Research Article

Displacement Approach to Determine the Effective Tensile and Torsional Modulus of Nanowires

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Surface elasticity and residual stress have a strong influence on the effective properties of nanowire (NW) due to its excessively large surface area-to-volume ratio. Here, the classical displacement method is used to solve the field equations of the core-surface layer model subjected to tension and torsion. The effective Young’s modulus is defined as the ratio of normal stress to axial strain, which decreases with the increase in NW radius and gradually reaches the bulk value. The positive or negative surface residual stresses will increase or decrease Young’s modulus and shear modulus due to the surface residual strains. Nonzero radial and circumferential strains enhance the influence of surface moduli on the effective modulus.

1. Introduction

Typical nanowires (NWs) are often referred to as 1D materials with nanometer-scale diameters or perimeters and excessively large surface area-to-volume ratio. NWs have considerable potential in various applications, such as molecular electronics, nanoelectromechanical systems, and novel building materials, for disaster prevention and mitigation [1–12]. The applications of NWs into future generation nanodevices require a complete understanding of the NW mechanical properties [2]. Many direct measurements have been performed to investigate the mechanical properties of NWs [3]. Unlike the mechanical testing of bulk materials, NW testing heavily depends on the experimental setup; in particular, manipulation procedure leads to substantial challenges due to the small NW dimensions [4]. In many experiments, such as in [1–6], the measured deflections are less than the diameter which can be classified small-deflection problem. In addition to experimental endeavors, theoretical prediction can also be used in NW mechanical analysis. Theoretical prediction is classified into two main categories as follows: first is the atomic modeling, which includes techniques such as tedious ab initio molecular dynamics calculations and density functional model [5], and second one is continuum mechanics modeling [6–10]. NWs are strongly influenced by their surface characteristics, thereby leading to distinct mechanical properties compared with their bulk counterpart. Consequently, in the continuum mechanics modeling of the mechanical properties of a solid NW, the role of surface stress must be considered. Zhang et al. analyzed the effect of surface residual stress and elasticity on the asymmetric yield strength of NWs on the basis of the potential energy method [6]. Chuang presented a simplistic theory to study the enhanced strength of a solid NW [7]. Gupta also presented a continuum formulation to investigate the finite deformation of nanorod/NWs [8]. The large-deflection deformation of NW implicates large rotational angle and infinitesimal strain. So, this situation will not be considered in our mode.

Although the classical continuum mechanics models can efficiently predict NW deformation, their applicability in identifying the surface effect on the effective modulus of NWs is tedious. Therefore, a relatively simple approach that can directly characterize the mechanical properties of a solid NW should be developed. In this work, the classical displacement method is used to study the tension and torsion of
NW and the influence of surface elasticity on the effective Young’s moduli and shear moduli.

2. Model Analysis

As schematically shown in Figure 1, we consider a stretched and twisted core-shell NW model viewed as a composite, comprising a cylindrical core (bulk) and surface layer. The equilibrium equations, strain-displacement relationships, and constitutive equations for the isotropic bulk materials are expressed as follows:

\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \]
\[ \sigma_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2G \varepsilon_{ij}, \]
\[ \sigma_{ij;j} = 0, \]

where \( \sigma_{ij} \), \( u_i \), and \( \varepsilon_{ij} \) denote the stresses, displacements, and strains in core, respectively, and \( \lambda \) and \( G \) are the Lamé constants of the bulk. For the elastic isotropic surface layer, the linear relationship of the surface stress and elastic strain can be expressed by Gurtin–Murdoch elasticity as follows [9]:

\[ \tau^s_{\alpha\phi} = \tau_0 \delta_{\alpha\phi} + \lambda s \varepsilon^s_{\xi\eta} \delta_{\alpha\phi} + 2G s \varepsilon^s_{\xi\eta}, \]

where \( \lambda_s \) and \( G_s \) are the surface modulus, \( \tau_0 \) is the surface residual stress, and \( \delta_{\alpha\phi} \) denotes the surface Christoffel symbols.

