 100\tau$. That is, when the cross-section size is far larger than the intrinsic length, the size-dependent effect can be neglected and the 1D nonlocal model can also be suitable.

For the case of an isotropic nanobar within uniform strain fields, the interaction force for any two symmetric points within the sphere with a cut-off radius can offset each other due to the symmetric distribution of the attenuation functions, as shown in Figure 5. As a result, the nonlocal effect is only possible to play a profound effect around the interface or surface zone [38]. This is the nature of the size-dependent phenomena in "equivalent moduli" shown in Figures 3 and 4.

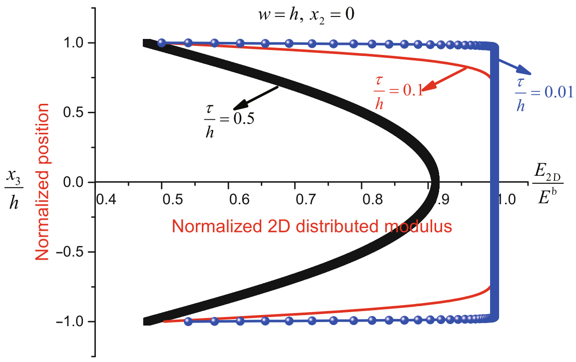


**Figure 3** (Color online) Effects of the intrinsic length $\tau$ and the cross-sectional position on the 2D distributed modulus ($x_2 = 0$ and $w = h$).

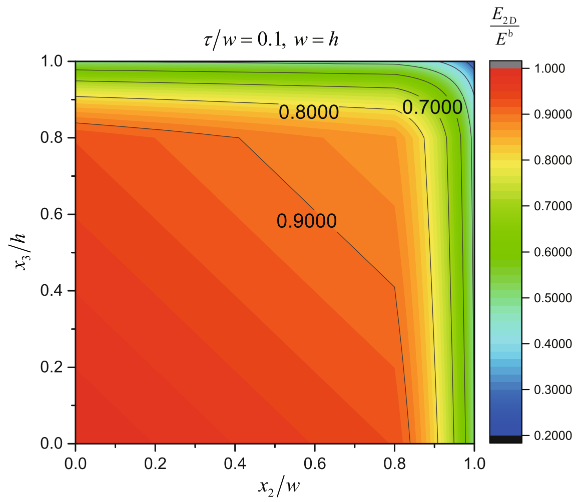


**Figure 4** (Color online) Nonlocal effect on the 2D distributed modulus (only 1/4 cross-section is plotted due to the symmetry).

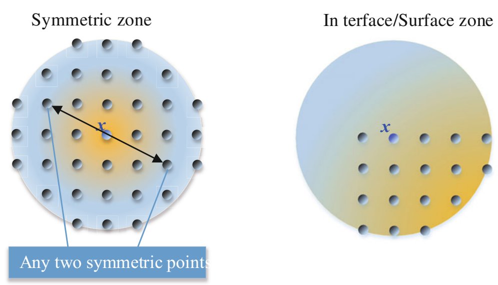


**Figure 5** (Color online) Schematic illustration of nonlocal interactions at different zones within uniform strain fields.

Thus, the nonlocal effect in the thickness direction will be larger than that in the width direction when the thickness is smaller than the width, and vice versa. Furthermore, when the cross-section feature length of a nanobar is smaller than its length, the nonlocal effect in the cross-section direction becomes more important than that in the length direction.

### 3.2 Governing equation

The virtual work principle is applied to set up the governing equations of the tension problem. Taking both the bulk and surface strain energies into consideration, the internal virtual work due to $\delta u(x_1)$ can be obtained as

$$\delta \mathcal{W}_I = \int_0^L \int_A \sigma_{11}^{\mathrm{b}}(\boldsymbol{x})\delta\varepsilon_{11}(x_1)\mathrm{d}A\mathrm{d}x_1 + \int_0^L \oint_{\partial A} \sigma_{11}^{\mathrm{s}}\delta\varepsilon_{11}(x_1)\mathrm{d}s\mathrm{d}x_1,$$

which can be rewritten as

$$\begin{aligned}\delta \mathcal{W}_I &= \int_0^L \int_A \sigma_{11}^{\mathrm{b}}(\boldsymbol{x})\mathrm{d}A\delta\varepsilon_{11}(x_1)\mathrm{d}x_1 + \int_0^L \oint_{\partial A} \sigma_{11}^{\mathrm{s}}\mathrm{d}s\delta\varepsilon_{11}(x_1)\mathrm{d}x_1 \\ &= \int_0^L N_b(x_1)\delta\frac{\mathrm{d}u}{\mathrm{d}x_1}\mathrm{d}x_1 + \int_0^L N_s(x_1)\delta\frac{\mathrm{d}u}{\mathrm{d}x_1}\mathrm{d}x_1, \quad (17)\end{aligned}$$

where the two extensional stress resultants are defined as

$$N_b(x_1) = \int_A \sigma_{11}^{\mathrm{b}}\mathrm{d}A,\ N_s(x_1) = \oint_{\partial A} \sigma_{11}^{\mathrm{s}}\mathrm{d}s. \quad (18)$$

