Research Article

Estimating the Thermal Conductivities and Elastic Stiffness of Carbon Nanotubes as a Function of Tube Geometry

Z. H. Zhang, N. Yu, and W. H. Chao

Department of Mechanical Engineering, Yuan Ze University, Jhongli 32003, Taiwan

Correspondence should be addressed to N. Yu, nyu@saturn.yzu.edu.tw

Received 15 October 2011; Accepted 18 March 2012

Academic Editor: Sulin Zhang

Copyright © 2012 Z. H. Zhang et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The thermal conductivities and elastic properties of carbon nanotubes (CNTs) are estimated by using the double-inclusion model, which is based on rigorous elasticity approach. The model regards a CNT as one inclusion (the inner cylindrical void) embedded in the other (the outer coaxial single-crystal graphite shell). The concept of homogenization is employed, and vital microstructural parameters, such as CNT diameter, length, and aspect ratio, are included in the present model. The relationship between microstructure and thermal conductivities and elastic stiffness of CNTs is quantitatively characterized. Our analytical results, benchmarked by experimental data, show that the thermal conductivities and elastic stiffness of CNTs are strongly dependent on the diameter of CNT with little dependence on the length of CNT.

1. Introduction

The present work employs and modifies the double-inclusion model [1] to estimate, from a microstructural point of view, the thermal conductivities and elastic stiffness of carbon nanotubes (CNTs). Several models based on molecular dynamics simulation are developed for estimating the thermal conductive and elastic properties of CNTs [2–7] yet are not very computationally efficient. Some of the existing models are based on beam theories [8, 9] and can only estimate the Young moduli of CNTs. Robertson et al. [10] and Lu [11] employ energy methods to estimate the elastic properties of CNTs. Finite deformation is considered in Gao and Li [12] where the formulation is aimed at single-walled CNTs. A multiscale shear-lag-based approach later is developed for estimating Young's moduli of CNTs as well as stresses in CNT-based composites [13]. Chantrenne and Barrat [14] derive analytical expressions for the thermal conductivities of a single graphene and a CNT as a function of their characteristic lengths. Their analytical estimates show good agreement for single graphene but not for CNTs.

The reported experimental data of thermal conductivities and Young's and shear moduli of CNTs from literature are summarized in Tables 1 and 2, respectively. It is noted that the reported data are significantly different from each other

as the thermal and elastic properties of CNTs are functions of the microstructure of CNTs [15–18]. Qian et al. [19] also collect many experimental data on the Young modulus of CNTs, and they range from 320 GPa to 5.0 TPa. It is the objective of the present work to develop an analytical model to delineate the relationship between the microstructure and thermal conductive and elastic stiffness of CNTs.

2. The Model

2.1. Mori-Tanaka Theorem. Consider an infinite medium B , embodying a subregion V , which includes an inclusion Ω undergoing a heat flux-free transformation temperature gradient $\nabla T^{*\Omega}$. The matrix is denoted by M , and $V = M \cup \Omega$, see Figure 1. In view of the concept of Eshelby [20], Mori and Tanaka [21], and Hatta and Taya [22], one may find the disturbance temperature gradient $\{\nabla T^d\} = \{\nabla T_x^d, \nabla T_y^d, \nabla T_z^d\}^T$ at a typical location, x , in V due to a transformation temperature gradient $\{\nabla T^{*\Omega}\} = \{\nabla T_x^{*\Omega}, \nabla T_y^{*\Omega}, \nabla T_z^{*\Omega}\}^T$ in Ω as follows:

$$\{\nabla T^d(x)\} = [S^\Omega] \{\nabla T^{*\Omega}\}, \quad (1)$$

where the case of ellipsoidal V and Ω are considered. Eshelby's matrix $[S^\Omega]$ is a 3×3 matrix and is a function of

TABLE 1: The reported data of thermal conductivity of CNTs.

	CNT diameter (nm)	CNT length (nm)	CNT thickness (nm)	K (W/m-K)	SWCNT/MWCNT
Hone et al. [28]	1.4	100	NA	1750 ~ 5850	SWCNT
Berber et al. [4]	NA	NA	NA	6600	SWCNT
Osman and Srivastava [5]	NA	NA	NA	1000 ~ 2500	SWCNT
Kim et al. [29]	14	2.5 μ m	NA	>3000	MWCNT
Maruyama [6]	NA	6 ~ 404	0.34	280 ~ 380	SWCNT
Bagchi and Nomura [30]	25	50 μ m	10	3000	MWCNT
Bi et al. [7]	NA	2.5 ~ 25	NA	400 ~ 600	SWCNT

TABLE 2: The reported experimental data of Young's and shear moduli of CNTs.

