

The size-dependent bending elastic properties of nanobeams with surface effects

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Abstract

A theoretical model is presented to investigate the size-dependent bending elastic properties of a nanobeam with the influence of the surface relaxation and the surface tension taken into consideration. The surface layer and its thickness of a nanostructure are defined unambiguously. A three-dimensional (3D) crystal model for a nanofilm with n layers of relaxed atoms is investigated. The four nonzero elastic constants of the nanofilm are derived, and then the Young's modulus for simple tension is obtained. Using the relation of energy equilibrium, the size-dependent effective elastic modulus and effective flexural rigidity of a nanobeam with two kinds of cross sections are derived, and their dependence on the surface relaxation and the surface tension is analysed.

1. Introduction

The Young's modulus E and the flexural rigidity EI are fundamental mechanical properties of structures, which are defined in the theory of continuum mechanics. Generally speaking, the Young's modulus of macroscopic materials related both with tension and bending is independent of the size of the structures. When the size of a structure comes down to nanoscale, however, it had been shown in many experiments [1–7], atomic simulation [8–13] and theoretical research [14–17] that the Young's modulus is size-dependent. The size dependence of the elastic moduli have been studied extensively, but with somewhat debatable results. At present, there were two opposite experimental results [1–7] about the size-dependent elastic modulus of nanostructures even for the same material [3, 5]. Some experiments [1–4] showed that elastic modulus increased with the decrease of characteristic dimension of the nanostructure, while others [5–7] showed that the reverse was true. Theoretical investigations also reached the two opposite conclusions. Until now, there was not yet a widely accepted theoretical model, which could explain the phenomena appropriately.

The size dependence of the elastic moduli is generally attributed to surface effects, which are so insignificant for macroscopic materials that they can be neglected. But for nanostructures, because of the very large surface-to-volume ratio, the surface effects can play important roles and can no longer be neglected. Thus the surface effects, including surface energy, surface tension, surface relaxation, surface reconstruction, etc, should be taken into consideration when the overall elastic properties of nanostructures are investigated. Villain *et al* [8] revealed a strong decrease of the Young's modulus by the atomistic simulation with the surface tension taken into consideration. Employing a molecular statics approach based on the embedded-atom-method interatomic potential, Wolf [9] and Liang [10] showed that elastic modulus could either increase or decrease at the nanoscale. The similar results were also obtained by Zhou and Huang [11] using a combination of molecular statics and *ab initio* calculations. Miller and Shenoy [12, 13] constructed a model taking account of surface tension to predict the size-dependent elastic properties of nanoscale plates and beams, and reached a conclusion that the effective stiffness is closely related to the values of surface elastic constants. Cammarata and Sieradzki [14] analysed the effects of surface energy on the elastic properties of nanomaterials and predicted the enhancement of elastic modulus of nanofilms.

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Table 1. The values of parameters in the calculation.

Symbol	Value	Symbol	Value
a [17]	1.74×10^{-10} m	L	100 nm
α_1 [17]	2.02 N m $^{-1}$	b	50 nm
α_2 [17]	1.10 N m $^{-1}$	ν	0.28
γ [18]	0.562 N m $^{-1}$	n	4

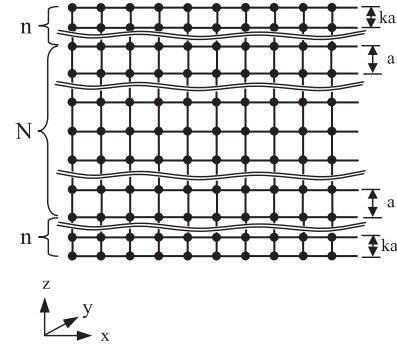
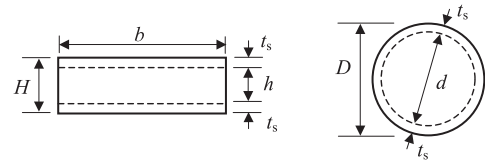
Dingreville *et al* [15] developed a framework to incorporate the surface energy into the continuum theory of mechanics and demonstrated that the overall elastic modulus of nanostructures could either increase or decrease. The present authors [17] also presented a 3D model with a layer of relaxed atoms taken into consideration to investigate the size-dependent elastic constants of nanofilm, and showed in theory that the elastic moduli of the nanofilm could enhance and reduce with the reduced thickness of the nanofilm, which was dependent on the surface relaxation coefficients.