The external virtual work is

$$\delta\mathcal{W}_E = -P\delta u(L). \quad (19)$$

The principle of virtual displacements then gives

$$\delta\mathcal{W}_I + \delta\mathcal{W}_E = 0, \quad (20)$$

which can be expressed as

$$-\int_0^L \frac{\mathrm{d}(N_b(x_1)+N_s(x_1))}{\mathrm{d}x_1}\delta u\mathrm{d}x_1 + (N_b(x_1)+N_s(x_1))\,\delta u\Big|_0^L - P\delta u(L) = 0. \quad (21)$$

By the Fundamental Lemma of Variational Calculus, the Euler equation is

$$N_b(x_1) + N_s(x_1) = C_0, \quad (22)$$

where $C_0$ is a constant to be determined. After substitution of eqs. (15), (5) and (18), eq. (22) can be expressed in terms of displacement as

$$(E^{\mathrm{b}}A\xi_1 + E^{\mathrm{s}}A^{\mathrm{s}})\frac{\mathrm{d}u}{\mathrm{d}x_1} + \frac{EA\xi_2}{2\tau}\int_0^L \exp\left(-\frac{|x_1-x_1'|}{\tau}\right)\frac{\mathrm{d}u}{\mathrm{d}x_1'}\mathrm{d}x_1' = C_0, \quad (23)$$

where

$$E = \int_{-w}^{w}\int_{-h}^{h} E_{2\mathrm{D}}(x_2,x_3)\,\mathrm{d}x'_2\mathrm{d}x'_3,\ E^{\mathrm{s}} = \lambda^{\mathrm{s}} + 2\mu^{\mathrm{s}}, \quad (24a)$$

$$A = 4wh,\ A^{\mathrm{s}} = \oint_{\partial A}\mathrm{d}s = 4(w+h). \quad (24b)$$

Substituting the expression of the 2D distributed modulus $E_{2\mathrm{D}}$ in eq. (16) into eq. (24a), we obtain the effective cross-sectional modulus in the bulk as

$$E(\tau/h,\tau/w) = \left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right)E^{\mathrm{b}}. \quad (25)$$

**Remark 3.1** The cross-sectional feature sizes of a bar, $(w,h)$, are generally smaller than its length $L$, which implies that classical mechanics is usually failed at first as the sizes of bars are down to nanoscale levels. Regarding this, the intrinsic length $\tau$ may be comparable to the cross-sectional feature size. As a result, the exponential terms in eq. (25) may not be neglectable, although it is exponentially small (often they are omitted in asymptotic approaches).

Clearly, the effective cross-sectional modulus $E$ in eq. (25) is a function of $\tau/w, \tau/h$. As shown in Figure 6, when $\tau \ll w$ and $\tau \ll h$, the cross-sectional nonlocal effect on the effective cross-sectional modulus can be neglected and therefore we arrive at $E \to E^{\mathrm{b}}$. Under such case, the 1D nonlocal model can also be suitable. However, caution must be drawn for the considerable differences between the effective cross-sectional modulus $E$ and the classical bulk modulus $E^{\mathrm{b}}$ where the intrinsic length is comparable to the cross-section feature size (the minimal value among width $2w$ or height $2h$). Moreover, the smaller the cross-sectional area is, the more significant

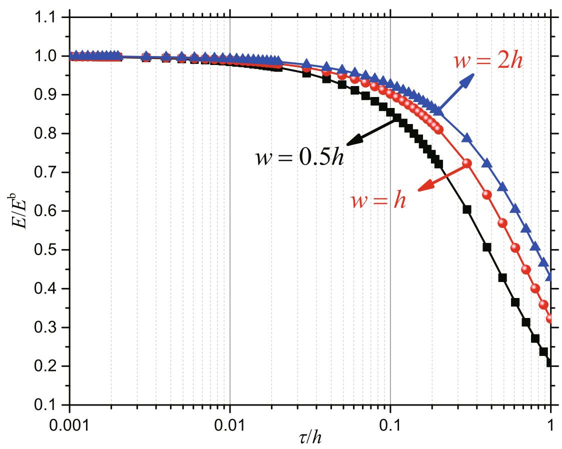


**Figure 6** (Color online) Effect of the intrinsic length $\tau$ on the effective cross-sectional modulus for various cross-sectional shapes.

the nonlocal effect becomes. To capture the significant cross-sectional nonlocality effect (“modulus-softening” effect), the 3D nonlocal model must be therefore employed.