	Length (nm)	Diameter (nm)	Thickness (nm)	SWCNT/MWCNT	Young's modulus (TPa)	Shear modulus (GPa)
Salvetat et al. [31]	180 ~ 370	4.5 ~ 20	0.34	SWCNT	0.067 ~ 0.5	0.7 ~ 6.5
Salvetat et al. [32]		26 ~ 76		MWCNT	1.28 $\pm$ 0.59	
Krishnan et al. [33]	23.4 ~ 36.8	1.12 ~ 1.5		SWCNT	1.25 (average)	0.1
Yu et al. [34]		19 ~ 41	0.34	SWCNT	0.32 ~ 1.47	
Yu et al. [35]	1800 ~ 10990	13 ~ 36		MWCNT	0.27 ~ 0.95

FIGURE 1: Mori-Tanaka model.

the geometry of inclusion Ω . In particular, the components of $[S^\Omega]$ for a circular cylindrical Ω are only functions of the aspect ratio of the cylinder [22]. It can be shown in a straightforward manner that the average temperature gradient of V , $\{\langle \nabla T^d \rangle_V\}$, is given by

$$\{\langle \nabla T^d \rangle_V\} = f \{\langle \nabla T^d \rangle_\Omega\} + (1-f) \{\langle \nabla T^d \rangle_M\}, \quad (2)$$

where the angle brackets $\langle \rangle$ represent an average quantity, $\{\langle \nabla T^d \rangle_\Omega\}$ is the average temperature gradient field of the inclusion, $\{\langle \nabla T^d \rangle_M\}$ is the average temperature gradient field of the matrix, and $f = \Omega/V$ is the inclusion volume

fraction. The average disturbance temperature gradient in region M due to $\nabla T^{*\Omega}$ is given by

$$\begin{aligned} \{\langle \nabla T^d \rangle_M\} &= \frac{1}{M} \int_M \{\nabla T^d(x)\} dV_x \\ &= \frac{1}{M} \left(\int_V \{\nabla T^d(x)\} dV_x - \int_\Omega \{\nabla T^d(x)\} dV_x \right) \\ &= \frac{1}{M} \left(\frac{\Omega}{V} \int_V [S^V] \{\nabla T^{*\Omega}\} dV \right) \\ &\quad - \frac{\Omega}{M} [S^\Omega] \{\nabla T^{*\Omega}\}, \end{aligned} \quad (3)$$

where S^V is Eshelby's matrix of inclusion V . Rearranging (3) gives

$$\{\langle \nabla T^d \rangle_M\} = \frac{\Omega}{M} ([S^V] - [S^\Omega]) \{\nabla T^{*\Omega}\}. \quad (4)$$

Substituting (1) and (4) into (2) gives the disturbance temperature gradient averaged over V due to a uniform transformation temperature gradient prescribed in Ω ,

$$\{\langle \nabla T^d \rangle_V\} = f [S^V] \{\nabla T^{*\Omega}\}. \quad (5)$$

Now consider a uniform transformation temperature gradient ∇T^{*M} in M . The heat flux and temperature gradient fields can be obtained by superposing two fields—one is due to $-\nabla T^{*M}$ and distributed over Ω , and the other is due to ∇T^{*M} and distributed over V . The average disturbance temperature gradient in Ω due to ∇T^{*M} in M is given by

$$\begin{aligned} \{\langle \nabla T^d \rangle_\Omega\} &= \frac{1}{\Omega} \int_\Omega [S(x; \Omega)] dV_x \{-\nabla T^{*M}\} \\ &\quad + \frac{1}{\Omega} \int_\Omega [S(x; V)] dV_x \{\nabla T^{*M}\} \\ &= ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}. \end{aligned} \quad (6)$$

The average disturbance temperature gradient in M due to ∇T^{*M} prescribed in M is given by

$$\begin{aligned} \{\langle \nabla T^d \rangle_M\} &= \frac{1}{M} \int_M [S(x; \Omega)] dV_x \{\langle -\nabla T^{*M} \rangle\} \\ &+ \frac{1}{M} \int_M [S(x; V)] dV_x \{\nabla T^{*M}\}. \end{aligned} \quad (7)$$