In many experimental approaches applied to determine the Young's modulus of nanostructures, a popular and effective one is by the measurements of deflections [1–3, 6] or the resonant frequencies [4, 5] of a nanobeam to acquire the Young's modulus. With that method, a bending theory for nanobeams is necessary. But in the present bending theory, there is not a model that takes the several surface effects into consideration simultaneously. Based on our previous work [17], the bending elastic properties of a nanobeam with the influence of the surface relaxation and the surface tension are studied in the present research. Compared with our previous work [17], there were mainly two improvements in the present work. In the first place, there was only a relaxed atomic layer taken into consideration in [17], while there are more relaxed atomic layers in the present study. Secondly, we consider the influence of both the surface relaxation and the surface tension on the elastic properties of the nanobeams in the present study, while only the influence of the surface relaxation was considered in our previous work [17].

2. The elastic moduli of the nanofilm with surface relaxation

In the section, we investigate the dependence of elastic moduli on the surface relaxation when more relaxed atomic layers are taken into consideration. In the first place, the concept of surface layer will be defined. It is a transition region between the uniform bulk material and the vacuum outside, where the rearrangement (e.g. surface relaxation, surface reconstruction) of atoms occurs. In the surface layer, the properties of the material are significantly different from those in the bulk material due to surface effects. Since the emphasis of this section is to discuss the influence of surface relaxation on the elastic properties, we may assume that there exists only surface relaxation in the surface layer. The influence of the surface tension will be studied in the next section.

The side-view schematic of a 3D nanofilm crystal model is shown in figure 1. There are n layers of relaxed atoms in the surface layer. A surface relaxation coefficient k_i is introduced [16]. It is known that the termination of the lattice periodicity in the normal direction of a surface will lead to imperfection of the coordination numbers (CNs) of a surface

**Figure 1.** The side-view schematic of the nanofilm crystal model.**Figure 2.** Two kinds of cross sections of the nanobeam.

atom, which will, in turn, relax the remaining bonds of lower-coordinated surface atoms. The CN-imperfection-induced bond relaxation can be defined as $a_i = k_i a$, ($i = 1, 2, \dots, n$), where a denotes the bulk value of bond length, subscript i is the i th atomic layer and k_i is the relaxation coefficient. The relaxation may be contractive ($k_i < 1$) or expansive ($k_i > 1$) [16]. In addition, the degree of the relaxation decays along the inner-normal direction of the free surface and there will be no CN reduction for $i > n$. Strictly speaking, the relaxation coefficient k_i for each atomic layer is different, but for the sake of simplification, an average value can be used: $k = \frac{1}{n} \sum_{i=1}^n k_i$. So the thickness of surface layer can be defined as $t_s = nka$. It is assumed that there are N layers of unrelaxed atoms in the bulk of nanobeam. So the thickness of the nanobeam (as shown in figure 2) is

$$H = t_0 + 2t_s = (N + 2nk)a. \quad (1)$$

Similar to the discussion in [17] for a relaxed atomic layer, we can derive the strain energy density of nanobeam with n layers of relaxed atoms in the surface layer as follows:

$$f = \frac{1}{2(N + 2nk)a} \left\{ (N - 1)\alpha_1(\varepsilon_x^2 + \varepsilon_y^2 + \varepsilon_z^2) + (2n + 1) \times \alpha_1(\varepsilon_x^2 + \varepsilon_y^2) + 2nk^2\alpha_3\varepsilon_z^2 + (N - 1)\alpha_2[(\varepsilon_y + \varepsilon_z)^2 + (\varepsilon_x + \varepsilon_z)^2] + \frac{4n\alpha_4}{1 + k^2}[(\varepsilon_x + k^2\varepsilon_z)^2 + (\varepsilon_y + k^2\varepsilon_z)^2] + (N + 2n)\alpha_2(\varepsilon_x + \varepsilon_y)^2 + 4(N + 2n)\alpha_2\varepsilon_{xy}^2 + \left[4(N - 1)\alpha_2 + \frac{16k^2\alpha_4}{1 + k^2} \right] (\varepsilon_{xz}^2 + \varepsilon_{yz}^2) \right\} \quad (2)$$

where α_1 and α_2 denote the spring constants of the nearest neighbours and the next-nearest neighbours between the unrelaxed atoms, respectively; α_3 and α_4 are those of the nearest neighbours and the next-nearest neighbours between the relaxed atoms, respectively. We have $\alpha_3 = \alpha_1/k$ and $\alpha_4 = \alpha_2/k$.

