Size effect of the elastic modulus of rectangular nanobeams: Surface elasticity effect*

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The size-dependent elastic property of rectangular nanobeams (nanowires or nanoplates) induced by the surface elasticity effect is investigated by using a developed modified core-shell model. The effect of surface elasticity on the elastic modulus of nanobeams can be characterized by two surface related parameters, i.e., inhomogeneous degree constant and surface layer thickness. The analytical results show that the elastic modulus of the rectangular nanobeam exhibits a distinct size effect when its characteristic size reduces below 100 nm. It is also found that the theoretical results calculated by a modified core-shell model have more obvious advantages than those by other models (core-shell model and core-surface model) by comparing them with relevant experimental measurements and computational results, especially when the dimensions of nanostructures reduce to a few tens of nanometers.

Keywords: size effects, elastic modulus, nanobeams, surface elasticity

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1. Introduction

Over the past decade, nanostructures such as nanowires,[1,2] nanofilms or nanoplates,[3] and nanotubes[4] have attracted much attention due to their novel and remarkable physical properties. They are widely used as the basic elements of nanoelectromechanical systems (NEMS). For long usage and reliability of nanodevices in the NEMS, it is necessary to understand the mechanical properties of nanostructures, especially the elastic properties.[5–20] Due to the large surface-to-volume ratios, the mechanical properties of nanostructures are different from those of their bulk forms.[5–19] Thus, the size effects of mechanical properties at nanoscale are very important, and more investigations are desirable.

Because the performances of many NEMS devices are highly dependent on the "effective" elastic modulus of nanostructures, a great amount of research has focused on studying the elastic characteristics of nanomaterials including experimental measurements,[5–7,14,19] theoretical analysis,[8,9,14,17] and atomistic and molecular simulation.[10–13,16,18] The common behavior was found that the elastic modulus is strongly dependent on size with the lateral dimension of nanostructure decreasing. Generally, the size effect of elasticity arises from the surface stress,[13,14] and surface elasticity.[5,17–19,21,22]

Theoretically, the Gurtin *et al.*'s theory on surface elasticity[21] is widely used and improved to account for surface effects of nanosized structures. In this theory, the surface of nanostructure is assumed to have a layer with zero thickness ideally adhering to the bulk material. This theoretical model is also called the core-surface model by some researchers. Subsequently, many researchers continued to extend this theoretical model to account for surface effects in various physical problems.[18,22,23] However, the zero thickness assumption might lead to an unrealistic physical picture in some cases and works only when the lateral size of nanostructure is relatively large. As is well known, the surface effect extending deep into the bulk of nanomaterial is a process that gradually fades. Therefore, nanostructures are modeled as a core-shell composite structure maybe more reasonably.[5,17] However, the traditional core-shell model considers the elasticity values in the bulk core and surface shell to be identical, which leads to a sudden jump of elastic modulus at the interface of core and shell of nanostructures. Therefore, in our previous work, we have improved the classical core-shell model proposing a modified core-shell model to illustrate the surface elasticity effect, which introduces a concept of inhomogeneity of surface elasticity under continuum theory framework. The size effect of effective elastic modulus for the circular nanowires was well investigated by this modified core-shell model.[24] The analytical results indicated that the modified core-shell model is able to predict the elastic behavior of the

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nanowires at the smaller size, especially below 20 nm.

In most previous research work, where nanowires or nanobeams with circular shape were often chosen to be representative study targets, there were many specific comparisons between the theoretical results and experimental measurements for the size dependency of the elasticity.[5,7,13,17,19] For the nanoelement with rectangular shape, the size dependency of elastic modulus was studied by Gurtin's theory of surface elasticity (i.e., core-surface model),[6,14,15,19] atomistic and molecular simulation,[10–12,16,18] and energy method.[8,9] However, the detailed analysis on the size effect of elastic modulus for the nanosized elements with rectangular cross section has not been discussed theoretically with consideration of the effects of surface thickness and surface elasticity. In the present work, we utilize the modified core-shell model to investigate the elastic property of rectangular nanobeams or nanoplates specifically with consideration of the effects of the thickness of the surface layer and the inhomogeneity of surface elasticity under bending condition.