The first term on the right-hand side of (7) is in essence identical to (3) except ∇T^{*M} being replaced by $(-\nabla T^{*M})$. Thus, (4) can be used to give

$$\begin{aligned} \{\langle \nabla T^d \rangle_M\} &= \frac{\Omega}{M} ([S^V] - [S^\Omega]) \{\langle -\nabla T^{*M} \rangle\} \\ &+ [S^V] \{\nabla T^{*M}\} \\ &= \frac{f}{1-f} [S^\Omega] \{\nabla T^{*M}\} \\ &+ \frac{1-2f}{1-f} [S^V] \{\nabla T^{*M}\}. \end{aligned} \quad (8)$$

Substituting (8) and (6) into (2), one obtains the disturbance temperature gradient averaged over V due to transformation temperature gradient ∇T^{*M} prescribed in M as follows:

$$\{\langle \nabla T^d \rangle_V\} = (1-f) [S^V] \{\nabla T^{*M}\}. \quad (9)$$

2.2. Extended Mori-Tanaka Theorem. Consider an infinite homogeneous solid B with a thermal conductivity $\{K\} = \{K_x, K_y, K_z\}^T$. The solid B contains two ellipsoidal inclusions, V and Ω ($\Omega \subset V$). Let Ω and M ($= V - \Omega$) undergo distinct heat flux-free transformation. The uniform transformation temperature gradient in the absence of the surrounding medium is $\nabla T^{*\Omega}$ and ∇T^{*M} in Ω and M , respectively. The average of the disturbance temperature gradient resulting from $\nabla T^{*\Omega}$ is given by (1) and (5), and the volume average of the corresponding heat flux field is given by

$$\{\langle q^d \rangle_\Omega\} = [K] ([S^\Omega] - [I]) \{\nabla T^{*\Omega}\}, \quad (10a)$$

$$\{\langle q^d \rangle_V\} = f[K] ([S^V] - [I]) \{\nabla T^{*\Omega}\}, \quad (10b)$$

where I is the 3×3 identity matrix.

Similarly, the temperature gradient resulted from ∇T^{*M} is given by (6) and (9), and the corresponding heat flux fields are given by

$$\{\langle q^d \rangle_\Omega\} = [K] ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}, \quad (11a)$$

$$\{\langle q^d \rangle_V\} = (1-f)[K] ([S^V] - [I]) \{\nabla T^{*M}\}. \quad (11b)$$

Combining (1), (6), (10a), and (11a) gives the average temperature gradient and heat flux in Ω due to $\nabla T^{*\Omega}$ and ∇T^{*M} ,

$$\{\langle \nabla T^d \rangle_\Omega\} = [S^\Omega] \{\nabla T^{*\Omega}\} + ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}, \quad (12a)$$

$$\begin{aligned} \{\langle q^d \rangle_\Omega\} &= [K] ([S^\Omega] - [I]) \{\nabla T^{*\Omega}\} \\ &+ [K] ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}. \end{aligned} \quad (12b)$$

The combination of (5), (9), (10b) and (11b) gives the average temperature gradient and heat flux in V due to $\nabla T^{*\Omega}$ and ∇T^{*M} ,

$$\begin{aligned} \{\langle \nabla T^d \rangle_V\} &= [S^V] \{f \{\nabla T^{*\Omega}\} + (1-f) \{\nabla T^{*M}\}\}, \end{aligned} \quad (13a)$$

$$\begin{aligned} \{\langle q^d \rangle_V\} &= [K] ([S^V] - [I]) \{f \{\nabla T^{*\Omega}\} + (1-f) \{\nabla T^{*M}\}\}. \end{aligned} \quad (13b)$$

The following relations can be derived in a straightforward manner:

$$\{\langle \nabla T^d \rangle_V\} = (1-f) \{\langle \nabla T^d \rangle_M\} + f \{\langle \nabla T^d \rangle_\Omega\}, \quad (14a)$$

$$\{\langle q^d \rangle_V\} = (1-f) \{\langle q^d \rangle_M\} + f \{\langle q^d \rangle_\Omega\}. \quad (14b)$$

Substituting (12a) and (12b), (13a) and (13b) into (14a) and (14b) gives

$$\begin{aligned} \{\langle \nabla T^d \rangle_M\} &= [S^V] \{\nabla T^{*M}\} \\ &+ \frac{f}{1-f} \{([S^V] - [S^\Omega]) (\{\nabla T^{*\Omega}\} - \{\nabla T^{*M}\})\}, \end{aligned} \quad (15a)$$

$$\begin{aligned} \{\langle q^d \rangle_M\} &= [K] ([S^V] - [I]) \{\nabla T^{*M}\} \\ &+ \frac{f}{1-f} [K] \{([S^V] - [S^\Omega]) (\{\nabla T^{*\Omega}\} - \{\nabla T^{*M}\})\}. \end{aligned} \quad (15b)$$