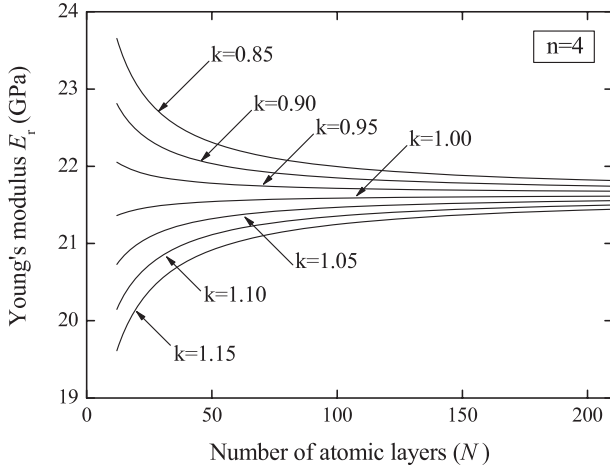


Figure 3. The variations of Young's modulus in the simple tension state with the decrease of atomic layer number for various relaxation coefficients.

Substitute equation (2) into the expression $C_{ij} = \partial^2 f / \partial \varepsilon_{ij}^2$, which relates strain energy density, stress and strain, and then four independent nonzero elastic constants can be obtained as:

$$C_{11} = \frac{(N + 2n)\alpha_1 + (2N + 2n - 1)\alpha_2 + \frac{4n\alpha_4}{1+k^2}}{(N + 2nk)a}, \quad (3)$$

$$C_{12} = \frac{(N + 2n)\alpha_2}{(N + 2nk)a}, \quad (4)$$

$$C_{13} = \frac{(N - 1)\alpha_2 + \frac{4nk^2\alpha_4}{1+k^2}}{(N + 2nk)a}, \quad (5)$$

$$C_{33} = \frac{(N - 1)(\alpha_1 + 2\alpha_2) + 2nk^2\alpha_3 + \frac{8nk^4\alpha_4}{1+k^2}}{(N + 2nk)a}. \quad (6)$$

Similar to the process in [17], a simple tension analysis can be performed. Then the Young's modulus of the nanobeam in the simple tension state can be derived with the surface relaxation taken into consideration:

$$E_r = \frac{(C_{11} - C_{12})(C_{11}C_{33} + C_{12}C_{33} - 2C_{13}^2)}{C_{11}C_{33} - C_{13}^2}. \quad (7)$$

The variations of the Young's modulus in the simple tension state with the decrease of atomic layer numbers are shown in figure 3. It can be seen that the size effect of the Young's modulus depends on the relaxation coefficient. When the atomic layer numbers are less than about 100, the Young's modulus varies with the decrease of the atomic layer numbers. It varies sharply as the atomic layer numbers are less than 50. More specifically, the Young's modulus increases with the decrease of the atomic layer number if relaxation coefficient $k < 1$; on the other hand, the Young's modulus decreases if relaxation coefficient $k > 1$.

3. The bending elastic properties of the nanobeam with the effects of surface relaxation and surface tension

In the section above, the elastic moduli of the nanofilm were obtained when the surface relaxation effects were taken into

consideration. As a matter of fact, in addition to the surface relaxation, the surface energy and surface tension also play important roles in the size-dependent mechanical properties of nanostructures. Surface energy and surface tension of the solids are two different concepts, which are often not well understood [18–20]. The surface energy is the reversible work per unit area needed to create a new surface. On the other hand, the surface tension is the reversible work per unit area needed to elastically stretch/compress a preexisting surface [18, 20]. The surface energy is usually positive, while the surface tension can be positive or negative [18]. For a beam, the surface tension dominates the surface deformation when the beam is bent. As a result, the work needed to vary the area of surface dS should be γdS , where γ is the surface tension. In this section, the bending elastic properties of a nanobeam will be investigated when the influence of both surface relaxation and the surface tension are taken into consideration.

