A Micromechanics Model for the Elastic Properties of Carbon Nanotubes

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Summary

The elastic properties of a carbon nanotube (CNT) are estimated by using the double-inclusion model, where one inclusion (the inner void) is embedded in the other inclusion (the outer tubular shell). The calculated results agree with experimental data. The effects of the tube diameter, length, and thickness on the elastic properties of CNTs are examined.

Introduction

Nanomaterials receive extensive attention in recent years. Carbon nanotubes (CNTs) are perhaps one of the namomaterials based on which practical applications might be developed soon.

Existing works on estimating the Young modulus of CNTs are mainly based on beam or shell thoeries. The double inclusion models based on elasticity theories are employed in the present model to predict the elastic constants of CNTs.

Basic Theories

Consider an ellipsoidal, elastic matrix M, containing an ellipsoidal, elastic inhomogeneity Ω. The matrix is embedded in an infinite elastic medium B. The elastic moduli of Ω, M, and B are given by

$$C = C(x) = \begin{cases} C^{\Omega} & \text{if } x \in \Omega \\ C^{M} & \text{if } x \in M \\ C & \text{otherwise} \end{cases} \tag{1}$$

One may replace the inhomogenieties by a reference material with elasticity C and prescribe transformation strains $\varepsilon^{*\Omega}$ and ε^{*M} in Ω and M, respectively, to compensate the material mismatch[1]. The average stress and strain fields produced in the double-inclusion $V\ (= M \cup \Omega)$ when the infinity domain B is subjected to far field strains ε^{∞}, are given by[2]

$$\langle\varepsilon_{ij}\rangle_\Omega = \varepsilon_{ij}^\infty + S_{ijmn}^\Omega\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega + (S_{ijmn}^V - S_{ijmn}^\Omega)\langle\varepsilon_{mn}^{*M}\rangle_M$$

$$\langle\sigma_{kl}\rangle_\Omega = C_{klij}\{\varepsilon_{ij}^\infty + (S_{ijmn}^\Omega - 1_{ijmn}^{(4s)})\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega + (S_{ijmn}^V - S_{ijmn}^\Omega)\langle\varepsilon_{mn}^{*M}\rangle_M\} \quad (2a, b)$$

$$\langle\varepsilon_{ij}\rangle_M = \varepsilon_{ij}^\infty + S_{ijmn}^V\langle\varepsilon_{mn}^{*M}\rangle_M + \frac{f}{1-f}(S_{ijmn}^V - S_{ijmn}^\Omega)(\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega - \langle\varepsilon_{mn}^{*M}\rangle_M)$$

$$\langle\sigma_{kl}\rangle_M = C_{klij}\{\varepsilon_{ij}^\infty + (S_{ijmn}^V - 1_{ijmn}^{(4s)})\langle\varepsilon_{mn}^{*M}\rangle_M + \frac{f}{1-f}(S_{ijmn}^V - S_{ijmn}^\Omega)(\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega - \langle\varepsilon_{mn}^{*M}\rangle_M)\} \quad (3a, b)$$

where the angle brackets represent averages, S^Ω and S^V are Eshelby's tensors of V and Ω, respectively.

Since the strain and stress fields must be preserved after homogenization, the following constraint conditions must be satisfied:

$$C_{klij}^\Omega\{\varepsilon_{ij}^\infty + S_{ijmn}^\Omega\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega + (S_{ijmn}^V - S_{ijmn}^\Omega)\langle\varepsilon_{mn}^{*M}\rangle_M\}$$
$$= C_{klij}\{\varepsilon_{ij}^\infty + (S_{ijmn}^\Omega - 1_{ijmn}^{(4s)})\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega + (S_{ijmn}^V - S_{ijmn}^\Omega)\langle\varepsilon_{mn}^{*M}\rangle_M\} \quad (4a)$$

$$C_{klij}^M\{\varepsilon_{ij}^\infty + S_{ijmn}^V\langle\varepsilon_{mn}^{*M}\rangle_M + \frac{f}{1-f}(S_{ijmn}^V - S_{ijmn}^\Omega)(\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega - \langle\varepsilon_{mn}^{*M}\rangle_M)\}$$
$$= C_{klij}\{\varepsilon_{ij}^\infty + (S_{ijmn}^V - 1_{ijmn}^{(4s)})\langle\varepsilon_{mn}^{*M}\rangle_M + \frac{f}{1-f}(S_{ijmn}^V - S_{ijmn}^\Omega)(\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega - \langle\varepsilon_{mn}^{*M}\rangle_M)\} \quad (4b)$$

