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# IMPROVED THERMOELASTIC COEFFICIENTS OF A NOVEL SHORT FUZZY FIBER-REINFORCED COMPOSITE WITH WAVY CARBON NANOTUBES

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The elastic response of a novel short fuzzy fiber-reinforced composite (SFFRC) has recently been investigated by the authors (*Mech. Mater.* **53** (2012), 47–60). The distinctive feature of the construction of this novel SFFRC is that straight carbon nanotubes (CNTs) are radially grown on the circumferential surfaces of unidirectional short carbon fiber reinforcements. The waviness of CNTs is intrinsic to many manufacturing processes and plays an important role in the thermomechanical behavior of CNT-reinforced composites. However, the effect of the waviness of CNTs on the thermoelastic response of a SFFRC has yet to be investigated. Therefore, we investigate the effect of wavy CNTs on the thermoelastic properties of this SFFRC, revealing that the axial thermoelastic coefficients of the SFFRC significantly increase when the wavy CNTs are coplanar with the longitudinal plane of the carbon fibers for higher values of the waviness factor and wave frequency of the CNTs. The effective values of the thermal expansion coefficients of this SFFRC are also found to be sensitive to change in temperature.

A list of abbreviations and symbols can be found starting on page 21.

# 1. Introduction

Research on the synthesis of molecular carbon structures by an arc-discharge method for the evaporation of carbon led to the discovery of an extremely thin, needle-like graphitic carbon nanotube (CNT) [Iijima 1991]. Researchers probably thought that CNTs might be useful as nanoscale fibers for developing novel CNT-reinforced nanocomposites, and this conjecture motivated them to accurately study the physical properties (mechanical, thermal, and electrical) of CNTs. Numerous experimental and numerical studies revealed that the axial Young's modulus of CNTs is in the terapascal range [Treacy et al. 1996; Natsuki et al. 2004; Shen and Li 2004; Liu et al. 2005; Li and Guo 2008]. The quest for utilizing these exceptional mechanical properties of CNTs and their high aspect ratio led to the emergence of a new area of research on the development of CNT-reinforced nanocomposites [Odegard et al. 2003; Ashrafi and Hubert 2006; Seidel and Lagoudas 2006; Esteva and Spanos 2009; Ray and Batra 2009; Meguid et al. 2010; Khondaker and Keng 2012].

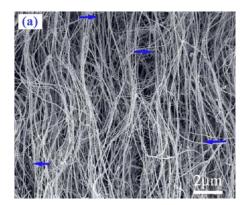
As nanoscale graphite structures, CNTs are of great interest not only for their mechanical properties but also for their thermal properties. For example, in several studies [Bandow 1997; Yosida 2000; Maniwa et al. 2001] the coefficients of thermal expansion (CTEs) of CNTs and their bundles are determined by using X-ray diffraction techniques. Bandow [1997] found that the CTE in the radial direction of multiwalled CNTs (MWCNTs) is almost the same as the CTE of graphite. Yosida [2000] and Maniwa

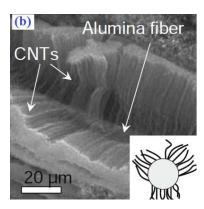
Keywords: short fuzzy fiber composite, wavy CNTs, micromechanics, thermoelastic coefficients.

et al. [2001] estimated the CTEs of single-walled CNT (SWCNT) bundles. Their results indicate that CNT bundles have a negative CTE at low temperatures and a positive CTE at high temperatures. Raravikar et al. [2002] estimated the CTEs of armchair (5, 5) and (10, 10) SWCNTs by using a molecular dynamics simulation (MDS) and found that the CTE of the CNT in the radial direction is less than that in the axial direction. Jiang et al. [2004] presented an analytical method to determine the CTEs of SWCNTs based on the interatomic potential and the local harmonic model. They found that all CTEs of SWCNTs are negative at low and room temperatures, and become positive at high temperatures. Kwon et al. [2004] performed a MDS and reported that the axial and radial CTEs of CNTs are nonlinear functions of change in temperature. Kirtania and Chakraborty [2009] presented a finite element (FE) analysis to estimate the CTEs of SWCNTs and demonstrated that the CTEs of SWCNTs increase uniformly with increase in the diameter of the SWCNT. The nonequilibrium Green's function method was employed by Jiang et al. [2009] to investigate the CTEs of SWCNTs and graphene. They found that the axial CTE is positive in the whole temperature range while the radial CTE is negative at low temperatures. Alamusi et al. [2012] investigated the axial CTEs of SWCNTs and MWCNTs by using a MDS, considering the effects of temperature and CNT diameter. For all CNTs, the obtained results revealed that axial CTEs are negative within a wide low-temperature range and positive in a high temperature range, and the temperature range for negative axial CTEs narrows as the diameter of the CNT decreases. Extensive research has also been carried out concerning the prediction of the CTEs of CNT-reinforced composites [Pipes and Hubert 2003; Kirtania and Chakraborty 2009]. In these studies, the results indicate that the addition of CNTs into the matrix causes significant improvement in the thermoelastic response of the CNT-reinforced composite as compared to that of the base composite.