The assumption of small deflection is applied, as the magnitude of the deflection of the nanofilm is small compared to its characteristic geometric size. The total bending strain energy can be expressed as:

$$U_{\text{tot}} = \int_0^L \frac{E_{\text{eff}}I}{2} (w''(x))^2 dx, \quad (8)$$

where L is the length of the nanobeam, E_{eff} the effective elastic modulus of nanostructures with the effects of surface relaxation and surface tension, I the moment of inertia, and $w(x)$ the deflection of the beam, and $w'(x) = dw(x)/dx$.

The total energy of the system can be expressed as the sum of the bending deformation energy with the influence of the surface relaxation and the surface deformation energy (see the appendix) resulted from the beam extension with the influence of the surface tension:

$$U_{\text{tot}} = \int_0^L \frac{E_r I}{2} (w''(x))^2 dx + \gamma \Omega \Delta L (1 - \nu), \quad (9)$$

where E_r is the elastic modulus of the nanobeam in the simple tension state with the surface relaxation effects taken into consideration, which is derived by equation (7), Ω the contour length of its cross section, ΔL its length variation and ν the Poisson's ratio. For a slight bending, the extension of the bending beam is given by:

$$\Delta L = \frac{1}{2} \int_0^L (w'(x))^2 dx. \quad (10)$$

By the energy balance, we have:

$$\int_0^L \frac{E_{\text{eff}}I}{2} (w''(x))^2 dx = \int_0^L \frac{E_r I}{2} (w''(x))^2 dx + \frac{\gamma \Omega (1 - \nu)}{2} \int_0^L (w'(x))^2 dx, \quad (11)$$

and then the effective flexural rigidity Γ_{eff} and the effective elastic modulus E_{eff} of the bending beam can be obtained as:

$$\Gamma_{\text{eff}} = E_{\text{eff}}I = E_r I + \gamma \Omega (1 - \nu) \frac{\int_0^L (w'(x))^2 dx}{\int_0^L (w''(x))^2 dx}, \quad (12)$$

$$E_{\text{eff}} = E_r + \frac{\gamma \Omega (1 - \nu)}{I} \frac{\int_0^L (w'(x))^2 dx}{\int_0^L (w''(x))^2 dx}. \quad (13)$$

Equations (12) and (13) can be applied to the nanobeams with arbitrary sectional profiles as well as arbitrary loads and support forms.

There are usually two kinds of cross sections (shown in figure 2) for a nanobeam, which are extensively used in most research. For convenience, we call the beam with quadrate section as a nanofilm, and the one with circular section as a nanowire. The contour length of cross section Ω and the moment of inertia I of a nanofilm and a nanowire can be obtained as follows, respectively. For the nanofilm with thickness $H = (N + 2nk)a$ and width b , we have:

$$\Omega_f = 2[b + (N + 2nk)a], \quad (14)$$

$$I_f = \frac{(N + 2nk)^3 a^3 b}{12}, \quad (15)$$

and

$$\frac{\Omega_f}{I_f} = \frac{24}{(N + 2nk)^3 a^3} \left[1 + \left(\frac{(N + 2nk)a}{b} \right) \right], \quad (16)$$

where the subscript f denotes the nanofilm. For a nanowire with diameter $D = d + 2t_s = (N + 2nk)a$, we have

$$\Omega_w = \pi(N + 2nk)a, \quad (17)$$

$$I_w = \frac{\pi(N + 2nk)^4 a^4}{64}. \quad (18)$$

Thus,

$$\frac{\Omega_w}{I_w} = \frac{64}{(N + 2nk)^3 a^3}, \quad (19)$$

where the subscript w denotes the nanowire.