2.3. Thermal Conductivities and Elastic Constants of Double Inclusion. Consider an ellipsoidal matrix M , containing an ellipsoidal inhomogeneity Ω . The matrix M is embedded in

FIGURE 2: Double-inclusion model.

an infinite medium B . The thermal conductivity of Ω , M , and B is given by

$$K = K(x) = \begin{cases} K^\Omega & \text{if } x \text{ in } \Omega, \\ K^M & \text{if } x \text{ in } M, \\ K & \text{otherwise,} \end{cases} \quad (16)$$

respectively; see Figure 2. To solve the double-inhomogeneity problem, one may replace the inhomogeneity, Ω , and the matrix, M , by a reference material with thermal conductivity $\{K\}$, which is the thermal conductivity of B . Then one could prescribe transformation temperature gradient $\nabla T^{*\Omega}$ and ∇T^{*M} in Ω and M , respectively, to compensate the material mismatch, which is essentially Eshelby's concept of equivalent inclusion [20]. When the infinity domain B is subjected to far-field temperature gradient $\{\nabla T^\infty\}$, the heat flux and temperature gradient fields of the double inclusion $V (= M \cup \Omega)$ are in general not uniform, and their averages are, with the help of (12a), (12b), and (15a) and (15b), given by

$$\begin{aligned} \{\langle \nabla T^d \rangle_\Omega\} &= \{\nabla T^\infty\} + [S^\Omega] \{\nabla T^{*\Omega}\} \\ &\quad + ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}, \end{aligned} \quad (17a)$$

$$\begin{aligned} \{\langle q^d \rangle_\Omega\} &= [K] \{\{\nabla T^\infty\} + ([S^\Omega] - [I]) \{\nabla T^{*\Omega}\} \\ &\quad + ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}\}, \end{aligned} \quad (17b)$$

$$\begin{aligned} \{\langle \nabla T^d \rangle_M\} &= \{\nabla T^\infty\} + [S^V] \{\nabla T^{*M}\} + \frac{f}{1-f} \\ &\quad ([S^V] - [S^\Omega]) (\{\nabla T^{*\Omega}\} - \{\nabla T^{*M}\}), \end{aligned} \quad (18a)$$

$$\begin{aligned} \{\langle q^d \rangle_M\} &= [K] \{\{\nabla T^\infty\} + ([S^V] - [I]) \{\nabla T^{*M}\} \\ &\quad + \frac{f}{1-f} ([S^V] - [S^\Omega]) \\ &\quad (\{\nabla T^{*\Omega}\} - \{\nabla T^{*M}\})\}. \end{aligned} \quad (18b)$$

Since the temperature gradient and the heat flux fields must be preserved after homogenization, the following constraint conditions must be satisfied:

$$\begin{aligned} [K^\Omega] \{\{\nabla T^\infty\} + [S^\Omega] \{\nabla T^{*\Omega}\} + ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}\} \\ = [K] \{\{\nabla T^\infty\} + ([S^\Omega] - [I]) \{\nabla T^{*\Omega}\} \\ + ([S^V] - [S^\Omega]) \{\nabla T^{*M}\}\}, \end{aligned} \quad (19a)$$

$$\begin{aligned} [K^M] \{\{\nabla T^\infty\} + [S^V] \{\nabla T^{*M}\} \\ + \frac{f}{1-f} ([S^V] - [S^\Omega]) (\{\nabla T^{*\Omega}\} - \{\nabla T^{*M}\})\} \\ = [K] \{\{\nabla T^\infty\} + ([S^V] - [I]) \{\nabla T^{*M}\} + \frac{f}{1-f} \\ ([S^V] - [S^\Omega]) (\{\nabla T^{*\Omega}\} - \{\nabla T^{*M}\})\}. \end{aligned} \quad (19b)$$