It has been reported in many experimental studies [Shaffer and Windle 1999; Qian et al. 2000; Zhang et al. 2008; Yamamoto et al. 2009; Tsai et al. 2011] that CNTs are actually curved cylindrical tubes. The use of long CNTs in CNT-reinforced nanocomposites has revealed that CNT curvature significantly reduces the effective properties of the CNT-reinforced composite [Fisher et al. 2002; Berhan et al. 2004; Shi et al. 2004; Anumandla and Gibson 2006]. The effect of CNT curvature on the polymer matrix nanocomposite stiffness has been investigated by Pantano and Cappello [2008]. They concluded that in the presence of weak bonding, enhancement of the nanocomposite stiffness can be achieved through the bending energy of CNTs rather than through their axial stiffness. Li and Chou [2009] studied the failure of CNT/polymer matrix composites by using a micromechanics model and conducting FE simulations. They found that CNT waviness tends to reduce the elastic modulus and tensile strength of the nanocomposite but increases its ultimate strain. Farsadi et al. [2013] developed a three-dimensional FE model to investigate the influence of the waviness of the CNTs on the elastic moduli of a CNT-reinforced composite.

In addition to the waviness of CNTs, significant technical and manufacturing challenges have hindered the development of large-scale CNT-enhanced structures [Ajayan and Tour 2007; Schulte and Windle 2007]. Alignment, dispersion, and adhesion of CNTs in polymer matrices are vital for structural composite applications [Thostenson et al. 2001; Ajayan and Tour 2007; Schulte and Windle 2007]. More success can be achieved in improving the transverse multifunctional properties of hybrid CNT-reinforced composites by growing short CNTs on the circumferential surfaces of advanced fibers [Bower et al. 2000; Veedu et al. 2006; Qiu et al. 2007; Garcia et al. 2008]. For example, Veedu et al. [2006] developed a multifunctional composite in which CNTs are grown on the circumferential surfaces of the fibers and found that the presence of CNTs on the surfaces of the fibers reduces the effective CTE





**Figure 1.** Left: SEM image of vertically aligned curved CNTs (adapted with permission from [Zhang et al. 2008]). Right: SEM image of aligned CNTs grown on alumina fiber (adapted with permission from [Yamamoto et al. 2009]).

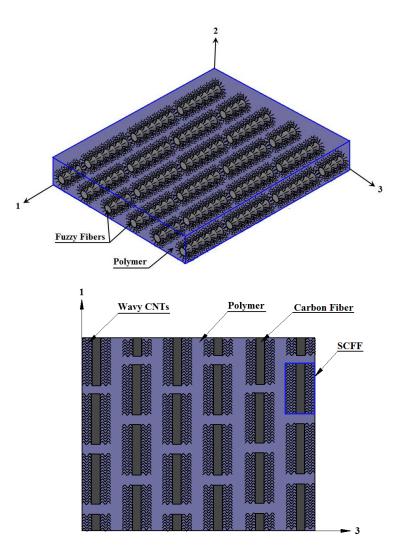
of the multifunctional composite up to 62% compared to that of the base composite (that is, without CNTs). Qiu et al. [2007] developed a multifunctional composite through an effective infiltration-based vacuum-assisted resin transfer moulding process. Their study indicated that the effective CTE of the multifunctional composite was reduced up to 25.2% compared with that of the composite without CNTs. A fiber coated with radially grown CNTs on its circumferential surface is called a "fuzzy fiber" [Garcia et al. 2008; Yamamoto et al. 2009; Chatzigeorgiou et al. 2012], and the resulting composite may be called a fuzzy fiber-reinforced composite (FFRC). Chatzigeorgiou et al. [2012] estimated the thermoelastic properties of fuzzy fiber composites in which a carbon fiber is coated with radially aligned straight CNTs by employing the asymptotic expansion homogenization method. They reported that the radial CTE of the fuzzy fiber composite is one order of magnitude less than its axial CTE. Recently, the elastic properties and the load transfer characteristics of a novel short fuzzy fiber-reinforced composite (SFFRC) have been extensively studied in [Kundalwal and Ray 2012; Kundalwal 2013].