One can solve Eq. (4a, b) for the transformation strains required for homogenization in terms of farfield strains ε^∞. Since

$$\langle\varepsilon_{ij}^d\rangle_V = (1-f)\langle\varepsilon_{ij}^d\rangle_M + f\langle\varepsilon_{ij}^d\rangle_\Omega$$

$$\langle\sigma_{kl}^d\rangle_V = (1-f)\langle\sigma_{kl}^d\rangle_M + f\langle\sigma_{kl}^d\rangle_\Omega \quad (5a, b)$$

substituting Eq. (2a, b) and Eq. (3a, b) into Eq. (5a, b) yields

$$\langle\varepsilon_{ij}\rangle_V = \varepsilon_{ij}^\infty + S_{ijmn}^V\{f\langle\varepsilon_{mn}^{*\Omega}\rangle_\Omega + (1-f)\langle\varepsilon_{mn}^{*M}\rangle_M\}$$

$$\langle \sigma_{kl} \rangle_V = C_{klij} \{ \varepsilon_{ij}^{\infty} + (S_{ijmn}^V - 1_{ijmn}^{(4s)})[f \langle \varepsilon_{mn}^{*\Omega} \rangle_{\Omega} + (1-f) \langle \varepsilon_{mn}^{*M} \rangle_M] \} \quad (6a, b)$$

The effective elastic properties $\overline{C}$ of the double inclusion V are defined by

$$\langle \sigma_{kl} \rangle_V = \overline{C}_{klij} \langle \varepsilon_{ij} \rangle_V \quad (7)$$

The combination of Eq. (6a, b) and Eq. (7) gives

$$\overline{C}_{klpq} = C_{klij} \{ 1^{(4s)} + (S^V - 1^{(4s)}) : [fB + (1-f)A] \}_{ijmn} \{ 1^{(4s)} + S^V : [fB + (1-f)A] \}_{mnpq}^{-1} \quad (8)$$

where

$$A_{mnpq} = [\frac{f}{1-f}(C^M : S^V - C^M : S^{\Omega} - C : S^V + C : S^{\Omega}) + (C : S^V - C - C^M : S^V)$$
$$+ \frac{f}{1-f}(C^M : S^V - C^M : S^{\Omega} - C : S^V + C : S^{\Omega})[C^{\Omega} : S^{\Omega} - C : (S^{\Omega}$$
$$- 1^{(4s)})]^{-1}(C : S^V - C : S^{\Omega} - C^{\Omega} : S^V + C^{\Omega} : S^{\Omega})]_{mnij}^{-1}[\frac{f}{1-f}(C^M : S^V$$
$$- C^M : S^{\Omega} - C : S^V + C : S^{\Omega})[C^{\Omega} : S^{\Omega} - C : (S^V - 1^{(4s)})]^{-1}(C - C^{\Omega})$$
$$- (C - C^M)]_{ijpq}^{-1} \quad (9)$$

$$B_{mnpq} = [C^{\Omega} : S^{\Omega} - C : (S^{\Omega} - 1^{(4s)})]_{mnij}^{-1}(C - C^{\Omega})_{ijpq} + [C^{\Omega} : S^{\Omega} - C : (S^{\Omega}$$
$$- 1^{(4s)})]_{mnkl}^{-1}[C : (S^V - S^{\Omega}) - C^{\Omega} : (S^V - S^{\Omega})]_{klij} A_{ijpq} \quad (10)$$

Two candidate for the reference elasticity tensor C are selected: $C = C^M$ and $C = \overline{C}$.

Results and Discussions

The elastic properties of a single-crystal graphite are given by[3]: $C_{11} = C_{22} = 1060$ GPa, $C_{12} = C_{21} = 180$ GPa, $C_{13} = C_{23} = 15$ GPa, $C_{44} = C_{55} = 4.5$ GPa, $C_{66} = 440$ GPa, and the other elastic moduli are zero.

As it is indicated in Figure 1, where the diameter and thickness of CNT are assumed to be 1.2 *nm* and 0.34 *nm*, respectively, the length of CNT does not affect Young's modulus of CNT significantly. The relationship between Young's modulus and the diameter of CNT is shown in Figure 2, where the length and thickness of CNT are assumed to be 100 *nm* and 0.34 *nm*, respectively. The predicted Young's modulus increasing with a decrease in tube diameter agrees with the available experimental data [4~7]. It is noted that Young's modulus drops significantly when the CNT diameter is longer than 1.2 *nm*. The relationship between CNT diameter and thickness, for a fixed Young's modulus of 1000 GPa is plotted in Figure 3, which agrees with the experimental results [8].

