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RESEARCH PAPER

Static analysis of ultra-thin beams based on a semi-continuum model

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Abstract A linear semi-continuum model with discrete atomic layers in the thickness direction was developed to investigate the bending behaviors of ultra-thin beams with nanoscale thickness. The theoretical results show that the deflection of an ultra-thin beam may be enhanced or reduced due to different relaxation coefficients. If the relaxation coefficient is greater/less than one, the deflection of micro/nano-scale structures is enhanced/reduced in comparison with macro-scale structures. So, two opposite types of size-dependent behaviors are observed and they are mainly caused by the relaxation coefficients. Comparisons with the classical continuum model, exact nonlocal stress model and finite element model (FEM) verify the validity of the present semi-continuum model. In particular, an explanation is proposed in the debate whether the bending stiffness of a micro/nano-scale beam should be greater or weaker as compared with the macro-scale structures. The characteristics of bending stiffness are proved to be associated with the relaxation coefficients.

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1 Introduction

Micro/nano-scale materials and structures have recently received considerable attention as these small-scale structures offer great potential applications. With the rapid development of current nanotechnology, miniaturized structures with micro/nano-scale features can be precisely manufactured and applied in the micro/nano-electromechanical systems (MEMS/NEMS). The widespread availability of MEMS/NEMS such as atomic force microscopes has resulted in renewed interest in micro/nano-systems as chemical, physical and biological sensors and devices. This demands higher precision for the sensors, higher frequency for the mixers, and the performance of these devices is extremely dependent on the properties of their ultra-thin beam-like elements. These properties need to be well characterized in order to control their functionality.

In comparison with the macro materials and structures, some effects which are not observed at macro-size appear in micro/nano-scale, such as the size-dependent effect. For instance, according to the classical continuum theory, the stress is singular at a crack tip despite how weak the external load is. However, each material has limited fatigue strength and in fact, atomic simulation and experiment proved its non-singularity at the crack tip [1]. In a phonon scattering experiment, it was demonstrated that the high frequency wave is dispersive and the propagation velocity is related to frequency [2] while, in comparison, the wave velocity is a constant in classical mechanics. To analytically investigate the size-dependent effect; the nonlocal theory [3], surface effect theory [4] and strain gradient theory [5] have been proposed. The nonlocal theory assumes that the stress at a point in the continuous body is not only the function of the strain at that

given point, but also related to the strains of all the points in the body. Eringen's nonlocal elasticity [3] allows one to account for the small scale effect that becomes significant when dealing with micro/nano-structures. Recently, Lim et al. [6–8] proposed a new exact nonlocal stress model and obtained some new conclusions according to Eringen's nonlocal field theory. The surface effect is present due to the high ratio of surface to bulk in the micro/nano-scale structures, and the mechanical behaviors of several atomic layers on surface really differ from the properties of the internal atoms. The strain gradient theory consists of two groups, the higher-order and lower-order sub-theories. For example, in the higher-order theory, higher-order stresses are defined to be the work-conjugate to strain gradient, thus leading to the necessity of using higher-order governing equations and boundary conditions. In recent years, a new strain gradient theory, which was built based on the energy nonlocal model, was presented by Yi et al. [9]. It was applied to investigate the size effects for torsion of thin metallic wire, ultra-thin beam bending and micro-indentation of polycrystalline copper. Many papers discussed the static or dynamic properties of nanobeams or carbon nanotubes (CNTs) based on nonlocal elasticity theory [6–8,10,11]. Disregard some disputes in the different conclusions according to the nonlocal nanoscale field [6–8,10,11]. It is indeed found that size-effects exist in the micro/nano-scale mechanical behaviors for buckling, bending, wave propagation and free or forced vibration etc. of micro/nano-scale structures.