In the experiments [1–3], to measure the effective elastic modulus of a nanobeam, the atomic force microscope (AFM) is used with a force acting on the span of the beam. The force is usually considered as a concentrated force applied to the mid-point of the beam [1–3]. However, since the diameter of the AFM tip in the experiments is about 10 nm, it may bring forth some error when the force of the AFM is considered as a concentrated force [1–3], which will be shown in the next section. Furthermore the acting point is not always at the mid-point of the beam. So a more general case will be considered in this paper. The beam is both-end clamped, and a uniform distributed load q is applied to its span (as shown in figure 4). The deflection of the beam is:

$$w(x) = \frac{1}{2EI} \left(-Mx^2 - \frac{Q}{3}x^3 + H(x - \lambda_1) \frac{q}{12}(x - \lambda_1)^4 - H(x - \lambda_2) \frac{q}{12}(x - \lambda_2)^4 \right), \quad (20)$$

where

$$M = \frac{q}{12L^2} [(L - \lambda_2)^3 (L + 3\lambda_2) - (L - \lambda_1)^3 (L + 3\lambda_1)], \quad (21)$$

$$Q = \frac{q}{2L^3} [(L - \lambda_1)^3 (L + \lambda_1) - (L - \lambda_2)^3 (L + \lambda_2)], \quad (22)$$

and λ_1, λ_2 is the distance from two ends of the acting points of the uniform distributed load to the origin, respectively, as

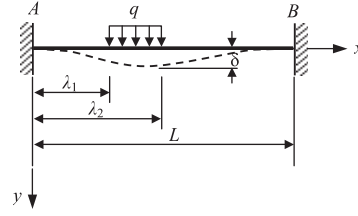


Figure 4. The schematic of the bending beam model.

shown in figure 4. $H(x - \lambda)$ is the Heaviside function, which is defined as:

$$H(x - \lambda) = \begin{cases} 0, & x < \lambda \\ 1, & x \geq \lambda. \end{cases} \quad (23)$$

Substituting equation (20) into equations (12) and (13), the effective flexural rigidity Γ_{eff} and the effective elastic modulus E_{eff} of the bending beam can be obtained, respectively. As a special example, the beam with a uniform distributed load applied to its middle span is discussed. The diameter of the AFM tip is specified as R , and it is assumed that $R = L/12$. Thus we have $\lambda_1 = (L - R)/2$ and $\lambda_2 = (L + R)/2$. Substituting λ_1, λ_2 and R into equations (20)–(23), we obtain:

$$\frac{\int_0^L (w'(x))^2 dx}{\int_0^L (w''(x))^2 dx} = \frac{L^2}{64}. \quad (24)$$

Substituting equations (14)–(19) and (24) into equations (12) and (13), the analytical expressions of the effective flexural rigidity Γ_{eff} and the effective elastic modulus E_{eff} of the nanofilm and the nanowire can be obtained, respectively, as

$$\Gamma_{\text{eff}}^f = \frac{(N + 2nk)^3 a^3 b}{12} E_r + \frac{[b + (N + 2nk)a](1 - \nu)L^2}{32} \gamma, \quad (25)$$

$$\Gamma_{\text{eff}}^w = \frac{\pi(N + 2nk)a}{64} [(N + 2nk)^3 a^3 E_r + (1 - \nu)L^2 \gamma], \quad (26)$$

$$E_{\text{eff}}^f = E_r + \frac{3\gamma L^2(1 - \nu)}{8(N + 2nk)^3 a^3} \left[1 + \left(\frac{(N + 2nk)a}{b} \right) \right], \quad (27)$$

$$E_{\text{eff}}^w = E_r + \frac{\gamma L^2(1 - \nu)}{(N + 2nk)^3 a^3}. \quad (28)$$

4. Discussion

It can be seen from equations (27) and (28) that the effective elastic modulus of a nanobeam is a function of the surface relaxation coefficient k and the surface tension γ . The values of the relaxation coefficient k and the surface tension γ determine the size effects of the effective elastic modulus. The values of parameters in the calculation are listed in table 1. Figures 5 and 6 show the variations of the effective elastic moduli of a nanofilm and a nanowire with atomic layer numbers. It can be seen from these figures that the effective elastic modulus varies when the atomic layer numbers are less than about 100, and it varies sharply as the atomic layer numbers are reduced further to less than 50. In addition, the sign of the surface tension dominates the direction of the variation, i.e. the elastic modulus is enhanced for a positive