According to the analysis of the mechanical equilibrium of surface layer and core, the generalized Young–Laplace equations for NW are expressed as follows [6, 10]:

\[ \sigma_{\alpha\beta} n_j + \tau^s_{\alpha\beta \phi} = 0, \]
\[ \sigma_{ij} n_j = \tau^s_{ij \phi} \]

where \( n_j \) is the unit normal vector and \( \varepsilon^s_{\alpha\phi} \) is the curvature tensor of the surface (Figure 2). The stress distribution of NW can be obtained using the classical displacement method on the basis of equations (1)–(6), that is, the bulk stress and the surface stress can be obtained by directly substituting the bulk displacement/strain formula into the constitutive equations. The global displacements dominant governing equations are established using generalized Young–Laplace equations. The solution of the field equations in the cylinder coordinate can be simplified if the NW is subjected to tension and torsion. We assume that \( u_z \) is function of \( z \) and \( u_\rho \) is function of \( \rho \). According to equation (1), the nonzero strains are

\[ \varepsilon_z = \frac{du_z}{dz}, \]
\[ \varepsilon_\rho = \frac{du_\rho}{d\rho}, \]
\[ \varepsilon_\phi = \frac{u_\phi}{\rho}, \]
\[ \gamma_{z\phi} = \frac{\partial u_\phi}{\partial z}, \]

where \( u_\phi \) is function of \( \phi \).

After substituting equation (7) into equation (2), the stress components in the bulk are

\[ \sigma_\rho = (\lambda + 2G) \frac{d u_\rho}{d \rho} + \lambda \varepsilon_z + \lambda \frac{u_\rho}{\rho}, \]
\[ \sigma_\phi = (\lambda + 2G) \frac{u_\rho}{\rho} + \lambda \varepsilon_z + \lambda \frac{du_\rho}{d \rho}, \]
\[ \sigma_z = (\lambda + 2G) \frac{du_z}{dz} + \lambda \varepsilon_z + \lambda \frac{d u_\rho}{d \rho}, \]
\[ \tau_{z\phi} = G \gamma_{z\phi}. \]

After substituting equations (8)–(11) into equation (3), it is noted that \( \sigma_\rho = \sigma_\phi \), and the stress components are found to be automatically satisfied the radial equilibrium equation. And, we get \( \varepsilon_\rho = \varepsilon_z \) and \( u_\rho \) is the linear distribution along the radial direction. The axial and circumferential equilibrium equation can be simplified into the following forms:

\[ \frac{d^2 u_z}{dz^2} = 0, \]
\[ \frac{\partial^2 u_\rho}{\partial \rho^2} = 0, \]

where the linear distribution along the axial direction of NW. Now, the displacement field can be expressed by

\[ u_\rho = \rho (a_1 z + b_1), \]
\[ u_z = a_2 z + b_2, \]
\[ u_\phi = a_3 \rho, \]

where \( a_1 \sim a_3 \) and \( b_1 \sim b_2 \) are constants related to boundary conditions. The surface of NW is assumed to be characterized by the deformation of the bulk solid so that surface strains can be expressed by

\[ \varepsilon^s_z = a_2, \]
\[ \varepsilon^s_\phi = a_3, \]
\[ \gamma^s_{z\phi} = R_0 a_1, \]

where \( R_0 \) is the radius of NW. Substituting equation (17) into equation (4), the surface stresses are

\[ \tau^s_{zz} = \tau_0 + (\lambda_s + 2G_s) a_2 + \lambda_s a_3, \]
\[ \tau^s_{\phi\phi} = \tau_0 + (\lambda_s + 2G_s) a_3 + \lambda_s a_2, \]
\[ \tau^s_{z\phi} = G_s R_0 a_1. \]

After substituting equations (18)–(20) into equations (5) and (6), the above surface stress components automatically satisfy the axial and circumferential generalized
Young–Laplace equations. The generalized Young–Laplace equation along the radial direction gives
\[
\sigma \rho = \tau_s \phi \phi / R_0 ,
\]
and it is
\[
\alpha_3 = - \frac{(\lambda + \lambda_p)\alpha_2}{2(\lambda + G) + \lambda_p + 2G_p}. \tag{21}
\]