As mentioned above, the classical continuum theory fails at micro/nano-scale, some new approaches should be constructed in addition to the traditional nonlocal theory, surface effect theory, strain gradient theory, etc. in order to suit for the development of new nanotechnology. As a result, the semi-continuum model emerged owing to the stringent requirements of engineering and nanotechnology. The semi-continuum model for lattice vibration of graphite was proposed by Nagamiya and Komatsu [12] in the middle of the 20th century and it was successful to express the dispersion relation of lattice vibration analytically. Based on this work, Nihira and Iwata [13] discussed the temperature dependence of lattice vibration and reported an analysis of the specific heat of graphite. The mechanical properties of ultra-thin films were initially addressed by Sun and Zhang [14] based on a semi-continuum model, and it was useful for the nanostructured materials that possess a plate-like geometry. The work presented by Sun and Zhang [14] indicated that the values of Young's modulus and Poisson's ratios strongly depend on the number of atomic layers. Bao et al. [15] investigated the elastic modulus of nanometer silicon membrane and concluded that the elastic modulus increases with increasing membrane thickness. A recent work by Tang et al. [16] pointed out two opposite types of size-dependence for elastic modulus, which concluded an increase or decrease with respect to thickness of the structures. The opposite effects were caused by long range attractive and repulsive interactions in pair potentials $u(r_{ij})$ between atoms i and j [16].

In the present paper, a semi-continuum based method for bending of an ultra-thin beam is developed. Two typical end supporting conditions, i.e. fully clamped and cantilever beams, are investigated. In contrast to the classical continuum mechanics, the semi-continuum model accounts for discrete nature in the thickness direction because the beam is ultra thin. The paper extends the works of Sun and Zhang [14] and Bao et al. [15] by building in relaxation and applying into each one atomic layer on the upper and lower surfaces. A comparison with classical mechanics shows that the relaxation coefficient is a key factor to the two opposite types of size-dependence mentioned by Tang et al. [16]. Comparisons with finite element method (FEM) and experiment, further determine the magnitude of relaxation coefficient in specific cases. In particular, special attention is paid to the influence of the relaxation coefficient on the deflection or bending stiffness of the ultra-thin beam subjected to a concentrated load.

2 Semi-continuum model

Consider an ultra-thin silicon beam, with length L, width B and thickness H, as shown in Fig. 1. The coordinate axes x and y locate on the mid-surface and the z-axis is perpendicular to this surface. The beam is assumed to be sufficiently restrained in order to prevent lateral torsional buckling and it is modeled in a regular tetrahedron lattice of atoms. The cross section of the beam is illustrated in Fig. 2, where the discrete black dots represent atoms and l denotes the atomic layer ordinal. The distance between two adjacent atomic layers is the crystal lattice parameter a. The beam is thus assumed to have $N + 1$ ($N = 0, 2, 4, \cdots$) atomic layers and N crystal lattices with the distance a between each lattice along the thickness. Although only odd atomic layers $N + 1$ are assumed for mathematical simplicity in theoretical deduction, the semi-continuum model is also applicable to ultra-thin materials composed of even atomic layers [14]. The traditional continuum mechanics is valid on the mid-plane and other parallel planes but it is not suitable in the thickness direction because of discreteness and divided layers of atom. In this model, the atom bond is assumed to be spring and the interatomic binding forces are equivalent to spring potential function with an elastic coefficient k and the elastic coefficient can be derived by the lattice dynamics for each material [17]. This model considers only the forces of adjacent atoms and the interaction among nonadjacent atoms is neglected.

Compared to the crystal lattice parameter, the thickness of each atomic layer is assumed small enough to be ignored. Note that much work on relaxation phenomenon have been studied and published [18,19]. Because atoms on the free surface have a smaller coordination number than its bulk, the relaxation phenomenon usually exists both at macro and

nano scales. Since the nano scale materials and structures have much smaller external characteristic scales, the relaxation phenomenon should be considered even further. Due to the relaxation effect, the atom bond in some surface atomic layers may be different from the inner atoms and the crystal lattice parameter in the surface could become ra, where r is the relaxation coefficient [19]. In this paper, each layer on the upper and lower surfaces is postulated to yield relaxation phenomenon, namely the distance of two adjacent atomic layers is ra on the upper and lower surfaces while the distance between the other adjacent atomic layers is still a. Therefore, we have $H = (N - 2 + 2r)a$.