2. Model and theoretical calculation

Consider a rectangular nanobeam with width w and height h composed of inner core (bulk) and external shell (surface) with equivalent surface thickness t as shown in Fig. 1.

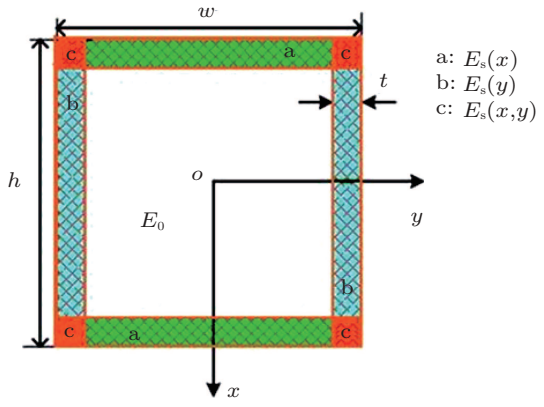


Fig. 1. (color online) Schematic sketch of rectangular cross section, in which the shadow represents the surface region. The regions represented by the letters 'a', 'b', and 'c' are surface regions with different elasticity values.

For simplicity, it is assumed that the elasticity of the bulk counterpart is harmonious and isotropic, and the elasticity of the surface is also isotropic, but its magnitude varies exponentially based on bulk elasticity of nanobeams. Due to the cross sections of the rectangular nanostructure in two dimensions being different, the forms of surface elasticity are different too. Moreover, the elasticity values at the four cross-sectional edges of the rectangular nanobeam are each overlapped by the horizontal and vertical surface elasticity. Thus, the specific expression forms of surface elasticity for the different surface regions are written as follows:

$$E_s(x,y)=\begin{cases} E_0\exp\left\{\alpha\left[|x|-\left(\frac{h}{2}-t\right)\right]\right\}, \\ \quad \frac{h}{2}-t\le|x|<\frac{h}{2},|y|\le\frac{w}{2}; \\ E_0\exp\left\{\alpha\left[|y|-\left(\frac{w}{2}-t\right)\right]\right\}, \\ \quad \frac{w}{2}-t\le|y|<\frac{w}{2},|x|\le\frac{h}{2}-t; \\ E_0\exp\left\{\alpha\left[|x|-\left(\frac{h}{2}-t\right)+|y|-\left(\frac{w}{2}-t\right)\right]\right\}, \\ \quad \frac{h}{2}-t<|x|\le\frac{h}{2},\frac{w}{2}-t<|y|\le\frac{w}{2}, \end{cases} \tag{1}$$

where E_0 is the bulk elastic modulus, and the parameter α is a surface factor related surface thickness t, which can be defined as $\alpha=\alpha_0/t$, with α_0 being a dimensionless constant, which describes the degree of the inhomogeneity of elasticity due to the transition from the bulk region to the external surface layer, and its sign (positive or negative) describes the properties of surface layer stiffening or softening. Moreover, the surface layer thickness t represents a transition region of this inhomogeneous degree. To calculate the total contributions of the different elasticity values at each point, the surface shell can be considered to be a superposition of many infinitesimal shells s_1, s_2, …, s_n, and also the continuum model is assumed. Consider that the nanobeam is bent to x-axis direction, according to the composite beam theory and the definition of the inertia moment of area, the bending stiffness is derived as

$$\begin{aligned} E_eI_e &= E_0I_0+\sum_{i=1}^{n}E_{si}I_{si} \\ &= E_0\cdot\frac{1}{12}(h-2t)^3(w-2t) \\ &\quad +\iint E_s(x,y)x^2\,\mathrm{d}x\mathrm{d}y, \end{aligned} \tag{2}$$

where E_e denotes the effective Young's modulus of the overall nanobeam and I is the inertia moment of cross section. Moreover, the subscripts 'e', '0', and 's' respectively represent the following meanings of 'effective', 'bulk', and 'surface'. Substituting Eq. (1) into Eq. (2), integrating and incorporating the definition of $\alpha=\alpha_0/t$, we have

$$\begin{aligned} E_e &= E_0\left[1-\frac{2t}{w}\left(1+\frac{1}{\alpha_0}-\frac{e^{\alpha_0}}{\alpha_0}\right)\right]\left\{\left(1-\frac{2t}{h}\right)^3\right. \\ &\quad +\frac{24t}{\alpha_0h}\left[\left(\frac{1}{4}-\frac{t}{\alpha_0h}+\frac{2t^2}{\alpha_0^2h^2}\right)(e^{\alpha_0}-1)\right. \\ &\quad \left.\left.+\frac{t}{h}\left(1-\frac{t}{h}-\frac{2t}{\alpha_0h}\right)\right]\right\}. \end{aligned} \tag{3}$$