Correspondingly, the boundary conditions are

$$\text{at } x_1 = 0 : u(0) = 0, \tag{26a}$$

$$\text{at } x_1 = L : N_b(L) + N_s(L) = P. \tag{26b}$$

By using the boundary condition (26b) and recalling eq. (22), we arrive at $C_0 = P$. With this, the governing eq. (23) can be rewritten as

$$(E^{\mathrm{b}}A\xi_1 + E^{\mathrm{s}}A^{\mathrm{s}})\frac{\mathrm{d}u}{\mathrm{d}x_1} + \frac{EA\xi_2}{2\tau}\int_0^L \exp\left(-\frac{|x_1 - x_1'|}{\tau}\right)\frac{\mathrm{d}u}{\mathrm{d}x_1'}\mathrm{d}x_1' = P. \tag{27}$$

Eqs. (27) and (26b) are the models for the tension problem of rods which incorporate both the long-ranged interactions (through 3D nonlocal integral elasticity) and the surface energy effect (via surface elasticity theory).

### 3.3 On the well-posed problem of bar problems

If the surface energy is not considered (i.e., $E^{\mathrm{s}} = 0$), eq. (27) reduces to

$$EA\xi_1\frac{\mathrm{d}u}{\mathrm{d}x_1} + \frac{EA\xi_2}{2\tau}\int_0^L \exp\left(-\frac{|x_1 - x_1'|}{\tau}\right)\frac{\mathrm{d}u}{\mathrm{d}x_1'}\mathrm{d}x_1' = P, \tag{28}$$

which is the two-phase 3D nonlocal bar model. When further considering the pure nonlocal model ($\xi_1 = 0$), eq. (28) reduces to

$$\frac{EA}{2\tau}\int_0^L \exp\left(-\frac{|x_1 - x_1'|}{\tau}\right)\frac{\mathrm{d}u}{\mathrm{d}x_1'}\mathrm{d}x_1' = P, \tag{29}$$

which is, however, ill-posed, although the 3D nonlocal effect is taken into account. If the cross-sectional nonlocal effect is neglected, the 3D nonlocal bar model (28) can be further simplified as the following form by simply setting $E = E^{\mathrm{b}}$.

$$E^{\mathrm{b}}A\xi_1\frac{\mathrm{d}u}{\mathrm{d}x_1} + \frac{EA\xi_2}{2\tau}\int_0^L \exp\left(-\frac{|x_1 - x_1'|}{\tau}\right)\frac{\mathrm{d}u}{\mathrm{d}x_1'}\mathrm{d}x_1' = P, \tag{30}$$

which is the governing equation for the uniaxial tension problem of bars using the 1D nonlocal model in refs. [10, 49].

If the 3D nonlocal effect is not considered (i.e., $\xi_1 = 1$ or $\xi_2 = 0$), eq. (27) reduces to

$$(E^{\mathrm{b}}A + E^{s}A^{\mathrm{s}})\frac{\mathrm{d}u}{\mathrm{d}x_1} = P, \tag{31}$$

which is the governing equation for tensile problem of nanobars considering surface energy effect. If both the nonlocal and surface energy effects are suppressed (i.e., $E^{\mathrm{s}} = 0$, $\xi_2 = 0$), eq. (27) reduces to the classical tensile problem of bars.

If $\xi_1 = 0$ (i.e., the pure nonlocal model (8) is adopted), eq. (27) reduces to

$$E^{\mathrm{s}}A^{\mathrm{s}}\frac{\mathrm{d}u}{\mathrm{d}x_1} + \frac{EA}{2\tau}\int_0^L \exp\left(-\frac{|x_1 - x_1'|}{\tau}\right)\frac{\mathrm{d}u}{\mathrm{d}x_1'}\mathrm{d}x_1' = P. \tag{32}$$

**Remark 3.2** The governing eq. (32) can account for the coupling influences of both the 3D nonlocality and surface elasticity. More importantly, unlike the pure 3D nonlocal model (29), the governing eq. (32) with the additional surface effect is an integral equation of the second kind and hence can be a well posed problem. For the sake of simplification, the governing eq. (32) is therefore used to model the bar problem taking the 3D nonlocality and surface elasticity effects into consideration.

### 3.4 A self-consistent variational and well-posed model

With the help of the reduction method [50, 51], eq. (32) can reduce to a specific differential-type governing equation from a viewpoint of mathematics. That is, we can arrive at the following proposition by following a similar procedure in ref. [11].

**Proposition 3.1** The well-posed governing equation shown in the integral-type expression (32), together with the pure three-dimensionally nonlocal kernel (eq. (12) with $\xi_1 = 0$), can be completely equivalent to a differential-type governing equation:

$$-\tau^2 E^{\mathrm{s}}A^{\mathrm{s}}\frac{\partial^2\varepsilon_{11}}{\partial x_1^2} + (EA + E^{\mathrm{s}}A^{\mathrm{s}})\,\varepsilon_{11} = P, \tag{33}$$

providing the following additional boundary conditions:

$$\begin{aligned} &\tau\frac{\partial\varepsilon_{11}}{\partial x_1} - \varepsilon_{11} = -\frac{P}{E^{\mathrm{s}}A^{\mathrm{s}}}, \text{ at } x_1 = 0, \\ &\tau\frac{\partial\varepsilon_{11}}{\partial x_1} + \varepsilon_{11} = \frac{P}{E^{\mathrm{s}}A^{\mathrm{s}}}, \text{ at } x_1 = L. \end{aligned} \tag{34}$$