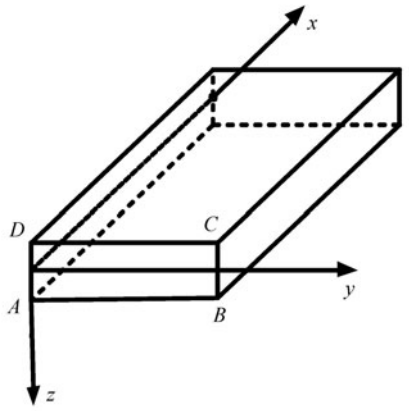

Fig. 1 Sketch of an ultra-thin beam

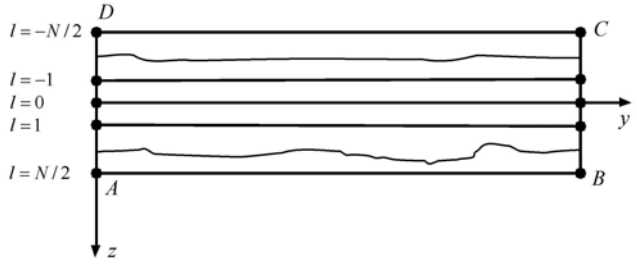

Fig. 2 The semi-continuum model for an ultra-thin beam

The displacements in x-, y- and z-axes are denoted by u, v and w, respectively. Based on the semi-continuum model and the equivalent spring method, the strain potential energy of unit volume in the l-th layer for the bending beam is derived similar to the approaches of Sun and Zhang [14] and Bao et al. [15], as

$$\begin{aligned} U^{(l)} = {} & \frac{k(N-1)}{6(N-2+2r)a}[(\varepsilon_{xx}^{(l)} + \varepsilon_{yy}^{(l)} + \varepsilon_{zz}^{(l)})^2 + \gamma_{xy}^{(l)2} + \gamma_{xz}^{(l)2} + \gamma_{yz}^{(l)2}] \\ & + \frac{k}{(N-2+2r)ar(r^2+2)}[(\varepsilon_{xx}^{(l)} + \varepsilon_{yy}^{(l)} + r\varepsilon_{zz}^{(l)})^2 \\ & + \gamma_{xy}^{(l)2} + r^2\gamma_{xz}^{(l)2} + r^2\gamma_{yz}^{(l)2}], \end{aligned} \tag{1}$$

where k is the elastic coefficient of the spring, the number of atomic layers N is assumed to satisfy $N > 2$, the superscript (l) denotes the l-th layer and the strain components are defined as [14]

$$\begin{aligned} \varepsilon_{xx}^{(l)} &= \frac{\partial u^{(l)}}{\partial x}, \\ \varepsilon_{yy}^{(l)} &= \frac{\partial v^{(l)}}{\partial y}, \\ \gamma_{xy}^{(l)} &= \frac{\partial u^{(l)}}{\partial y} + \frac{\partial v^{(l)}}{\partial x}, \\ \varepsilon_{zz}^{(l)} &= \frac{w^{(l+1)} - w^{(l)}}{a}, \\ \gamma_{xz}^{(l)} &= \frac{\partial w^{(l)}}{\partial x} + \frac{u^{(l+1)} - u^{(l)}}{a}, \\ \gamma_{yz}^{(l)} &= \frac{\partial w^{(l)}}{\partial y} + \frac{v^{(l+1)} - v^{(l)}}{a}. \end{aligned} \tag{2}$$

3 Linear model

The displacements are assumed to be small and, hence, the axial load yielding by the bending can be ignored. Here, only the strain potential energy due to bending deformation is accounted for and the displacements in x- and y- axes are much smaller than the one in z- direction. Because of very thin atomic layers, we further have $u^{(l+1)} \approx u^{(l)}$, $v^{(l+1)} \approx v^{(l)}$ and $w^{(l+1)} \approx w^{(l)}$. For simplicity, the strain tensor in Eq. (2) has only one nonzero component, given as

$$\varepsilon_{xx}^{(l)} = -z\frac{\mathrm{d}^2 w}{\mathrm{d}x^2}. \tag{3}$$

The linear model which neglects axial elongation is built for fully clamped and cantilever beams. Some comparisons of the linear semi-continuum model with the classical continuum model, exact nonlocal stress model and linear FEM are presented below in detail.