Scanning electron microscopy (SEM) images analyzed in [Zhang et al. 2008] and [Yamamoto et al. 2009] are shown in Figure 1. They show clearly that CNTs remain highly curved when they are grown on the surfaces of advanced fibers. It is hypothesized that their affinity to becoming curved is due to their high aspect ratio and associated low bending stiffness. Since the addition of CNTs in hybrid CNT-reinforced composites influences the thermoelastic properties of the hybrid nanocomposites, the waviness of the CNTs may also affect the effective thermoelastic response of the SFFRC. However, the thermoelastic response of such a hybrid nanocomposite, being composed of short fuzzy fiber reinforcements coated with wavy CNTs, has not yet been investigated. Therefore, in this study we have endeavored to investigate the effect of waviness of CNTs on the effective thermoelastic properties of a SFFRC.

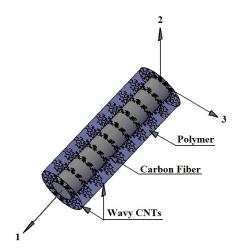
The outline is as follows: Section 2 briefly describes the architecture of the SFFRC containing wavy CNTs coplanar with either of the two mutually orthogonal planes. Section 3 presents the development of the Mori–Tanaka (MT) models for estimating the effective thermoelastic properties of the SFFRC and its constituent phases. In Section 4, numerical results are presented. Finally, Section 5 delineates the conclusions drawn from this study.

# 2. Architecture of a novel SFFRC

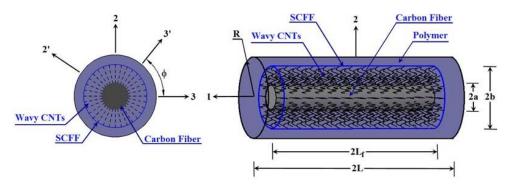
The top part of Figure 2 represents a lamina of a SFFRC in which the short fuzzy fibers are uniformly reinforced in the polymer matrix. Its in-plane cross section is illustrated in Figure 2, bottom. The short fuzzy fiber coated with sinusoidally wavy CNTs [Fisher et al. 2002; Berhan et al. 2004; Anumandla and Gibson 2006; Pantano and Cappello 2008; Zhang et al. 2008; Tsai et al. 2011; Farsadi et al. 2013] reinforced in the polymer matrix can be viewed as a circular cylindrical short composite fuzzy fiber (SCFF), as illustrated in Figure 3. The SCFFs are assumed to be uniformly dispersed over the volume of a lamina of the SFFRC in such a way that the three orthogonal principal material coordinate axes (1-2-3) exist in the composite as shown in Figure 2, top. The architecture of the representative volume element



**Figure 2.** Top: schematic diagram of a lamina made of the SFFRC containing wavy CNTs. Bottom: In-plane cross section of the SFFRC lamina. (Wavy CNTs are coplanar with the longitudinal plane of the carbon fiber.)



**Figure 3.** Fuzzy fiber coated with wavy CNTs reinforced in the polymer matrix (wavy CNTs are coplanar with the transverse plane of the carbon fiber).