Equation (3) provides a universal relation between the effective and the bulk modulus for nanobeams with rectangular

cross section. If $w \gg h > t$, namely, for the nanoplate, the effective modulus form is simplified into

$$E_{\mathrm{e}} = E_0 \left\{ \left(1 - \frac{2t}{h}\right)^3 + \frac{24t}{\alpha_0 h} \left[\left(\frac{1}{4} - \frac{t}{\alpha_0 h} + \frac{2t^2}{\alpha_0^2 h^2} \right) \times (\mathrm{e}^{\alpha_0} - 1) + \frac{t}{h} \left(1 - \frac{t}{h} - \frac{2t}{\alpha_0 h} \right) \right] \right\}. \quad (4)$$

Evidently, from Eqs. (3) and (4) we can see that the effective elasticity of rectangular nanobeams exhibits strong size dependence with the dimensions of cross section decreasing. Moreover, it is found that two crucial surface factors, i.e., inhomogeneous degree constant α_0 and surface layer thickness (transition region) t, play important roles in the effective Young's modulus of nanobeams.

3. Results and discussion

First of all, we investigate the size dependency of the effective Young's modulus with the variation of dimensions of cross section for a rectangular nanowire. The theoretical solutions for the overall effective Young's modulus E_{e} of nanowires, normalized by the Young's modulus E_0 of the bulk materials, are plotted in Figs. 2(a) and 2(b). As a theoretical example for discussion, we adopt the representative surface parameters: the transition region of surface inhomogeneity (namely surface thickness) $t = 2.0$ nm, the inhomogeneous degree constant $\alpha_0 = 2.0$ for the surface stiffening materials and $\alpha_0 = -2.0$ for the surface softening materials. Obviously, with the decreases of the width w and the height h, the magnitude of the normalized modulus E_{e}/E_0 varies more and more intensively. Especially, when the characteristic size of the rectangular nanowire reduces below 100 nm, a distinct size dependency of the elastic modulus is shown. At several tens of nanometers or several nanometers, this phenomenon displays more prominently due to the effect of surface elasticity from the surface layer.

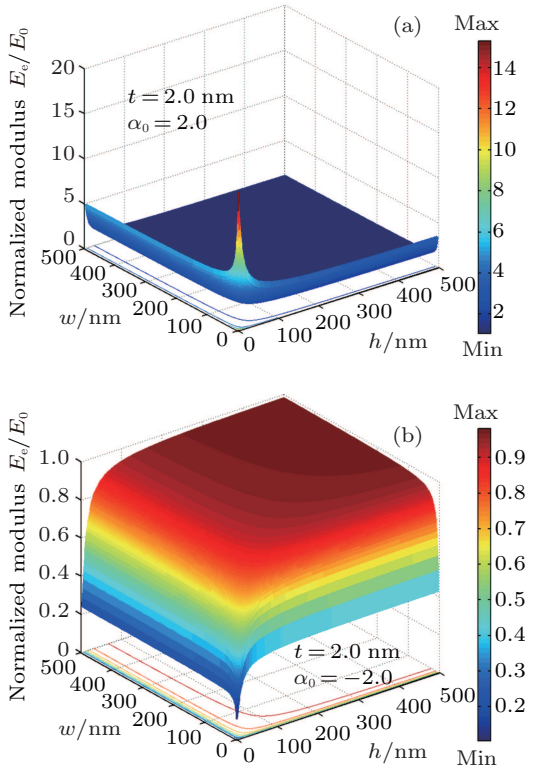


Fig. 2. (color online) Normalized elastic modulus versus width w and height h of cross section for the rectangular nanowire (a) for the case of surface stiffening, where the inhomogeneous degree $\alpha_0 = 2.0$, and (b) for the case of surface softening, where the inhomogeneous degree $\alpha_0 = -2.0$.