3.1 Fully clamped beams

For a fully clamped ultra-thin beam subjected to a downward concentrated load P at the mid-point ($x = L/2$), the deflection function may be expressed as

$$w_{\mathrm{s}}(x) = \frac{w_{0\mathrm{s}}}{2}\left(1 - \cos\frac{2\pi x}{L}\right), \quad (0 \le x \le L), \tag{4}$$

where $w_{0\mathrm{s}}$ is the maximum deflection occurring at the mid-point.

The strain potential energy is defined as

$$E_{\mathrm{int}} = \sum_{z=-Na/2}^{Na/2} \int_0^B \int_0^L U^{(l)} a\mathrm{d}x\mathrm{d}y. \tag{5}$$

From Eqs. (1) to (5) above, one obtains

$$E_{\mathrm{int}} = \frac{kB\pi^4 a^2 N(N+1)(N+2)w_{0\mathrm{s}}^2}{6(N-2+2r)L^3}\left[\frac{N-1}{6} + \frac{1}{r(r^2+2)}\right]. \tag{6}$$

For an ultra-thin beam with a concentrated load, the external work done by the concentrated load is given by

$$W_{\text{ext}} = \int_0^{w_{0s}} P(w_s)\mathrm{d}w_s. \tag{7}$$

According to the work-energy theorem, the work done by the external load is converted to the strain potential energy. Energy in the two forms should be equal, or the variation $\delta(E_{\text{int}} - W_{\text{ext}}) = 0$. Hence, we have the following formulae of static behaviors for the dimensional and dimensionless deflections w_{0s} and $\bar{w}_{0s}$, and the bending stiffness D_{0s}, respectively

$$w_{0s} = \frac{3(N-2+2r)PL^3}{kB\pi^4 a^2 N(N+1)(N+2)}\left[\frac{N-1}{6} + \frac{1}{r(r^2+2)}\right]^{-1}, \tag{8a}$$

$$\bar{w}_{0s} = \frac{3(N-2+2r)\bar{P}}{\pi^4\tau^2 N(N+1)(N+2)}\left[\frac{N-1}{6} + \frac{1}{r(r^2+2)}\right]^{-1}, \tag{8b}$$

$$D_{0s} = \frac{kB\pi^4 a^2 N(N+1)(N+2)}{3(N-2+2r)L^3}\left[\frac{N-1}{6} + \frac{1}{r(r^2+2)}\right], \tag{9}$$

where $\bar{w}_{0s} = w_{0s}/L$, $\bar{P} = P/kB$ and $\tau = a/L$ is a parameter common in nonlocal theory to be interpreted in detail in due course.

The relation between dimensionless maximum deflection and the number of atomic layers is shown in Fig. 3 for some different dimensionless loads and relaxation coefficients. The maximum deflection decreases quickly with increasing atomic layers, especially when the number of atomic layers is very small. When the number of atomic layers becomes large enough, deflection changes very slowly and its value is close to the macro beam solution as will be shown in the next part for a cantilever ultra-thin beam. Therefore, the micro/nano-scale materials and structures with fewer layers have significantly marked deflection. For instance, when there are 10 atomic layers, the mid-point deflection of the ultra-thin beam is more than 200 times that of 70 atomic layers.

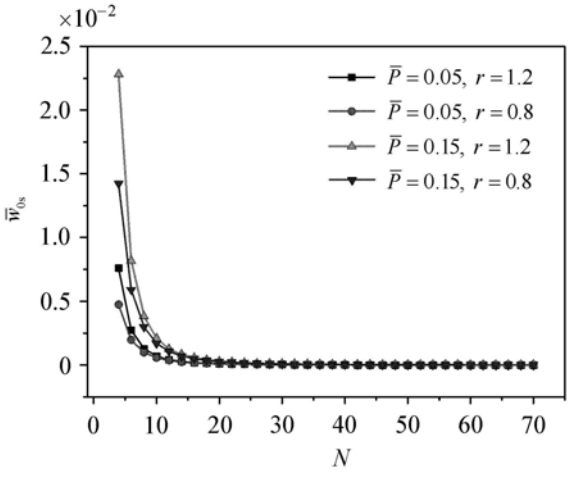

Fig. 3 Dimensionless maximum deflection versus the number of atomic layers for a fully clamped beam with $\tau = 0.1$