**Figure 4.** Architecture of the RVE of the SFFRC in which the SCFF is embedded in the polymer material.

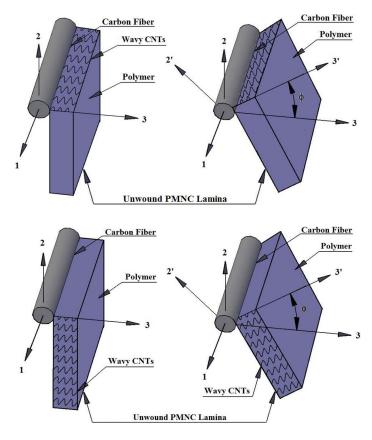
(RVE) of the SFFRC in which the SCFF embedded in the polymer material is schematically illustrated in Figure 4. The orientation of the plane of the wavy CNTs radially grown on the circumferential surface of the carbon fiber is an important issue because the planar orientations of the wavy CNTs may influence the thermoelastic properties of the SFFRC; this issue needs to be carefully addressed. Two possible planar orientations of the wavy CNTs are considered herein. The wavy CNTs are coplanar with either the longitudinal (that is, the 1-3 or 1'-3') or the transverse (that is, the 2-3 or 2'-3') plane of the carbon fiber, as shown in Figures 2 and 3, respectively. Investigation of the effect of all other planar orientations of the wavy CNTs is beyond the scope of the present study.

# 3. Modeling of the effective thermoelastic properties of a novel SFFRC and its constituent phases

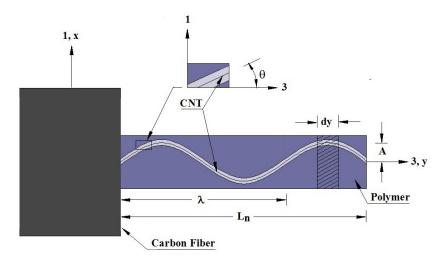
This section deals with the procedures of employing the MT model to predict the effective thermoelastic properties of the SFFRC and its constituent phases. The various steps involved in the computation of the effective thermoelastic properties of the SFFRC are outlined as follows.

- The first step in modeling the SFFRC is to determine the effective thermoelastic properties of a polymer matrix nanocomposite (PMNC) containing wavy CNTs coplanar with either the longitudinal (that is, the 1-3 or 1'-3') or the transverse (that is, the 2-3 or 2'-3') plane of the carbon fiber.
- Subsequently, considering the PMNC material as the matrix phase and the short carbon fibers as the reinforcement, the effective thermoelastic properties of the SCFF can be computed.
- Finally, using the effective thermoelastic properties of the SCFF and the polymer matrix, the effective thermoelastic properties of the SFFRC can be obtained.

**3.1.** Effective thermoelastic properties of the PMNC. From the constructional features of the SCFF, it may be seen that the carbon fiber is wrapped by a lamina of PMNC material, as illustrated in Figure 5. The average effective thermoelastic properties of the annular portion of the PMNC material surrounding the carbon fiber can be approximated by estimating the effective thermoelastic properties of the unwound lamina containing wavy CNTs. Hence, the effective elastic coefficient matrix  $[\overline{C}^{NC}]$  and the effective thermal expansion coefficient vector  $\{\overline{\alpha}^{NC}\}$  of the unwound lamina containing wavy CNTs are to be estimated a priori. Subsequently, appropriate transformations and homogenization procedures can be



**Figure 5.** Unwound lamina of PMNC containing wavy CNTs coplanar with the longitudinal (top) or transverse (bottom) plane of the carbon fiber.



**Figure 6.** RVE of unwound PMNC material containing a wavy CNT coplanar with the longitudinal (that is, 1-3) plane of the carbon fiber (adapted with permission from [Kundalwal and Ray 2013]).

carried out on  $[\overline{C}^{NC}]$  and  $\{\overline{\alpha}^{NC}\}$  to determine the effective thermoelastic properties of the annular portion of PMNC surrounding the carbon fiber.

Wavy CNTs coplanar with the longitudinal plane of the carbon fiber. We first consider the wavy CNTs to be coplanar with the longitudinal plane (the 1-3 or 1'-3' plane) of the carbon fiber, as shown in Figures 2 and 4, while computing the thermoelastic properties of the PMNC. An appropriate RVE of unwound PMNC material containing a wavy CNT can be considered to investigate the thermoelastic properties of the unwound PMNC material. Such an RVE is schematically illustrated in Figure 6. The RVE shown in Figure 6 can be divided into infinitesimally thin slices of thickness dy and each slice can be treated as an off-axis unidirectional lamina in which the CNT axis makes an angle  $\theta$  with the radial direction. The CNT waviness is assumed to be sinusoidal in the longitudinal plane of the carbon fiber and is defined by

$$x = A\sin(\omega y), \quad \omega = n\pi/L_n,$$
 (1)

in which A and  $L_n$  are the amplitude of the CNT wave and the linear distance between the CNT ends, respectively, and n represents the number of CNT waves. The running length,  $L_{nr}$ , of the CNT is given by