We further examine the validity of the present model by comparing with the classical core-shell model, taking zinc oxide (ZnO) nanowires for example. At first, the hexangular cross section of ZnO nanowires is assumed to be square, i.e., $w = h$, while the nanowire in core-shell structure in Ref. [5] is assumed to be circular. Using Eq. (3), the values of normalized Young's modulus (E_{e}/E_0) as a function of nanowire cross section (the height h or the diameter D) are plotted in Fig. 3. Since the smallest diameter of ZnO nanowires tested experimentally[5] is limited to about 17 nm, below this size, a new numerical approach-molecular statistical thermodynamics (MST) method is proposed to fill this gap and provide a very good connection to the experimental results.[25] It is noted that for large diameters (about > 500 nm), the theoretical values of elastic modulus for both core-shell model and modified core-shell model are almost close to the value of the bulk material. While the dimension decreases down to about 100 nm, the effective elastic modulus continuously increases, especially, when the dimension reduces below 50 nm, the value of elastic modulus increases remarkably due to the surface elasticity effect. However, the differences between core-shell model and modified core-shell model are observed clearly from the inset of Fig. 3. At smaller size (about 10 nm), the theoretical lines of the normalized Young's modulus obtained by the above mentioned two models exhibit different trends. It is found that the theoretical result given by core-shell model[5] does not accord with the MST results below 10 nm due to the limitation of the model, while our solutions, whether the cross section of nanowire is assumed to be rectangular or circular, both fit the experimental results as well as they accord with the trend of MST results to some extent. Here, we adopt the fitted surface parameters equally for two kinds of cross sections of the nanowire (rectangular and circular) as follows: surface thickness $t = 2.0$ nm, and inhomogeneous degree $\alpha_0 = 1.0$ for the rectangular cross section; surface thickness $r_{\mathrm{s}} = 2.0$ nm, and inhomogeneous degree $\alpha_0 = 1.0$ for the circular cross section. In addition, we also find that the distinct difference in the normalized Young's modulus, E_{e}/E_0, starts at about 20 nm between rectangular cross section and circular

cross section for the nanowire. It is seen that the theoretical line for the nanowire assumed to be circular shape is closer to the MST data than that assumed to be rectangular. This means that the hexangular cross section of the ZnO nanowire assumed to be circular shape is more reasonable than rectangular shape. Therefore, the effect of the nanowire geometry is also important at an extremely small size. That is mainly because the influences from the bulk part of materials become weaker and weaker with dimension of the nanowire decreasing, until finally what is left is the influence coming only from the surface layer. At this time, the effect of geometry of the nanowire starts to work, and determines the degree of surface effect at the extremely small size.

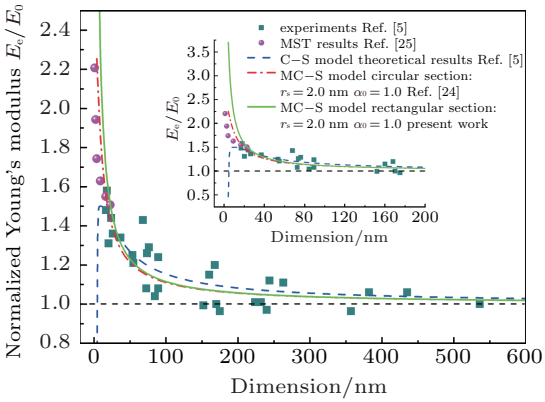


Fig. 3. (color online) Plots of normalized modulus E_e/E_0 as a function of dimension of ZnO nanobeams (h or D). The inset gives the enlarged graph of normalized modulus E_e/E_0 versus the dimension of the nanowire at a smaller size. The abbreviated word 'C-S' means core-shell, and 'MC-S' refers to modified core-shell.