To demonstrate the size-dependent effect clearly, deflection without relaxation ($r = 1.0$) should be eliminated. The ratio of dimensionless maximum deflection is shown in Fig. 4, where the deflection with $r = 1.0$ is used as a normalized denominator. Two kinds of size-dependence are observed in Fig. 4, i.e. the deflection ratio decreases with increasing atomic layers (for $r > 1.0$) and the deflection ratio increases with increasing atomic layers (for $r < 1.0$). This observation is similar to the size-dependence of elastic modulus proposed by Tang et al. [16] through intermolecular potentials. The similar conclusion is obtained via two different ways. This is because the relaxation coefficient is related to molecular potential. Moreover, in tensile or compressive tests at macro-scale, the stress-strain ratio (i.e. Young's modulus) is a constant for a specific material even for test pieces of varying sizes, namely, it is size-independent for materials of macro-sizes. On the contrary, size-dependence is significant for test pieces at micro/nano-scales. For linear deformation, relaxation coefficients induce changes of the thickness and it is the main reason for size-dependence.

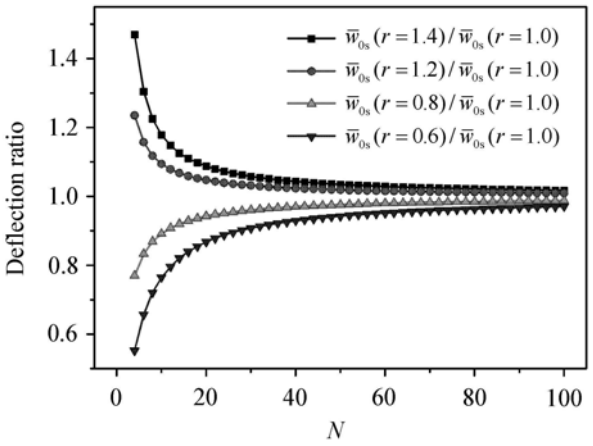

Fig. 4 Size-dependence for a fully clamped beam with $\tau = 0.1$

Table 1 presents a comparison between the present linear semi-continuum model and the linear FEM, where the latter employs a commercial package ANSYS for a fully clamped silicon nanobeam by Sundararajan and Bhushan [20]. In their example, the upper width of the beam was assumed to be a little different from the lower one. For proper comparison, the following parameters [20] are adopted: $L = 6\,\mu$m, $B = 389.5$ nm, $H = 255$ nm, and the other parameters for the linear silicon model are $a = 0.543\,1$ nm and $k = 261.432$ N/m [15,17]. Because the width includes the upper width of 295 nm and the lower width of 484 nm [20], an averaged value is assumed to make an approximate comparison.

The results obtained by the present semi-continuum linear model are found to be consistent with linear FEM for

$r = 0.3$. Equivalently, in this FEM case [20], the relaxation coefficient of each atomic layer on the upper and lower surfaces of silicon beam is 0.3 or so. Note that the magnitude of the relaxation coefficient calculated here is related to both the model assumption, such as the number of atomic layers to be relaxed, and the specific parameters used in the FEM example.

Table 1 Comparison of the linear semi-continuum model and linear FEM with $a = 0.543\,1$ nm, $k = 261.432$ N/m, $L = 6\,\mu$m, $B = 389.5$ nm and $H = 255$ nm

P/μN	W_{0s}/nm						
	Linear FEM [20]	$r = 1.2$	$r = 1.0$	$r = 0.8$	$r = 0.3$	$r = 0.1$	$r = 0.05$
0	0	0	0	0	0	0	0
20	247.7	255.7	254.5	253.2	247.6	236.8	223.2
40	492.8	511.5	509.1	506.5	495.2	473.6	446.3
60	739.6	767.2	763.7	759.8	742.8	710.3	669.5

According to classical continuum mechanics, the bending stiffness of a fully clamped beam with a concentrated load at its mid-point is given by

$$D_{0c} = \frac{192EI}{L^3} = \frac{16EB(N-2+2r)^3a^3}{L^3}, \tag{10}$$

where E is the elastic modulus, and $I = BH^3/12 = B(N-2+2r)^3a^3/12$ is the moment of area for a rectangular cross section of beam.