$$L_{nr} = \int_0^{L_n} \sqrt{1 + A^2 \omega^2 \cos^2(\omega y)} \, dy,$$
 (2)

where the angle  $\theta$  shown in Figure 6 is given by

$$\tan \theta = dx/dy = A\omega \cos(\omega y). \tag{3}$$

The effective thermoelastic properties at any point of any slice of the unwound lamina of PMNC containing sinusoidally wavy CNTs where the CNT axis makes an angle  $\theta$  with the radial direction (3 or 3') can be approximated by transforming the effective thermoelastic properties of the unwound lamina of PMNC containing straight CNTs. Hence, in what follows the MT model for predicting the effective

thermoelastic properties of the unwound lamina of PMNC with straight CNTs will be presented first. Due to difficulties in the atomistic modeling of CNTs inside the polymer matrix environment, researchers have considered CNTs as equivalent solid fibers for estimating the effective thermoelastic properties of CNT-reinforced composites [Fisher et al. 2002; Pipes and Hubert 2003; Berhan et al. 2004; Anumandla and Gibson 2006; Pantano and Cappello 2008; Tsai et al. 2011; Farsadi et al. 2013]. Thus, considering CNTs as solid fibers, the MT model [Mori and Tanaka 1973] can be utilized to estimate the effective elastic coefficient matrix  $[C^{nc}]$  of the unwound lamina of PMNC with straight CNTs [Benveniste 1987]:

$$[C^{nc}] = [C^p] + v_n([C^n] - [C^p])([\tilde{A}_1][v_p[I] + v_n[\tilde{A}_1]]^{-1}), \tag{4}$$

in which

$$[\tilde{A}_1] = [[I] + [S^n]([C^p])^{-1}([C^n] - [C^p])]^{-1},$$

where  $v_n$  and  $v_p$  represent the volume fractions of the CNT fiber and polymer material, respectively, present in the RVE of the PMNC. The square matrix  $[S^n]$  represents the Eshelby tensor for the cylindrical CNT. The elements of the Eshelby tensor  $[S^n]$  for the cylindrical CNT reinforcement in the isotropic polymer matrix are explicitly written as [Qiu and Weng 1990]

$$[S^{n}] = \begin{bmatrix} S_{1111}^{n} & S_{1122}^{n} & S_{1133}^{n} & 0 & 0 & 0 \\ S_{2211}^{n} & S_{2222}^{n} & S_{2233}^{n} & 0 & 0 & 0 \\ S_{3311}^{n} & S_{3322}^{n} & S_{3333}^{n} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{2323}^{n} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{1313}^{n} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{1212}^{n} \end{bmatrix},$$
 (5)

in which

$$S_{1111}^{n} = S_{2222}^{n} = \frac{5 - 4v^{p}}{8(1 - v^{p})}, \quad S_{3333}^{n} = 0, \qquad S_{1122}^{n} = S_{2211}^{n} = \frac{4v^{p} - 1}{8(1 - v^{i})},$$

$$S_{1133}^{n} = S_{2233}^{n} = \frac{v^{p}}{2(1 - v^{p})}, \quad S_{3311}^{n} = S_{3322}^{n} = 0, \quad S_{1313}^{n} = S_{2323}^{n} = 1/4, \qquad S_{1212}^{n} = \frac{3 - 4v^{p}}{8(1 - v^{p})},$$

where  $v^p$  denotes the Poisson's ratio of the polymer matrix.

Using the effective elastic coefficient matrix  $[C^{nc}]$ , the effective thermal expansion coefficient vector  $\{\alpha^{nc}\}$  for unwound PMNC with straight CNTs can be derived in the form of [Laws 1973] as

$$\{\alpha^{nc}\} = \{\alpha^n\} + ([C^{nc}]^{-1} - [C^n]^{-1})([C^n]^{-1} - [C^p]^{-1})^{-1}(\{\alpha^n\} - \{\alpha^p\}), \tag{6}$$

where  $\{\alpha^n\}$  and  $\{\alpha^p\}$  are the thermal expansion coefficient vectors of the CNT fiber and the polymer material, respectively. The effective elastic coefficient matrix  $[C^{NC}]$  and the effective thermal expansion coefficient vector  $\{\alpha^{NC}\}$  at any point of any slice of the unwound lamina of PMNC where the CNT is inclined at an angle  $\theta$  with the 3 (3')-axis can be derived by employing the appropriate transformations:

$$[C^{\text{NC}}] = [T_1]^{-T} [C^{nc}] [T_1]^{-1}, \quad \{\alpha^{\text{NC}}\} = [T_1]^{-T} \{\alpha^{nc}\},$$
 (7)

in which

$$[T_1] = \begin{bmatrix} k^2 & 0 & l^2 & 0 & kl & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ l^2 & 0 & k^2 & 0 & -kl & 0 \\ 0 & 0 & 0 & k & 0 & -l \\ -2kl & 0 & 2kl & 0 & k^2 - l^2 & -n \\ 0 & 0 & 0 & l & 0 & k \end{bmatrix},$$

with

$$k = \cos \theta = [1 + \{n\pi A/L_n \cos(n\pi y/L_n)\}^2]^{-1/2}$$

and

$$l = \sin \theta = n\pi A/L_n \cos(n\pi y/L_n) [1 + (n\pi A/L_n \cos(n\pi y/L_n))^2]^{-1/2}.$$

Subsequently, the average effective elastic coefficient matrix  $[\overline{C}^{NC}]$  and the thermal expansion coefficient vector  $\{\overline{\alpha}^{nc}\}$  of the lamina of unwound PMNC material containing wavy CNTs can be obtained by averaging the transformed elastic coefficients  $(C_{ij}^{NC})$  and the thermal expansion coefficients  $(\alpha_{ij}^{NC})$  over the linear distance between the CNT ends as [Hsiao and Daniel 1996]

$$[\overline{C}^{NC}] = \frac{1}{L_n} \int_0^{L_n} [C^{NC}] dy, \quad \{\overline{\alpha}^{NC}\} = \frac{1}{L_n} \int_0^{L_n} \{\alpha^{NC}\} dy.$$
 (8)

When the carbon fiber is viewed to be wrapped by such an unwound lamina of PMNC, the matrix  $[\overline{C}^{\text{NC}}]$  and the vector  $\{\overline{\alpha}^{\text{NC}}\}$  as given by (8) also provide the effective properties at a point located in the PMNC with respect to the 1'-2'-3' coordinate system, where the wavy CNT is grown at an orientation angle  $\phi$  with the 3-axis in the 2-3 plane as shown in Figures 4 and 5. Hence, at any point in the PMNC surrounding the carbon fiber, the effective elastic coefficient matrix  $[\overline{C}^{\text{PMNC}}]$  and the effective thermal expansion coefficient vector  $\{\overline{\alpha}^{\text{PMNC}}\}$  of the PMNC with respect to the 1-2-3 coordinate system turn out to be dependent on the CNT orientation angle  $\phi$  and can be determined by the following transformations:

$$[\overline{C}^{\text{PMNC}}] = [T]^{-T} [\overline{C}^{\text{NC}}] [T]^{-1}, \quad {\{\overline{\alpha}^{\text{PMNC}}\}} = [T]^{-T} {\{\overline{\alpha}^{\text{NC}}\}},$$
 (9)

where

$$[T] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & m^2 & n^2 & mn & 0 & 0 \\ 0 & n^2 & m^2 & -mn & 0 & 0 \\ 0 & -2mn & 2mn & m^2 - n^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & m & -n \\ 0 & 0 & 0 & 0 & n & m \end{bmatrix}, \quad \text{with } m = \cos \phi \text{ and } n = \sin \phi.$$

From (9) it is obvious that the effective thermoelastic properties at any point in the PMNC surrounding the carbon fiber with respect to the principle material coordinate axes of the SFFRC vary over the annular cross section of the PMNC phase of the RVE of the SCFF. However, without loss of generality, it may be considered that the volume average of these effective thermoelastic properties over the volume of the PMNC can be treated as the constant effective elastic coefficient matrix  $[C^{PMNC}]$  and the constant effective thermal expansion coefficient vector  $\{\alpha^{PMNC}\}$  of PMNC containing sinusoidally wavy CNTs

surrounding the carbon fiber with respect to the 1-2-3 coordinate axes of the SFFRC. These are given by

$$[C^{\text{PMNC}}] = \frac{1}{\pi (b^2 - a^2)} \int_0^{2\pi} \int_a^b [\overline{C}^{\text{PMNC}}] r \, dr \, d\phi,$$

$$\{\alpha^{\text{PMNC}}\} = \frac{1}{\pi (b^2 - a^2)} \int_0^{2\pi} \int_a^b \{\overline{\alpha}^{\text{PMNC}}\} r \, dr \, d\phi.$$
(10)