Under a constant external load \( P \), the average normal stress on the cross section of NW is
\[
\bar{\sigma} = \frac{P}{\pi R_0^2} = \frac{2\tau_0}{R_0} + \left[ (\lambda + 2G) + 2(\lambda_p + 2G_p) \right] a_2 + 2(\lambda + \lambda_p) a_3 , \tag{22}
\]
where \( \lambda_p = \lambda / R_0 \) and \( G_p = G / R_0 \). Under a constant external torsion \( T \), the shear stress on the cross section of NW satisfy the following equation:
\[
\left( G I_p + G s \right) \alpha_1 = T , \tag{23}
\]
where \( I_p = \pi R_0^4 / 32 \) and \( I_s = 2\pi R_0^3 \). Combining equations (17), (22), and (23), the constants can be confirmed as follows:
\[
\alpha_1 = \frac{T}{G I_p + G s} \tag{24}
\]
\[
\alpha_2 = \frac{(\sigma - (2\tau_0 / R_0)) \left( 2\lambda + 2G + \lambda_p + 2G_p \right)}{2G(2G + 3\lambda) + \lambda_p (6G + \lambda) + 2G_p \left( 6G + 5\lambda + 4G_p + 4\lambda_p \right)} \tag{25}
\]
\[
\alpha_3 = \frac{-(\sigma - (2\tau_0 / R_0))(\lambda + \lambda_p)}{2G(2G + 3\lambda) + \lambda_p (6G + \lambda) + 2G_p \left( 6G + 5\lambda + 4G_p + 4\lambda_p \right)} . \tag{26}
\]

We next determine the distribution of the surface residual strain and then consider the effective modulus of NW. If nonzero surface residual stress is present on the NW surface and let \( \sigma = 0 \) in equations (25) and (26), then the relaxed surface axial strain and circumferential strain are expressed as follows:
\[
\varepsilon_{zz} = \frac{-2\tau_0 / R_0 \left( 2\lambda + 2G + \lambda_p + 2G_p \right)}{2G(2G + 3\lambda) + \lambda_p (6G + \lambda) + 2G_p \left( 6G + 5\lambda + 4G_p + 4\lambda_p \right)} , \tag{27}
\]
\[
\varepsilon_{\phi\phi} = \frac{-2\tau_0 / R_0 \left( \lambda + \lambda_p \right)}{2G(2G + 3\lambda) + \lambda_p (6G + \lambda) + 2G_p \left( 6G + 5\lambda + 4G_p + 4\lambda_p \right)} .
\]
The surface residual stresses of the NW are inherent and in the self-equilibrium state, that is, independent of the external load. If the NW is subjected to tension and torsion, then the strain and stress analysis of NW can be also performed using equations (7)–(26). Let $u_{ax}$ and $u_{aj}$ be the axial displacements of the two NW ends and $l_0$ be the initial length of NW, the average axial strain is

$$\varepsilon = \frac{u_{ax} - u_{ez0}}{l_0} = a_2.$$ (28)

The effective strains of NW are the difference between average axial strain and surface radial strain, as expressed below:

$$\varepsilon_{eff} = \varepsilon_{zz} - \varepsilon_{zz0}$$
$$\varepsilon_{eff} = \varepsilon_{pp} - \varepsilon_{zz0}.$$ (29)

Consequently, the effective Young’s modulus of NW is obtained as follows:

$$E_{eff} = \frac{\sigma}{\varepsilon_{eff}} = \frac{2G(2G + 3\lambda_p) + \lambda_p(6G + \lambda_p) + 2G_p(6G + 5\lambda + 4G_p + 4\lambda_p)}{2\lambda + 2G + \lambda_p + 2G_p}.$$ (30)

The effective Poisson’s ratio of NW is

$$E_{eff} = \frac{-a_3}{a_2} = \frac{\lambda + \lambda_p}{2\lambda + 2G + \lambda_p + 2G_p}.$$ (31)

The effective shear modulus of NW is

$$G_{eff} = \frac{T}{I_p a_1} = G + \frac{G_p I_p}{I_p}.$$ (32)