When there are many atomic layers, bending stiffness predicted by the semi-continuum and classical continuum models should be identical. From Eqs. (9) and (10), we obtain the elastic modulus for bulk material as $E = \pi^4 k/288a$. It can be applied approximately to calculate the bulk Young's modulus from some micro parameters. For instance, $a = 0.543\,1$ nm and $k = 261.432$ N/m are taken into account for silicon, and the value is thus found to be 162.81 GPa. It is consistent with Young's modulus of the bulk silicon obtained by experimentation or other approaches.

The difference of classical and semi-continuum bending stiffness $(D_{0c} - D_{0s})/D_{0s}$ with respect to the thickness of a fully clamped beam H is shown in Fig. 5 for a silicon beam with $a = 0.543\,1$ nm, $k = 261.432$ N/m and for classical bending stiffness the Young's modulus $E = 162$ GPa.

The difference between classical and semi-continuum bending stiffness is strongly dependent on relaxation coefficients. It is interesting that the stiffness in both models is approximately equal when $r \approx 1.36$. For relaxation coefficients below 1.36, the semi-continuum bending stiffness is larger than the classical continuum result, while for relaxation coefficient above 1.36, the classical continuum bending stiffness is larger than the semi-continuum one. It provides a possible explanation for a current argument that the bending stiffness of nano scale structures should be enhanced or weakened in comparison with that predicted by classical continuum model [6–8,10,11,21]. Meanwhile, for increasing atomic layers, the thickness of the beam size is no longer within nanometer scale and hence the bending stiffness with all relaxation coefficients shows good agreement.

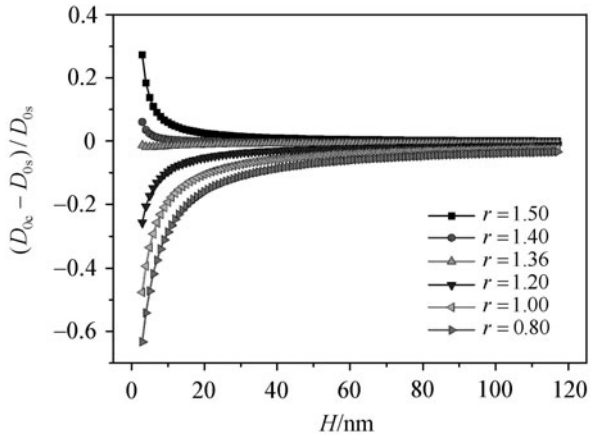

Fig. 5 Effects of the thickness and relaxation coefficients on the difference of bending stiffness with $a = 0.543\,1$ nm, $k = 261.432$ N/m and $E = 162$ GPa

3.2 Cantilever beam

For an ultra-thin cantilever beam with a downward concentrated load P at the free end ($x = L$), the deflection function is assumed as

$$w_s(x) = w_{0s} \sin\frac{\pi x}{2L}, \quad (0 \le x \le L). \tag{11}$$

Substituting Eq. (11) into Eq. (3), and using Eqs. (1), (2) and (5), one obtains

$$E_{\text{int}} = \frac{kB\pi^4 a^2 N(N+1)(N+2)w_{0s}^2}{384(N-2+2r)L^3}\left[\frac{N-1}{6} + \frac{1}{r(r^2+2)}\right]. \tag{12}$$

The deflection function and the dimensionless maximum deflection from Eqs. (7) and (12) are, respectively, given by

$$w_s(x) = \frac{192(N-2+2r)PL^3}{kB\pi^4 a^2 N(N+1)(N+2)}$$

$$\times\left[\frac{N-1}{6}+\frac{1}{r(r^2+2)}\right]^{-1}\sin\frac{\pi x}{2L}, \tag{13}$$

$$\bar{w}_{0s}=\frac{192(N-2+2r)\bar{P}}{\pi^4\tau^2N(N+1)(N+2)}\left[\frac{N-1}{6}+\frac{1}{r(r^2+2)}\right]^{-1}. \tag{14}$$

Equations (13) and (14) imply similar size-dependence and deformation capability with respect to those of the fully clamped beams.