Thus the effective constitutive relations for the PMNC material surrounding the carbon fiber with respect to the principle material coordinate (1-2-3) axes of the SFFRC can be expressed as

$$\{\sigma^{\text{PMNC}}\} = [C^{\text{PMNC}}](\{\epsilon^{\text{PMNC}}\} - \{\alpha^{\text{PMNC}}\}\Delta T), \tag{11}$$

in which  $\Delta T$  represents the temperature deviation from a reference temperature.

Wavy CNTs coplanar with the transverse plane of the carbon fiber. Now the CNT waviness is assumed to be sinusoidal in the transverse plane (2-3 or 2'-3') of the carbon fiber, as shown in Figure 3, and is characterized by

$$z = A\sin(\omega y), \quad \omega = n\pi/L_n,$$
 (12)

in which the angle  $\theta$  shown in Figure 7 is given by

$$an \theta = dz/dy = A\omega \cos(\omega y). \tag{13}$$

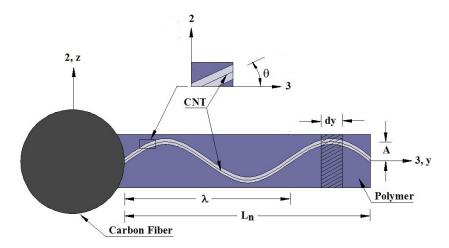
The procedure of utilizing the MT model presented in Section 3.1 for determining the effective thermoelastic properties of the unwound lamina of PMNC with straight CNTs can be utilized to estimate the effective thermoelastic properties of the unwound lamina of PMNC with wavy CNTs coplanar with the transverse plane of the carbon fiber. Once  $[C^{nc}]$  and  $\{\alpha^{nc}\}$  are computed by (4) and (6), respectively, the effective elastic coefficient matrix  $[C^{NC}]$  and the effective thermal expansion coefficient vector  $\{\alpha^{NC}\}$  at any point of any slice of the unwound lamina of PMNC where the CNT is inclined at an angle  $\theta$  with the 3 (3')-axis can be derived by employing the appropriate transformations for the wavy CNTs coplanar with the transverse plane of the carbon fiber:

$$[C^{\text{NC}}] = [T_2]^{-T} [C^{nc}] [T_2]^{-1}, \quad \{\alpha^{\text{NC}}\} = [T_2]^{-T} \{\alpha^{nc}\},$$
 (14)

in which

$$[T_2] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & k^2 & l^2 & kl & 0 & 0 \\ 0 & l^2 & k^2 & -kl & 0 & 0 \\ 0 & -2kl & 2kl & k^2 - l^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & k & -l \\ 0 & 0 & 0 & 0 & l & k \end{bmatrix}.$$

Subsequently, (8) and (10) can be used to estimate the effective elastic coefficient matrix  $[C^{PMNC}]$  and thermal expansion coefficient vector  $\{\alpha^{PMNC}\}$  of the PMNC material surrounding the carbon fiber when the wavy CNTs are coplanar with the transverse plane of the carbon fiber.



**Figure 7.** RVE of the unwound PMNC material containing a wavy CNT to be coplanar with the transverse plane (that is, 2-3 plane) of the carbon fiber (adapted with permission from [Kundalwal and Ray 2013]).

**3.2.** Effective thermoelastic properties of the SCFF. The second step in modeling the SFFRC is to estimate the effective thermoelastic properties of the SCFF. Utilizing the effective elastic properties of PMNC containing wavy CNTs derived in the previous section as the matrix material properties and with the carbon fiber aligned along the 1-direction as the reinforcement, the MT model presented for the unwound PMNC can be augmented to derive the effective elastic coefficient matrix  $[C^{SCFF}]$  of a lamina made of the SCFF:

$$[C^{\text{SCFF}}] = [C^{\text{PMNC}}] + \bar{v}_f([C^f] - [C^{\text{PMNC}}])([\tilde{A}_2][v_{\text{PMNC}}[I] + v_f[\tilde{A}_2]]^{-1}), \tag{15}$$