Note that eq. (33) can be viewed as a self-consistent variational formulation of the governing eq. (32) or eq. (32) by employing specific boundary conditions in eq. (34). Currently, the frequently-employed differential-type constitutive relation given in eq. (10) without employing specific boundary conditions is an inconsistent variational model and therefore shows, however, a considerable difference with its differential-type counterpart for any boundary value problem [12, 40], although the differential-type and integral-type constitutive laws can predict the same results for non-boundary-value problems (such as dispersion of waves, screw dislocations, as originally suggested by ref. [16]).

## 4 Closed-form solutions of displacement

In this section, we shall derive the closed form solutions for eq. (32) or its equivalent formulation (33) under the clamped-free boundary condition. Note that we assume that the long-ranged interactions are described by the pure 3D nonlocal integral model, and the surface elastic modulus $E^s > 0$ [52].

The solution of the strain in eq. (33) can be expressed as

$$\varepsilon_{11}(x_1) = C_1 e^{-\alpha x_1} + C_2 e^{\alpha x_1} + \frac{1}{EA + E^s A^s} P, \tag{35}$$

where use has been made of the boundary condition (26b) at $x_1 = L$, and

$$\alpha = \sqrt{\frac{(EA + E^s A^s)}{\tau^2 E^s A^s}} = \frac{1}{\tau}\sqrt{1 + \frac{1}{\Omega}}, \tag{36}$$

with

$$\Omega = E^s A^s/(EA). \tag{37}$$

The constants $C_1, C_2$ can be determined from eq. (34) as follows:

$$C_1 = \frac{EAe^{L\alpha}P}{E^s A^s (EA + E^s A^s)(e^{L\alpha}(\alpha\tau + 1) - \alpha\tau + 1)}, \quad C_2 = C_1 e^{-L\alpha}. \tag{38}$$

Consequently, with the boundary condition (26b) ($u(0) = 0$), $u(x_1)$ can be exactly solved as

$$u(x_1) = \int_0^{x_1} \varepsilon_{11}(x_1')\mathrm{d}x_1' \tag{39}$$

$$= \frac{P\left\{e^{L\alpha} + e^{\alpha x_1} - e^{\alpha(L - x_1)} - 1 + x_1\alpha\left[e^{L\alpha}(\alpha\tau + 1) - \alpha\tau + 1\right]\Omega\right\}}{EA\alpha\Omega(1 + \Omega)\left[e^{L\alpha}(\alpha\tau + 1) - \alpha\tau + 1\right]}. \tag{40}$$

The maximum displacement takes place at $x_1 = L$ and can be given by

$$u_m = \frac{P\left\{2\left(e^{L\alpha} - 1\right) + L\alpha\Omega\left[e^{L\alpha}(\alpha\tau + 1) - \alpha\tau + 1\right]\right\}}{EA\alpha\Omega(1 + \Omega)\left[e^{L\alpha}(\alpha\tau + 1) - \alpha\tau + 1\right]}. \tag{41}$$

### 4.1 Asymptotic solution of displacement

As $\tau/L$ is usually considered to be relatively small, $e^{-\alpha L}$ should be exponentially small (cf. (36)). Thus, some approximations can be given for solutions (39) and (41). By omitting exponentially small terms, the displacement (39) can be expressed as

$$u(x_1) = \frac{P\left[1 - e^{-\alpha x_1} + e^{-(L - x_1)\alpha} + x_1(\alpha\tau + 1)\alpha\Omega\right]}{EA\Omega(1 + \Omega)(\alpha\tau + 1)\alpha} + E.S.T., \tag{42}$$

where "$E.S.T.$" denotes exponentially small terms. Note that $\Omega$ and $\alpha$ have been defined in eqs. (37) and (36), respectively. To explicitly show the cross-sectional nonlocal effect, $\Omega$ can be expressed as the following form by substituting eq. (25) into eq. (37).

$$\Omega = \frac{E^s A^s}{E^b A}\left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)^{-1}\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right)^{-1}. \tag{43}$$

Correspondingly, the asymptotic displacement is

$$u(x_1) = \frac{P\left[1 - e^{-\alpha x_1} + e^{-(L - x_1)\alpha} + x_1(\alpha\tau + 1)\alpha\Omega\right]}{E^b A\Omega(1 + \Omega)(\alpha\tau + 1)\alpha} \times \left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)^{-1}\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right)^{-1},$$

and the asymptotic maximum displacement occurring at $x_1 = L$ can be expressed as

$$u_m = \frac{PL\left(1 + \Omega + \sqrt{\Omega + \Omega^2} + 2\frac{\tau}{L}\right)}{E^b A(1 + \Omega)\left(1 + \Omega + \sqrt{\Omega + \Omega^2}\right)}\left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)^{-1} \times \left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right)^{-1}. \tag{44}$$

Note that the effective cross-sectional modulus $E$ has been expressed using the bulk modulus $E^b$ according to relation (25).