The deflection function and maximum deflection based on the classical continuum model, and the maximum deflection based on an exact nonlocal stress model [7] are, respectively, given by

$$w_c(x)=\frac{Px^2}{6EI}(3L-x), \tag{15a}$$

$$w_{0c}=\frac{PL^3}{3EI}, \tag{15b}$$

$$w_{0n}=\frac{PL^3}{12EI}\left[4+12\tau^2+\frac{3\tau(4-\tau^2)(1-e^{2/\tau})-30\tau^2e^{1/\tau}}{1+e^{2/\tau}}\right], \tag{16}$$

where τ, in nonlocal theory, is a dimensionless parameter associated with the ratio of the internal to the external characteristic scales of the material (e.g. the ratio of crystal lattice parameter to the length of the beam a/L).

The difference between the semi-continuum and classical continuum models from Eqs. (13) and (15a), using the normalized form, is shown in Fig. 6. The parameters for silicon beams are $a = 0.543\,1$ nm, $k = 261.432$ N/m, and the Young's modulus $E = 162$ GPa is adopted for the classical deflection in Eq. (15a). It reveals that the difference is strongly dependent on the position, the thickness and the relaxation coefficient.

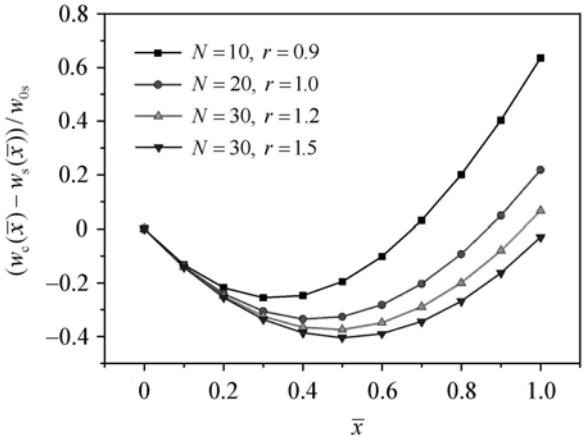

Fig. 6 The normalized difference between semi-continuum and classical continuum deflections, where $\bar{x} = x/L$, $a = 0.543\,1$ nm, $k = 261.432$ N/m and $E = 162$ GPa

Table 2 illustrates a comparison among the semi-continuum, classical continuum and exact nonlocal stress models for a fully clamped silicon beam. It is found that the difference between the classical continuum model and semi-continuum model or exact nonlocal stress model is obvious when there are fewer atomic layers. With increasing atomic layers, the thickness goes beyond micro/nano scale and there is no obvious difference. The classical continuum model overestimates deflection as compared with the semi-continuum model under certain conditions, i.e. $r = 0.8$ in this case. Similar conclusions were reported via other approaches, such as the exact nonlocal stress model [7], or a modified couple stress theory [21].

Table 2 Comparison of the semi-continuum, classical continuum and exact nonlocal stress solutions for a cantilever silicon beam with $a = 0.543\,1$ nm, $k = 261.432$ N/m, $L = 1\mu$m, $B = 200$ nm, $P = 10^{-5}\,\mu$N, $E = 162$ GPa, $r = 0.8$ and $\tau = 0.1$

N	10	20	30	40	90
w_{0s}/nm	4.71	0.74	0.24	0.11	0.01
w_{0c}/nm	8.71	1.02	0.30	0.12	0.01
w_{0n}/nm	5.39	0.75	0.22	0.10	0.01

4 Conclusions

The static bending behaviors of ultra-thin beams are studied via a new linear semi-continuum model. The bending stiffness may be enhanced or reduced due to a different relaxation coefficient. If the relaxation coefficient is greater or less than one, the deflection based on the semi-continuum model could be larger or smaller than that based on the classical continuum model. Good agreement for deflection is demonstrated for the semi-continuum, classical continuum and exact nonlocal stress models when the beam is in macroscopic size. Two opposite trends of size-dependence are observed in the semi-continuum model and they are caused by relaxation coefficients. The results reported in this paper could be useful for designing MEMS/NEMS using fully clamped or cantilever beam-like structures.

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