Solving (19a) and (19b) simultaneously, one finds

$$\{\langle \nabla T^{*M} \rangle_M\} = [A] \{\nabla T^\infty\}, \quad (20a)$$

$$\{\langle \nabla T^{*\Omega} \rangle_\Omega\} = [B] \{\nabla T^\infty\}, \quad (20b)$$

where

$$\begin{aligned} [A] &= \left[\frac{f}{1-f} ([K^M][S^V] - [K^M][S^\Omega] \right. \\ &\quad \left. - [K][S^V] + [K][S^\Omega]) \right. \\ &\quad \left. + ([K][S^V] - [K] - [K^M][S^V]) \right. \\ &\quad \left. + \frac{f}{1-f} \right. \\ &\quad \left. ([K^M][S^V] - [K^M][S^\Omega] \right. \\ &\quad \left. - [K][S^V] + [K][S^\Omega]) \right. \\ &\quad \left. [[K^\Omega][S^\Omega] - [K]([S^\Omega] - [I])]^{-1} \right. \\ &\quad \left. ([K][S^V] - [K][S^\Omega] \right. \\ &\quad \left. - [K^\Omega][S^V] + [K^\Omega][S^\Omega]) \right]^{-1} \end{aligned}$$

$$\begin{aligned}
& \left[\frac{f}{1-f} ([K^M][S^V] - [K^M][S^\Omega]) \right. \\
& \quad \left. - [K][S^V] + [K][S^\Omega] \right) \\
& \quad \left[[K^\Omega][S^\Omega] - [K]([S^V] - [I]) \right]^{-1} \\
& \quad \left. ([K] - [K^\Omega]) - ([K] - [K^M]) \right], \tag{21}
\end{aligned}$$

$$\begin{aligned}
[B] &= \left[[K^\Omega][S^\Omega] - [K]([S^\Omega] - [I]) \right]^{-1} \left[([K] - [K^\Omega]) \right. \\
& \quad \left. + \left[[K^\Omega][S^\Omega] - [K]([S^\Omega] - [I]) \right]^{-1} \right. \\
& \quad \left. [K]([S^V] - [S^\Omega]) - [K^\Omega]([S^V] - [S^\Omega]) \right] [A]. \tag{22}
\end{aligned}$$

Substituting (17a) and (17b) and (18a) and (18b) into (14a) and (14b), one finds

$$\begin{aligned}
\{ \langle \nabla T^d \rangle_V \} &= \{ \nabla T^\infty \} \\
&+ [S^V] \{ f \{ \nabla T^{*\Omega} \} + (1-f) \{ \nabla T^{*M} \} \}, \tag{23a}
\end{aligned}$$

$$\begin{aligned}
\{ \langle q^d \rangle_V \} &= [K] \{ \{ \nabla T^\infty \} \\
&+ ([S^V] - [I]) \\
&[f \{ \nabla T^{*\Omega} \} + (1-f) \{ \nabla T^{*M} \}] \}. \tag{23b}
\end{aligned}$$

The thermal conductivities $\bar{K}$ of the double inclusion V are defined by

$$\{ \langle q^d \rangle_V \} = [\bar{K}] \{ \langle \nabla T^d \rangle_V \}. \tag{24}$$

The combination of (20a) and (20b), (23a) and (23b), and (24) gives

$$\begin{aligned}
[\bar{K}] &= [K] \left[\{ [I] + ([S^V] - [I]) [f[B] + (1-f)[A]] \} \right. \\
& \quad \left. \{ [I] + [S^V] [f[B] + (1-f)[A]] \} \right]^{-1}. \tag{25}
\end{aligned}$$

A reasonable choice for the reference material for homogenization is the matrix material. Thus, $\nabla T^{*M} = 0$. Letting $[A] = 0$ in (25) gives

$$\begin{aligned}
[\bar{K}] &= [K^M] \left[\{ [I] + f([S^V] - [I]) \right. \\
& \quad \left. [([K^M] - [K^\Omega])[S^\Omega] - [K^M]]^{-1} \right. \\
& \quad \left. ([K^\Omega] - [K^M]) \} \right] \\
& \quad \left[\{ [I] + f[S^V] \right. \\
& \quad \left. [([K^M] - [K^\Omega])[S^\Omega] - [K^M]]^{-1} \right. \\
& \quad \left. ([K^\Omega] - [K^M]) \} \right]^{-1}. \tag{26}
\end{aligned}$$

In the case of CNT, the inner inclusion Ω is a void, and the outer M is a graphene. Therefore, the $[K^\Omega]$ in (26) may be neglected as the thermal conductivity of air is much less than that of the graphene, or $[K^\Omega] = 0$ in the case of a vacuum. Therefore, the thermal conductivities of a CNT can be estimated by

$$\begin{aligned}
[\bar{K}] &= [K^M] ([S^\Omega] - [I] - f([S^V] - [I])) \\
& \quad ([S^\Omega] - [I] - f[S^V])^{-1}. \tag{27}
\end{aligned}$$