The size dependence of displacements predicted by exact and approximate solutions is studied based on eqs. (39) and (42). The classical displacement for bars under tension is $u_c = Px_1/E^b A$. To only show the axially size-dependent effect, we set $L \gg h$ and $L \gg w$ (leading to $E = E^b$), and then Figure 7 shows the normalized displacement ($u/u_c$). It is clear that the displacement increases as the axially nonlocal parameter $\tau$ increases, and the axially nonlocal parameter $\tau$ has the softening size effect on the displacement. Owing to the stiffening effect of surface elastic modulus $E^s$, the

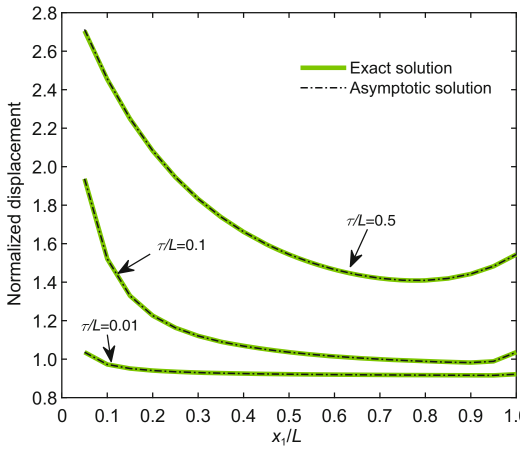


**Figure 7** (Color online) Size dependence of displacement predicted by exact and asymptotic solutions ($\Omega = 0.1$).

displacement may be hardening or softening. Furthermore, the size effect on the displacement near two ends is very significant. And the size effect on the displacement near the clamped end is more significant than that near the free end. More importantly, the approximate method (42) can predict the displacements which are in very good agreement with the exact solution (39) for all the cases of interest.

### 4.2 1D nonlocal model versus 3D nonlocal model

When neglecting the cross-sectional nonlocal effect ($\ell = 0$ or $E = E^{\mathrm{b}}$), the displacement solution (42) can reduce to

$$u_{1D}(x_1) = \frac{P\left[1 - e^{-\beta x_1} + e^{-(L-x_1)\beta} + x_1(\beta\tau + 1)\beta\chi\right]}{E^{\mathrm{b}}A\chi(1+\chi)(\beta\tau + 1)\beta}, \tag{45}$$

where

$$\beta = \sqrt{\frac{E^{\mathrm{b}}A + E^{\mathrm{s}}A^{\mathrm{s}}}{\tau^2 E^{\mathrm{s}}A^{\mathrm{s}}}} = \frac{1}{\tau}\sqrt{1 + \frac{1}{\chi}}, \quad \chi = \frac{E^{\mathrm{s}}A^{\mathrm{s}}}{E^{\mathrm{b}}A}. \tag{46}$$

Eq. (45) is the closed-form solution for the displacement of the bar modeled using the pure axially-nonlocal model and the surface elasticity. Note that $\chi$ and $\Omega$ has the following relation:

$$\Omega = \chi\left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)^{-1}\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right)^{-1}.$$

Figure 8 shows the displacement predicted by classical results, the 1D and 3D nonlocal models with surface effect. As expected, the maximum displacement takes place at $x = L$. Furthermore, unlike the classical displacement, the size-dependent displacement is no long linearly changed along the length direction of nanobars. More importantly, the 1D nonlocal model may cause unacceptable errors when the cross-sectional nonlocal effect is significant ($\tau/h = 0.5$).

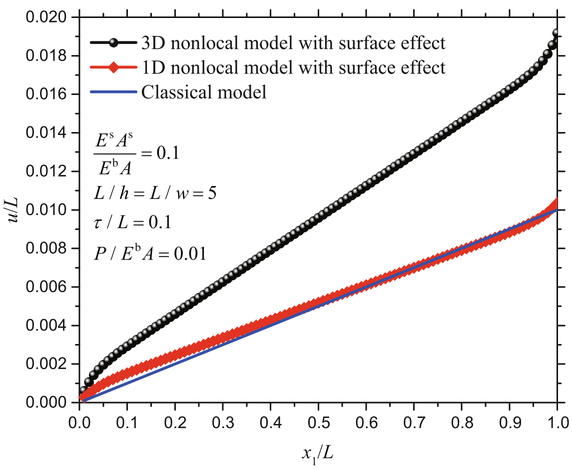


**Figure 8** (Color online) Displacement predicted by classical results, the 1D and 3D nonlocal models with surface effect.

## 5 Predictions for effective elastic modulus

It is not clear whether the elastic modulus wound reduce or rise with the decreasing size of the cross-section of nanobars. Now, we consider the size dependence of elastic modulus. The size dependence may be attributed to bulk periodic nanostructures and surface elasticity.