Additionally, another material with surface softening, silicon nitride (SiN_x) nanoplates,[15] is considered. Figures 4(a) and 4(b) display a comparison of the normalized modulus (E_e/E_0) between theoretical solutions and experimental results. Two experimental flexural modes are investigated in Figs. 4(a) and 4(b). It is seen that the theoretical solutions of E_e/E_0 either by core-surface model (i.e., Gurtin's surface elastic model) or modified core-shell model, each exhibit a distinct dependence on the characteristic size of the nanoplates. The reasons for size effects for both models arise from the influence of surface elasticity. As can also be seen from Figs. 4(a) and 4(b), the theoretical results given by Eq. (4) each have a greater advantage than those from Ref. [15] at a small size. The fitted values of surface elasticity in core-surface model[15] are -1170 N/m for the first flexure mode and -950 N/m for the second flexure mode. Meanwhile, in our modified core-shell model, we obtain a group of nice surface parameters from the fits: $t = 6.0$ nm and $\alpha_0 = -3.6$ for the first flexure mode; $t = 6.0$ nm and $\alpha_0 = -2.3$ for the second flexure mode. For the two flexure modes, it is noted that the values of inhomogeneous degree constant are different when the surface thickness values are the same, which probably suggests that the depth of relaxation under the surface might be the same but the degree of surface relaxation differs in physics. Moreover, it is worth noting from the insets of Figs. 4(a) and 4(b) that the value of effective Young's modulus by the core-surface model approaches to zero or even negative ($E_e \leq 0$) when the thickness of silicon nitride cantilevers is below about 20 nm. This phenomenon disobeys the physical reality which means that the results are unreasonable, in other words, it yields an invalid modulus in physics. However, our theoretical results obtained by the modified core-shell model not only show a good agreement with the experimental results within error range but also can predict a valid Young's modulus at a small size.

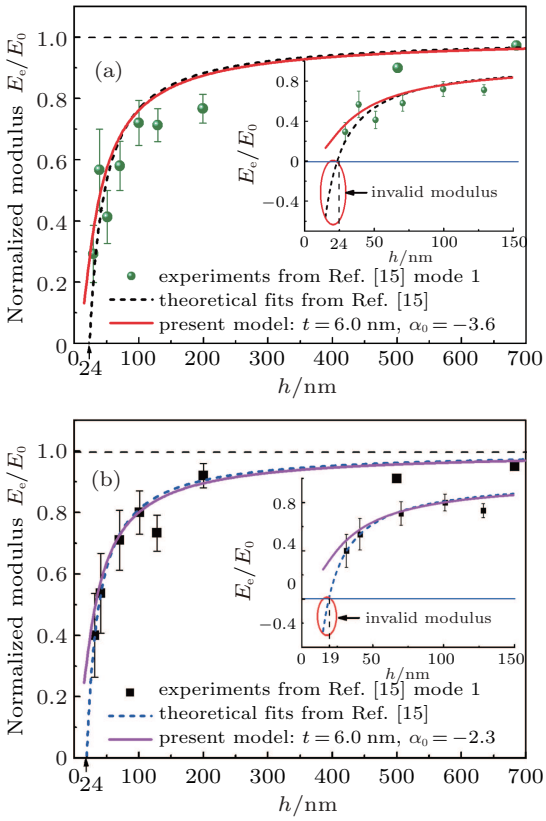


Fig. 4. (color online) Comparisons of the theoretical solutions by the present model with the existing theoretical results (core-surface model) and relevant experimental results for silicon nitride nanoplates. Panel (a) is for the first flexure mode and panel (b) is for the second flexure mode. The insets show the enlarged curve sections of the E_e/E_0 for both experimental flexure modes.

4. Summary

In summary, we have determined the effective normalized Young's modulus for the bending of rectangular nanowires or nanoplates incorporating the effect of surface elasticity by a proposed modified core-shell model. It is shown that a strong size-dependent effect of elastic modulus for rectangular nanobeams is demonstrated with the decrease of the characteristic size (the width w and the height h) of the nanobeams, especially, below 100 nm, the size effect of elastic modulus

is indicated more prominently due to the surface elasticity of the surface region. Moreover, from the comparisons of the existing theoretical models (core-shell model and core-surface model) with relevant experimental and computational results (MST), it is demonstrated that our surface elasticity model (modified core-shell model) can better predict the size effect of elasticity and is more reasonable especially when the dimensions of nanostructures reduce to a few tens of nanometers. Therefore, this study might be helpful for interpreting various phenomena associated with the size effect of elastic properties of rectangular nanobeams. However, our model also has its limitation when the surface layers are mutually overlapped; the mechanical properties of nanostructures at such a small size are still an open issue, which deserves further study and explanation.

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