Specifically,

$$\bar{K}_{ii} = K_{ii}^M \left(1 - \frac{f}{1 - S_{ii}^\Omega + f S_{ii}^V} \right) \quad i = 1 \sim 3; \text{ no sum on } i. \tag{28}$$

In view of the analogy between heat conduction and linear elasticity, the elastic constants $[\bar{C}]$, which is a 6×6 matrix, of a CNT can be estimated by

$$\begin{aligned}
[\bar{C}] &= [C^M] ([C^\Omega] - [I] - f([C^V] - [I])) \\
& \quad ([C^\Omega] - [I] - f[C^V])^{-1}, \tag{29}
\end{aligned}$$

where $[C^M]$ is the stiffness matrix of a single-crystal graphite, $[I]$ is the 6×6 identity matrix, and the components of Eshelby's matrix for anisotropic elastic inclusions are given by Mura [23]. In particular, the shear moduli of a CNT can be estimated by

$$\bar{C}_{ii} = C_{ii}^M \left(1 - \frac{f}{1 - S_{ii}^\Omega + f S_{ii}^V} \right) \quad i = 4 \sim 6; \text{ no sum on } i. \tag{30}$$

FIGURE 3: Young's modulus as a function of CNT length for $t = 0.34$ nm and $D = 1.2$ nm.

3. Results

The following elastic properties of a single-crystal graphite are used in our calculations [24]:

$$[C^M] = \begin{bmatrix} 1060 & 15 & 180 & 0 & 0 & 0 \\ 15 & 36.5 & 15 & 0 & 0 & 0 \\ 180 & 15 & 1060 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 440 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.5 \end{bmatrix} \text{ GPa.} \quad (31)$$

As it is indicated in Figure 3, 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 its axial and transverse Young's moduli significantly. The relationship between axial Young's modulus and the diameter of CNT is shown in Figure 4, where the length and thickness of CNT are assumed to be 1 μm and 0.34 nm, respectively. The predicted axial Young's modulus increases with a decrease in CNT diameter, which is consistent with the available experimental data, yet is in contrast with what is predicted by Li and Chou [18]. It is noted that axial Young's modulus drops significantly when the CNT diameter is greater than 1.2 nm. The transverse Young modulus of CNT exhibits a similar relation with CNT diameter. The relationship between CNT diameter and thickness, for a fixed axial Young's modulus of 1 TPa, is shown in Figure 5, which agrees with Thostenson et al. [25].

The in-plane and out-of-plane thermal conductivities of graphene are assumed to be equal to 2,000 and 10 W/m-K, respectively [26] in the present calculations. The thermal conductivity of air varies from 0.02 to 0.08 W/m-K as the temperature varies from -55°C to $1,000^\circ\text{C}$ and is negligible. As it is indicated in Figure 6, where the diameter of CNT is assumed to be 1.2 nm and 1.4 nm and the CNT thickness is

FIGURE 4: Young's modulus versus CNT diameter for $t = 0.34$ nm and $L = 1000$ nm.

FIGURE 5: The relationship between CNT diameter and CNT thickness for $\bar{E} = 1$ TPa.

assumed to be 0.34 nm, the length of CNT does not affect its axial thermal conductivity significantly, which is consistent to the findings of Yang et al. [27] and Hone et al. [28]. The relationship between CNT diameter and its thermal conductivity for a fixed length of 100 nm is shown in Figure 7, where the thickness of CNT is assumed to be 0.34 nm, and the axial thermal conductivity of CNT decreases dramatically with an increase in CNT diameter when the CNT diameter is less than 10 nm. When the CNT diameter is greater than 10 nm, the decrease in axial thermal conductivity of CNT becomes gradual. Figure 8 shows the relationship between CNT aspect ratio and its axial thermal conductivity. The axial thermal conductivity increases with an increase in the aspect ratio of CNT [17]. The relationship between the axial thermal conductivity of MWCNT and its number of layers is shown in Figure 9, where the MWCNT outer diameter, length, and thickness of each layer are assumed to be 14 nm, 100 nm, and 0.34 nm, respectively.

FIGURE 6: Axial thermal conductivity of CNT as a function of CNT length for $t = 0.34$ nm, $D = 1.2$ nm, and $D = 1.4$ nm.

FIGURE 7: Axial thermal conductivity as a function of CNT outer diameter for $t = 0.34$ nm and $L = 100$ nm.