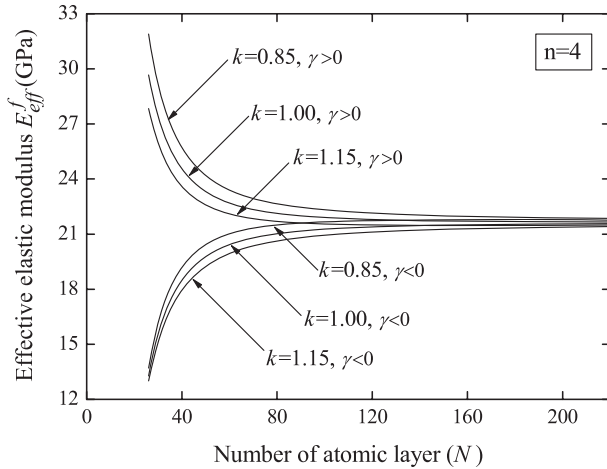


Figure 5. The size-dependent effective elastic modulus of the nanofilm.

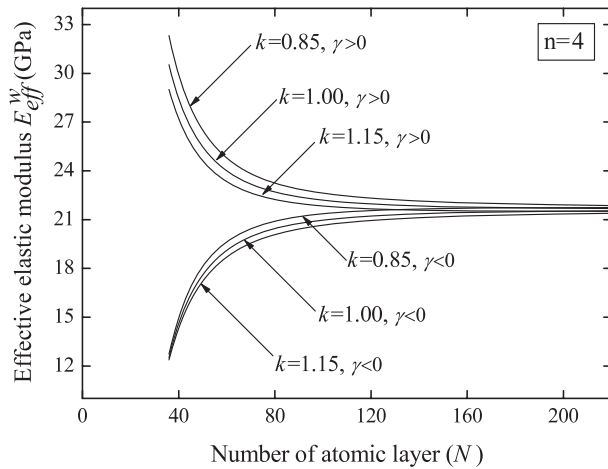


Figure 6. The size-dependent effective elastic modulus of the nanowire.

surface tension, which is qualitatively consistent with the experimental results of [1–4], and it is weakened for a negative surface tension, which is qualitatively consistent with the experimental results of [5–7]. On the other hand, the surface relaxation coefficient k also influences the effective bending elastic modulus. In fact, when the surface relaxation coefficient k is equal to unity, i.e. $k = 1$, equation (28) becomes:

$$E_{\text{eff}}^w = E + \frac{\gamma L^2(1-\nu)}{D^3}, \quad (29)$$

which is similar to the result, $E_{\text{eff}}^w = E + \frac{8}{5} \frac{\gamma L^2(1-\nu)}{D^3}$, in [3], where the load of AFM was approximately considered as a concentrated force. Let $\delta E_{\text{eff}}^w = E_{\text{eff}}^w - E$, we show the error caused by the approximation in figure 7. It can be seen that the difference is large when the characteristic size of the nanostructure is small enough, i.e. the atomic layer numbers are less than 50.

It can also be seen from figures 5 and 6 that the curves with the relaxation coefficient $k < 1$ and $k > 1$ are, respectively, above and below the curves with the relaxation coefficient $k = 1$. That is to say, the surface relaxation can make the

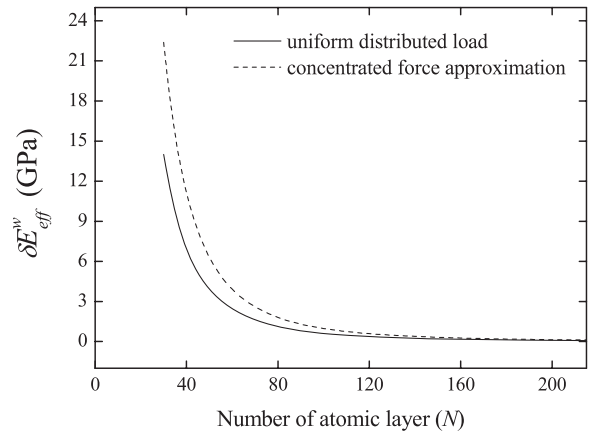


Figure 7. The difference between the uniform distributed load and the concentrated force approximation.