In the case of classical elasticity, the axial displacement can be expressed as

$$u_c(x_1) = \frac{Px_1}{E^{\mathrm{b}}A},$$

and the maximum axial displacement can be given by

$$u_c(L) = \frac{PL}{E^{\mathrm{b}}A}, \tag{47}$$

for bars under tension (with a concentrated load $P$ at free end). The classical results can also be determined by setting $\tau = 0$ and $E^{\mathrm{s}} = 0$ in eqs. (42) and (44).

By comparing the size-dependent maximum axial displacement (44) and with its classical counterpart (47), the effective elastic modulus $E_{\mathrm{eff}}$ can be given by

$$E_{\mathrm{eff}} = \frac{E^{\mathrm{b}}(1+\Omega)\left(1 + \Omega + \sqrt{\Omega + \Omega^2}\right)}{\left(1 + \Omega + \sqrt{\Omega + \Omega^2} + 2\frac{\tau}{L}\right)} \times \left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right). \tag{48}$$

By using the effective elastic modulus, the maximum axial displacements of the size-dependent nanobars can be determined by using a traditional tensile analysis in a familiar manner used in classical bars in tension. This will be helpful for determining the nonlocal and surface parameters from experimental studies which are often carried out in a familiar manner used in classical (macroscopic) approaches [53].

When considering the case of a long nanobar where its length is far larger than its cross-sectional feature size ($L \gg \min\{w, h\}$ and $\tau/L \to 0$), the axially nonlocal effect is neglectable. Under such case, the effective elastic modulus (48) reduces to

$$E_{\mathrm{eff}}^{\mathrm{long}} = E^{\mathrm{b}}(1+\Omega)\left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right). \tag{49}$$

To explicitly show both the surface and cross-sectional nonlocal effects, the effective elastic modulus of a long nanobar can be, alternatively, expressed as the following form by substituting eq. (43) into the previous expression.

$$E_{\mathrm{eff}}^{\mathrm{long}} = E^{\mathrm{b}}\left(1 + \frac{\tau}{2w}e^{-\frac{2w}{\tau}} - \frac{\tau}{2w}\right)\left(1 + \frac{\tau}{2h}e^{-\frac{2h}{\tau}} - \frac{\tau}{2h}\right)$$

$$+\frac{E^{\mathrm{s}}(w+h)}{wh}. \tag{50}$$

Note that when $w/\tau = 4$ (or $h/\tau = 4$), the exponential term $\exp(-8) = 0.0003$. Thus, when considering the case of $\ell/R < 0.25$ where $R \doteq \min(w, h)$ is the cross-sectional feature size, the exponential term can be approximate as 0. Under the circumstance, the effective elastic modulus of a long nanobar can be approximately obtained as

$$E_{\mathrm{eff}}^{\mathrm{long}} = E^{\mathrm{b}}\left(1-\frac{\tau}{2w}\right)\left(1-\frac{\tau}{2h}\right)+\frac{E^{\mathrm{s}}(w+h)}{wh},$$

and the size-dependent effect can be characterized by

$$\frac{E_{\mathrm{eff}}^{\mathrm{long}}}{E^{\mathrm{b}}} = \left(1-\frac{\tau}{2w}\right)\left(1-\frac{\tau}{2h}\right)+\chi.$$

As observed, the surface elasticity has a "modulus-hardening" effect; however, the cross-sectional nonlocality has a "modulus-softening" effect. That is, the effective elastic modulus may be softening or hardening, depending on the competition between the surface and nonlocal effects.

By making use of eq. (50), Figure 9 shows the "modulus-softening" or "modulus-hardening" effective elastic modulus due to the competition between the surface and nonlocal effects. As observed from Figure 9, the "modulus-softening" effect is more significant as $\tau/h$ (or $\tau/w$) increases, and the "modulus-hardening" effect can increase when enlarging $\chi$. These observations can be, to a certain extent, consistent with the size-dependent phenomena on the effective elastic moduli in both experimental investigations [53] and analytical models [23, 54–57].

When considering the case of a short nanobar where its cross-sectional feature size is far larger than its length ($L \ll R$), the size-dependent contribution due to both the cross-sectional nonlocal effect and the surface effect can be neglected ($E^{\mathrm{s}}/R = 0$ and $\tau/R = 0$). Under such case, the effective elastic modulus (48) reduces to

$$E_{\mathrm{eff}}^{\mathrm{short}} = E^{\mathrm{b}}\left(1+2\frac{\tau}{L}\right)^{-1}, \tag{51}$$

which shows a "modulus-softening" behavior.