4. Conclusion

In the present work, the double-inclusion model [1], which is based on elasticity solutions [20, 21] and is originally presented in the context of linear elasticity, is employed and extended to predict the thermal conductivities and elastic constants of CNTs. Though the theorem proposed by Mori and Tanaka [21] is not restricted to ellipsoidal inclusions, the present work regards a CNT as a circular cylindrical shell containing a concentric circular cylindrical void, that is, two coaxial circular cylindrical inclusions—one is embedded in the other. The outer shell is composed of a single-crystal graphite sheet.

Our results indicate that (1) the length of CNT does not significantly affect its thermal conductivities, axial and transverse Young's and shear moduli; (2) with an increase in CNT diameter, axial and transverse Young's moduli and thermal conductivities as well as shear moduli decrease. This may

FIGURE 8: Relationship between axial thermal conductivity and CNT aspect ratio.

FIGURE 9: Relationship between axial thermal conductivity of MWCNT and its number of layers.

explain why the reported experimental data in the literature (see Tables 1 and 2) are scattered when the thermal conductivity and elastic properties of a CNT are considered as functions of its microstructure, in particular, its diameter. The results derived from the present model agree quite well with the available experimental measurement and observation.

Acknowledgment

This work is supported by the National Science Council in Taiwan under Grant no. NSC95-2221-E-155-016 to Yuan Ze University, Taiwan.

References

- [1] M. Hori and S. Nemat-Nasser, "Double-inclusion model and overall moduli of multi-phase composites," *Mechanics of Materials*, vol. 14, no. 3, pp. 189–206, 1993.
- [2] B. I. Yakobson, C. J. Brabec, and J. Bernholc, "Nanomechanics of carbon tubes: instabilities beyond linear response," *Physical Review Letters*, vol. 76, no. 14, pp. 2511–2514, 1995.
- [3] G. Gao, T. Çağın, and W. A. Goddard, "Energetics, structure, mechanical and vibrational properties of single-walled carbon nanotubes," *Nanotechnology*, vol. 9, no. 3, pp. 184–191, 1998.
- [4] S. Berber, Y. K. Kwon, and D. Tománek, "Unusually high thermal conductivity of carbon nanotubes," *Physical Review Letters*, vol. 84, no. 20, pp. 4613–4616, 2000.