### 3. Results and Discussion

All the displacements, strains, bulk stresses, and surface stresses of the NW have been determined using the classical displacement approach. Figure 3 shows the variation in the effective Young’s moduli of the NW compared with its radius. For example, in Al NW, the surface moduli are $\lambda_s = 6.8415$ N/m and $G_s = -0.3755$ N/m [6]. The bulk parameters are $\lambda = 59.2$ GPa and $G = 25.4$ GPa [6]. The solid curve on the basis of our continuum formula (equation (16)) matches Zhang et al. [6] approach (the dotted curve). The effect of surface stresses on the effective Young’s modulus of NW is illustrated, where Young’s modulus decreases with the increase in the NW radius ($R_0$) and gradually reaches a constant value of 69 GPa. As shown in Figure 3, the two approaches provide slightly different results with small radius (<5 nm). Our formula offers small effective Young’s modulus and rapid reduction because the potential energy method adds to the influence of radial and circumferential strains in the definition of Young’s modulus. Homogenization theory of nanocomposites can provide a rigorous definition to define effective properties [10]. As depicted in equation (28), the surface residual stresses ($\tau_{nj}$) also affects Young’s modulus. The surface residual stresses are inherent and in the self-equilibrium state, that is, independent of the external load, due to the surface residual strain (equation [10]). Hence, the positive or negative surface residual stresses will increase (or decrease) Young’s modulus of NW.

Surface moduli also have strong influence on Young’s modulus. The absolute value of the NW surface elasticity is generally <1000 N/m, but it is difficult to accurately quantify. A minimal difference is observed between the experimental approach and numerical atomistic analysis even with small radius. For reference, we also present the variation of the effective modulus of NW compared with its surface moduli in Figure 4. The NW with a large radius is considered ($R = 10$ nm, 20 nm, 30 nm, 40 nm) solely for computational purpose. Figure 4 illustrates the increase in Young’s modulus with the increase in the surface moduli ($\lambda_s$). Equations (8)–(11) show that the surface shear strains are zero, but the surface area expansion is nonzero. Equation (4) implies high surface stress values with high surface moduli, thereby resulting in large NW Young’s modulus. However, the amplification of the surface moduli on Young’s modulus is controlled by the NW radius, that is, the surface area-to-volume ratio increases with the decrease in NW radius. This result suggested that the effective modulus of NW is enhanced by the surface stress. Size dependence is the general characteristics of nanomaterials. Classical displacement approach can provide the surface strain and stress and simplifies the analysis of the effect of surface elasticity on Young’s modulus.
4. Conclusions

NW can be viewed as a composite structure, with the inner core having the normal properties and the surface layer having surface elasticity on the basis of the Gurtin–Murdoch elasticity. The generalized Young–Laplace equations for NW are required in addition to the field equations for core and surface layer. Classical displacement approach in the cylinder coordinate has been used to determine the stress distribution of NW. The nominal normal stress and axial strain are defined in the initial NW configuration with initial length ($l_0$) and radius ($R_0$). The $l_0/R_0$ ratio shows that the effective Young's modulus decreases with the increase in $R_0$ of the nanowire and gradually reachesthe bulk value. The positive or negative surface residual stresses will increase (or decrease) Young’s modulus of NW due to the surface residual strain. Surface moduli also have strong influence on the effective Young’s modulus. Nonzero radial and circumferential strains lead to nonzero area expansion, which enhances the influence of surface moduli effective Young’s modulus.

The radial displacement in the NW is finite [8], and the present model can be easily extended to analyze the effective properties if true strain is used. NW torsion and bending may also be modeled if we consider a proper assumption of the displacement distribution in equation (7). In conclusion, classical displacement approach can obtain NW displacements, strains, and stress distributions and as well as its effective properties. The mechanism underlying the influence of the general characteristics of NW on Young’s modulus can also be easily considered.

Data Availability

The cited data, about surface elastic constants of silver nanowire, used to support the findings of this study are included within the article. The data have been used to verify our theoretical prediction.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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