If the 1D nonlocal model (30) is used, the effective elastic modulus can be obtained in a similar way as that of the 3D nonlocal model given by eq. (48). The effective elastic modulus of the 1D nonlocal model can be given by

$$E_{\mathrm{eff}}^{\mathrm{1D}} = \frac{E^{\mathrm{b}}(1+\chi)\left(1+\chi+\sqrt{\chi+\chi^2}\right)}{1+\chi+\sqrt{\chi+\chi^2}+2\frac{\tau}{L}}. \tag{52}$$

Recalling that $\chi$, which has been defined in eq. (46), is a dimensionless parameter to characterize the surface effect. Furthermore, if the pure surface elasticity is considered, we have

$$E_{\mathrm{eff}}^{\mathrm{surface}} = E^{\mathrm{b}}+\frac{E^{\mathrm{s}}(w+h)}{wh},$$

which is the effective elastic modulus of the pure surface model.

Figure 10 shows the size-dependent effect on the normalized effective elastic modulus predicted by the classical model, the 1D nonlocal model with surface effect, the pure surface model, and the 3D nonlocal model with surface effect. As expected, the pure surface model produces an enlarging effective modulus. While the 1D nonlocal model takes the surface effect into consideration, it processes also a considerable difference with the 3D nonlocal model when the cross-sectional nonlocal effect is significant. However, the difference can decrease as $\tau/h$ (or $\tau/w$) increases. This is because the axially nonlocal effect may be neglectable when

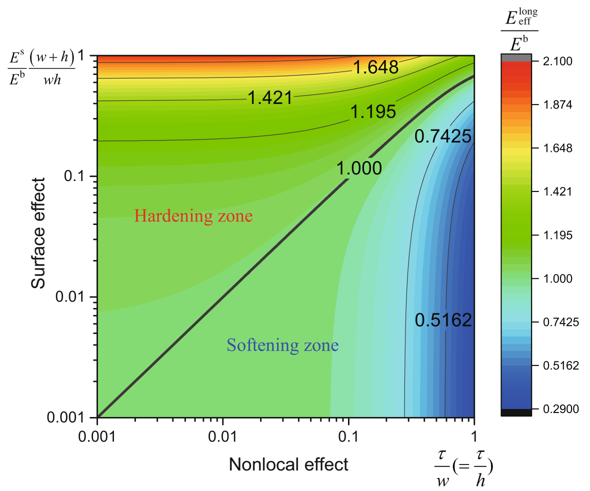


**Figure 9** (Color online) Surface-nonlocality map for the effective elastic modulus of long nanobars.

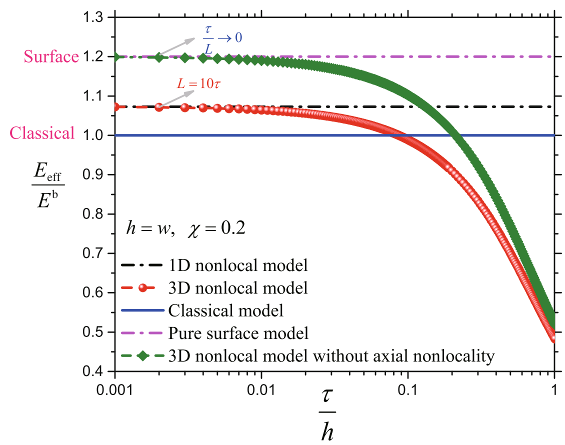


**Figure 10** (Color online) Size-dependent effect on the normalized effective elastic modulus predicted by the classical model, the 1D nonlocal model with surface effect, the pure surface model, and the 3D nonlocal model with surface effect.

the cross-sectional nonlocal effect plays a dominant role in the effective modulus.

Considering pure nonlocal effects ($\chi = 0$), Figure 11 shows the competition relation between axial nonlocality versus cross-sectional nonlocality for the effective elastic moduli as a function of the ratio of length to the cross-sectional feature size. To compare the axial and cross-sectoinal nonlocal effects, the error defined as the absolute value between the nonlocal and classical models is also calculated and plotted. It is found out from Figure 11 that both the nonlocal cross-sectional and axial interactions become significant when the length-to-height ratio of nanobars is small. If the length-to-height ratios are relatively large (considering slender bars), the main nonlocal effect stems, however, from the nonlocal cross-sectional effect, rather than the axial nonlocal effect as it is commonly believed.

Figure 12 shows the size-dependent effect on the normalized effective elastic modulus as the ratio of length to height

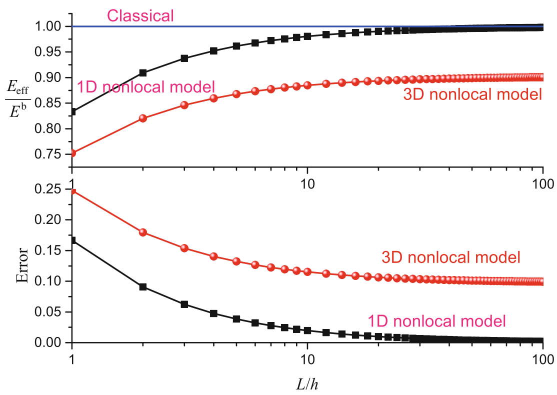


**Figure 11** (Color online) Axial nonlocality versus cross-sectional nonlocality for the effective elastic moduli as a function of the ratio of length to the cross-sectional feature size ($h = w = R$, $\tau/R = 0.1$).