- [5] M. A. Osman and D. Srivastava, "Temperature dependence of the thermal conductivity of single-wall carbon nanotubes," *Nanotechnology*, vol. 12, no. 1, pp. 21–24, 2001.
- [6] S. Maruyama, "A molecular dynamics simulation of heat conduction in finite length SWNTs," *Physica B*, vol. 323, no. 1–4, pp. 193–195, 2002.
- [7] K. Bi, Y. Chen, J. Yang, Y. Wang, and M. Chen, "Molecular dynamics simulation of thermal conductivity of single-wall carbon nanotubes," *Physics Letters A*, vol. 350, no. 1–2, pp. 150–153, 2006.
- [8] S. Govindjee and J. L. Sackman, "On the use of continuum mechanics to estimate the properties of nanotubes," *Solid State Communications*, vol. 110, no. 4, pp. 227–230, 1999.
- [9] V. M. Harik, "Ranges of applicability for the continuum beam model in the mechanics of carbon nanotubes and nanorods," *Solid State Communications*, vol. 120, no. 7–8, pp. 331–335, 2001.
- [10] D. H. Robertson, D. W. Brenner, and J. W. Mintmire, "Energetics of nanoscale graphitic tubules," *Physical Review B*, vol. 45, no. 21, pp. 12592–12595, 1992.
- [11] J. P. Lu, "Elastic properties of carbon nanotubes and nanoropes," *Physical Review Letters*, vol. 79, no. 7, pp. 1297–1300, 1997.
- [12] X.-L. Gao and K. Li, "Finite deformation continuum model for single-walled carbon nanotubes," *International Journal of Solids and Structures*, vol. 40, no. 26, pp. 7329–7337, 2003.
- [13] X. L. Gao and K. Li, "A shear-lag model for carbon nanotube-reinforced polymer composites," *International Journal of Solids and Structures*, vol. 42, no. 5–6, pp. 1649–1667, 2005.
- [14] P. Chantrenne and J.-L. Barrat, "Analytical model for the thermal conductivity of nanostructures," *Superlattices and Microstructures*, vol. 35, no. 3–6, pp. 173–186, 2004.
- [15] P. Poncharal, Z. L. Wang, D. Ugarte, and W. A. De Heer, "Electrostatic deflections and electromechanical resonances of carbon nanotubes," *Science*, vol. 283, no. 5407, pp. 1513–1516, 1999.
- [16] M. C. Llaguno, J. Hone, A. T. Johnson, and J. E. Fischer, "Thermal conductivity of single wall carbon nanotubes: diameter and annealing dependence," in *Proceedings of the AIP Conference*, vol. 591, pp. 384–387, 2001.
- [17] P. Grassberger and L. Yang, "Heat conduction in low dimensions: from fermi-pasta-ulam chains to single-walled nanotubes," 2002, <http://arxiv.org/abs/cond-mat/0204247v1>.
- [18] C. Li and T. W. Chou, "A structural mechanics approach for the analysis of carbon nanotubes," *International Journal of Solids and Structures*, vol. 40, no. 10, pp. 2487–2499, 2003.
- [19] D. Qian, G. J. Wagner, W. K. Liu, M. F. Yu, and R. S. Ruoff, "Mechanics of carbon nanotubes," *Applied Mechanics Reviews*, vol. 55, no. 6, pp. 495–533, 2002.
- [20] J. D. Eshelby, "The determination of elastic field of an ellipsoidal inclusion and related problems," *Proceedings of the Royal Society of London A*, vol. 241, no. 1226, pp. 376–396, 1957.
- [21] T. Mori and K. Tanaka, "Average stress in matrix and average elastic energy of materials with misfitting inclusions," *Acta Metallurgica*, vol. 21, no. 5, pp. 571–574, 1973.
- [22] H. Hatta and M. Taya, "Equivalent inclusion method for steady state heat conduction in composites," *International Journal of Engineering Science*, vol. 24, no. 7, pp. 1159–1172, 1986.
- [23] T. Mura, *Micromechanics of Defects in Solids*, Martinus Nijhoff, Boston, Mass, USA, 1982.
- [24] J. Z. Liu, Q. Zheng, and Q. Jiang, "Effect of a rippling mode on resonances of carbon nanotubes," *Physical Review Letters*, vol. 86, no. 21, pp. 4843–4846, 2001.
- [25] E. T. Thostenson, W. Z. Li, D. Z. Wang, Z. F. Ren, and T. W. Chou, "Carbon nanotube/carbon fiber hybrid multiscale composites," *Journal of Applied Physics*, vol. 91, no. 9, pp. 6034–6037, 2002.
- [26] Electronics Cooling 2007, http://www.electronics-cooling.com/articles/2001/2001_august_techbrief.php.
- [27] D. J. Yang, S. G. Wang, Q. Zhang, P. J. Sellin, and G. Chen, "Thermal and electrical transport in multi-walled carbon nanotubes," *Physics Letters, Section A*, vol. 329, no. 3, pp. 207–213, 2004.
- [28] J. Hone, A. Zettl, and M. Whitney, "Thermal conductivity of single-walled carbon nanotubes," *Synthetic Metals*, vol. 103, no. 1–3, pp. 2498–2499, 1999.
- [29] P. Kim, L. Shi, A. Majumdar, and P. L. McEuen, "Mesoscopic thermal transport and energy dissipation in carbon nanotubes," *Physica B*, vol. 323, no. 1–4, pp. 67–70, 2002.
- [30] A. Bagchi and S. Nomura, "On the effective thermal conductivity of carbon nanotube reinforced polymer composites," *Composites Science and Technology*, vol. 66, no. 11–12, pp. 1703–1712, 2006.
- [31] J. P. Salvetat, G. A. D. Briggs, J. M. Bonard et al., "Elastic and shear moduli of single-walled carbon nanotube ropes," *Physical Review Letters*, vol. 82, no. 5, pp. 944–947, 1998.
- [32] J. P. Salvetat, J. M. Bonard, N. B. Thomson et al., "Mechanical properties of carbon nanotubes," *Applied Physics A*, vol. 69, no. 3, pp. 255–260, 1999.
- [33] A. Krishnan, E. Dujardin, P. N. Yianilos, and M. M. J. Treacy, "Young's modulus of single-walled nanotubes," *Physical Review B*, vol. 58, no. 20, pp. 14013–14019, 1998.
- [34] M. F. Yu, B. S. Files, S. Arepalli, and R. S. Ruoff, "Tensile loading of ropes of single wall carbon nanotubes and their mechanical properties," *Physical Review Letters*, vol. 84, no. 24, pp. 5552–5555, 2000.
- [35] M. F. Yu, T. Kowalewski, and R. S. Ruoff, "Investigation of the radial deformability of individual carbon nanotubes under controlled indentation force," *Physical Review Letters*, vol. 85, no. 7, pp. 1456–1459, 2000.