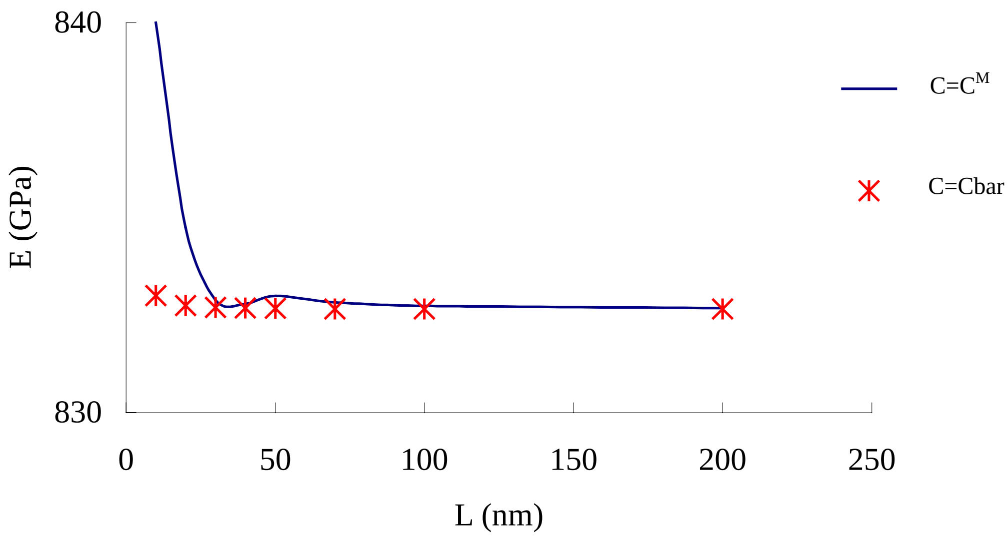

Figure 1: Young's modulus vs. CNT length for t = 0.34 nm and D = 1.2 nm

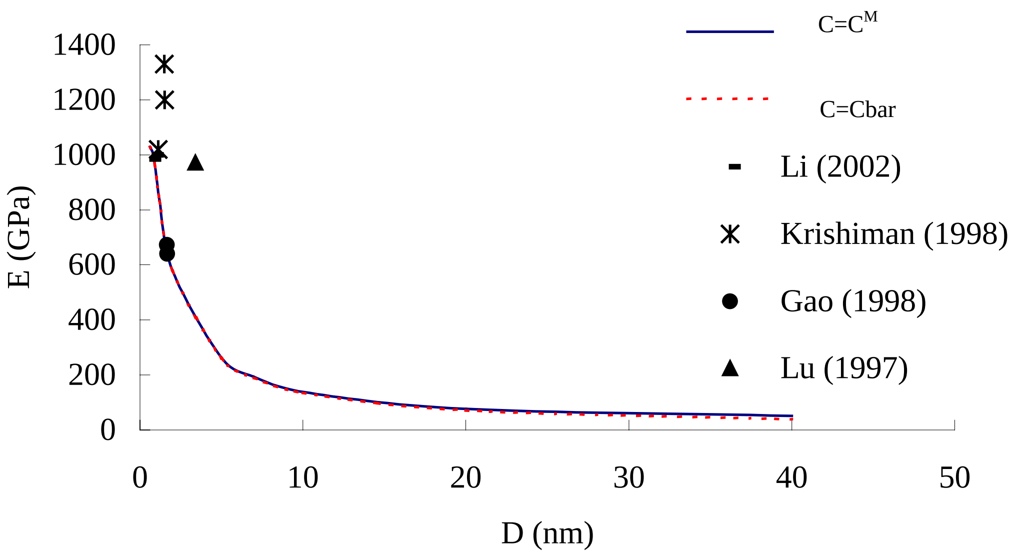

Figure 2: Young's modulus vs. CNT diameter for t = 0.34 nm and L = 100 nm

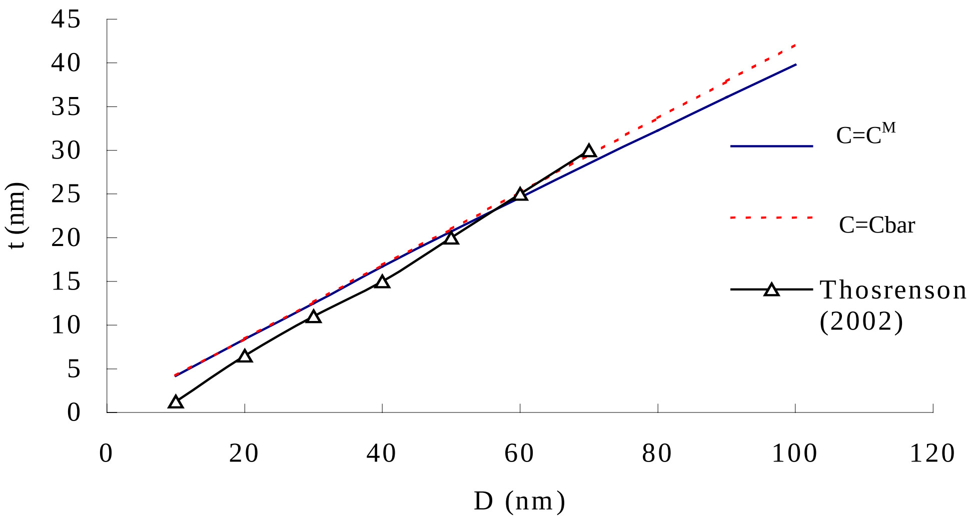

Figure 3: The relationship between CNT diameter and CNT thickness

for $\overline{E}$ = 1000 GPa

Conclusions

In the present work, a CNT is modeled as a double inclusion and its elastic properties are estimated using elasticity theories. The effects of tube diameter, length , and thickness on the elastic properties of CNTs are examined.

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