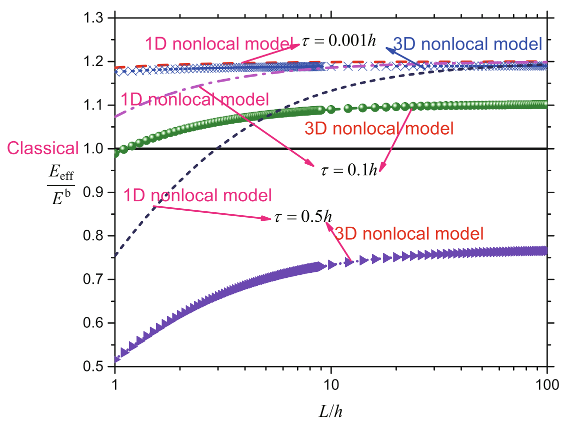


**Figure 12** (Color online) Size-dependent effect on the normalized effective elastic modulus as a function of $L/h$ predicted by the classical model, the 1D and 3D nonlocal models with surface effect ($h = w = R$, $\tau/R = 0.1$, $\chi = 0.2$).

increases. The 1D and 3D nonlocal models incorporating the surface effect are used for predicting the normalized effective elastic modulus. There exists a considerable difference between the 1D and 3D nonlocal models, especially for the case where bar's height is comparable to its intrinsic lengths. More importantly, the cross-sectional nonlocal effect always plays a significant role in the modulus-softening effect. As shown in the case of $\tau = 0.1h$, both the axial nonlocality and the cross-sectional nonlocality show important influences on the effective elastic modulus when considering a small ratio of length to height; the effect of axial nonlocal effect can, however, be neglected when we consider the case of $L/h \geqslant 10$ where the modulus-softening effect due to the cross-sectional nonlocality may still be significant.

Clearly, the effective elastic modulus $E_{\rm eff}$ suggests the following remarks as discussed previously.

(1) Both the axial nonlocality and the cross-sectional nonlocality show a modulus-softening effect, resulting in a smaller bulk (core) modulus in comparison of classical elastic modulus.

(2) The surface elastic modulus $E^s$ has a stiffening size effect on the effective elastic modulus. Thus, the effective elastic modulus may be softening or hardening, depending on the competition between the surface and nonlocal effects.

(3) There exists a considerable difference between the 1D and 3D nonlocal models for predicting the effective elastic modulus, especially for the case where bar's radius is comparable to its intrinsic lengths.

(4) When the length-to-height ratio is relatively large, the main nonlocal effect stems from the nonlocal cross-sectional effect, rather than the axial (1D) nonlocal effect as it is commonly believed.

(5) The 1D nonlocal model can be adopted if and only if the cross-sectoinal feature size (the minimal value between its height and its width) is far larger than its length and, of course, its intrinsic length.

## 6 Conclusions

Nanoscale bars are naturally discrete, and therefore the continuum assumption is failed. Also, surface-to-volume ratio is very large for nanoscale bars, and as a result, the surface effect becomes significant and has to be taken into consideration. The nonlocal theory of elasticity releasing the continuum assumption and the surface theory of elasticity are therefore employed to model nanobars under tension.

As commonly believed in the current practice, the axial (1D) nonlocal effect is only taken in account to analyze the mechanical behaviors of nanobars, regardless of their 3D inherent atomistic interactions. This study suggests a three-dimensional nonlocal constitutive law to model the true nonlocal effect of nanobars, and based on which and the surface theory of elasticity, a self-consistent variational and well-posed governing equation has been established for modeling tensile nanobars. It has revealed for the first time how both the cross-sectional nonlocal interactions and the 1D axial nonlocality affect the tensile behaviors of nanobars. It is found that both the nonlocal cross-sectional and axial interactions become significant when the length-to-height ratio of nanobars is small. If the length-to-height ratio is relatively large (slender bars), the main nonlocal effect stems, however, from the nonlocal cross-sectional effect, rather than the commonly believed axial nonlocal effect. It can be concluded that the nonlocal influence predicted by the currently axial nonlocal bar model is grossly underestimated. This implies that the currently axial nonlocal bar model is suitable only for bar's length far smaller than its cross-sectional feature size where both the surface and cross-sectionally nonlocal effects are neglectable.

This work also shows that it is possible to overcome the ill-posed problem of the pure nonlocal integral elasticity by employing both the pure nonlocal integral elasticity and surface elasticity. A well-posed size-dependent governing equation has been established for modeling nanobars under tension, and closed-form solutions are derived for the displacement field of nanobars under tension.

According to the closed-form solutions, the effective elastic modulus is obtained and will be useful for calibrating the physical quantities in the "discrete-continuum" transition region for a span-scale modeling approach. It is found that the effective elastic modulus may be softening or hardening, depending on the competition between the surface and nonlocal effects.

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