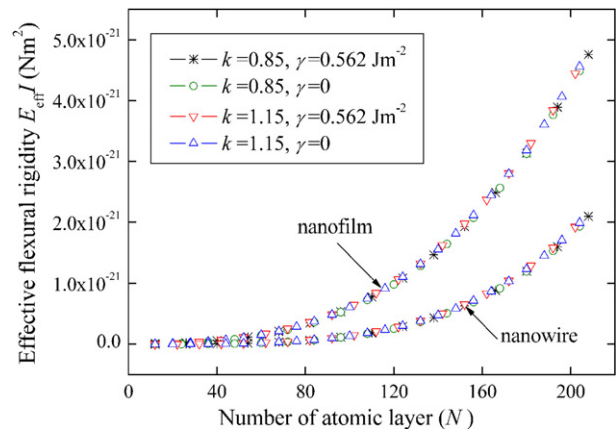


Figure 8. The effective flexural rigidity of the nanobeam for two kinds of cross section.

(This figure is in colour only in the electronic version)

surface stiffer when the surface relaxes into the plane ($k < 1$), and softer when the surface relaxes out of the plane ($k > 1$). So one can conclude that the size effects of the effective elastic modulus of nanobeam depend on the surface tension γ and the relaxation coefficient k . How and how much it depends on them is determined by the interaction between the surface relaxation and surface tension.

Figure 8 shows the variations of the effective flexural rigidity of the nanofilm and the nanowire with the atomic layer numbers. It can be seen that the curves coincide for the surface tension with opposite sign and relaxation coefficients with different value, which shows that the influence of the surface relaxation and surface tension on the effective flexural rigidity is negligible. It is because that, with the moment of inertia being multiplied, the effective flexural rigidity becomes not sensitive to the difference between the macroscopic bulk and the nanostructures due to the decrease of scale.

5. Conclusion

A more generalized 3D crystal model for the elastic properties of the nanofilm is established with the consideration of n layers

of relaxed atoms. Four nonzero elastic constants of the model are derived, and the Young's modulus of the nanofilm in the simple tension state is obtained. The size effects of the Young's modulus are dependent on the relaxation coefficient. It does not vary obviously with the atomic layer number until the atomic layer numbers are less than about 100. Moreover the elastic modulus varies sharply as the atomic layer numbers are less than 50. More specifically, the value of Young's modulus increases with the decrease of the atomic layer number if relaxation coefficient $k < 1$; it is the other way round if relaxation coefficient $k > 1$.

When the effects of both the surface relaxation and the surface tension are taken into consideration, the effective flexural rigidity and effective elastic modulus of a bending beam are derived by energy equilibrium. The size effects of the effective elastic modulus of a nanobeam are dependent on the relaxation coefficient k and the surface tension γ . How much it depends on them is determined by the interaction between the surface relaxation and surface tension. The influences of the surface relaxation and the surface tension on the effective flexural rigidity are so negligible that they can be neglected even at the nanoscale.

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Appendix

The surface area of a nanobeam with length L and contour Ω before the deformation is

$$S = L\Omega. \quad (\text{A.1})$$

The surface area of the nanobeam after the deformation is

$$S' = L \left(1 + \frac{\Delta L}{L} \right) \left(1 - \frac{\Delta L}{L} \nu \right) \Omega, \quad (\text{A.2})$$

where ΔL is the extension of the nanobeam. Due to the small deformation assumption, the deformed surface area can be

written approximately as:

$$S' \approx L\Omega \left[1 + \frac{\Delta L}{L}(1 - \nu) \right] = L\Omega + \Omega\Delta L(1 - \nu). \quad (\text{A.3})$$

Thus the variation of surface area of the nanobeam is

$$\Delta S = S' - S = \Omega\Delta L(1 - \nu), \quad (\text{A.4})$$

and then the surface deformation energy resulting from beam extension with the effects of surface tension (γ) can be obtained as

$$U_{st} = \gamma\Omega\Delta L(1 - \nu). \quad (\text{A.5})$$

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