where

$$[\tilde{A}_2] = [[I] + [S_f]([C^{PMNC}])^{-1}([C^f] - [C^{PMNC}])]^{-1},$$

and where  $\bar{v}_f$  and  $v_{\text{PMNC}}$  are the volume fractions of the carbon fiber and PMNC, respectively, with respect to the volume of the RVE of the SCFF, and the Eshelby tensor,  $[S^f]$ , is determined based on the elastic properties of the PMNC and the shape of the carbon fiber. It should be noted that the PMNC material is transversely isotropic and, consequently, the Eshelby tensor [Li and Dunn 1998] corresponding to transversely isotropic material is utilized to compute the matrix  $[S^f]$ . The elements of the Eshelby tensor for the cylindrical carbon fiber embedded in the transversely isotropic PMNC material are explicitly given by [Li and Dunn 1998]:

$$[S^f] = \begin{bmatrix} S_{1111}^f & S_{1122}^f & S_{1133}^f & 0 & 0 & 0 \\ S_{2211}^f & S_{2222}^f & S_{2233}^f & 0 & 0 & 0 \\ S_{3311}^f & S_{3322}^f & S_{3333}^f & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{2323}^f & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{1313}^f & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{1212}^f \end{bmatrix},$$
(16)

in which

$$S_{1111}^f = S_{2222}^f = \frac{5C_{11}^{\text{PMNC}} + C_{12}^{\text{PMNC}}}{8C_{11}^{\text{PMNC}}}, \quad S_{1122}^f = S_{2211}^f = \frac{3C_{12}^{\text{PMNC}} - C_{11}^{\text{PMNC}}}{8C_{11}^{\text{PMNC}}}, \quad S_{1133}^f = S_{2233}^f = \frac{C_{13}^{\text{PMNC}}}{2C_{11}^{\text{PMNC}}}, \\ S_{3311}^f = S_{3322}^f = 0, \quad S_{1313}^f = S_{2323}^f = 1/4, \quad S_{3333}^f = 0, \quad S_{1212}^f = \frac{3C_{11}^{\text{PMNC}} - C_{12}^{\text{PMNC}}}{8C_{11}^{\text{PMNC}}}.$$

Using the effective elastic coefficient matrix [ $C^{\text{SCFF}}$ ], the effective thermal expansion coefficient vector { $\alpha^{\text{SCFF}}$ } for the SCFF can be determined as follows [Laws 1973]:

$$\{\alpha^{\text{SCFF}}\} = \{\alpha^f\} + ([C^{\text{SCFF}}]^{-1} - [C^f]^{-1})([C^f]^{-1} - [C^{\text{PMNC}}]^{-1})^{-1}(\{\alpha^f\} - \{\alpha^{\text{PMNC}}\}), \tag{17}$$

where  $[C^f]$  and  $\{\alpha^f\}$  are the elastic coefficient matrix and thermal expansion coefficient vector of the carbon fiber, respectively.

**3.3.** Effective thermoelastic properties of the SFFRC. Considering the SCFF as the cylindrical reinforcement embedded in the isotropic polymer matrix, the effective elastic properties [C] of the SFFRC can be determined by utilizing the MT model as follows:

$$[C] = [C^p] + v_{\text{SCFF}}([C^{\text{SCFF}}] - [C^p]) ([\tilde{A}_3][\bar{v}_P[I] + v_{\text{SCFF}}[\tilde{A}_3]]^{-1}), \tag{18}$$

in which

$$[\tilde{A}_3] = [I] + [S^{\text{SCFF}}]([C^p])^{-1}([C^{\text{SCFF}}] - [C^p])]^{-1}$$

and where  $v_{\text{SCFF}}$  and  $\bar{v}_p$  are the volume fractions of the SCFF and polymer material, respectively, with respect to the volume of the RVE of the SFFRC. The elements of the Eshelby tensor [ $S^{\text{SCFF}}$ ] for the cylindrical SCFF reinforcement in the isotropic polymer matrix are given by [Qiu and Weng 1990]

$$[S^{\text{SCFF}}] = \begin{bmatrix} S_{1111} & S_{1122} & S_{1133} & 0 & 0 & 0 \\ S_{2211} & S_{2222} & S_{2233} & 0 & 0 & 0 \\ S_{3311} & S_{3322} & S_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{1212} \end{bmatrix},$$
(19)

in which

$$S_{1111} = 0, \qquad S_{2222} = S_{3333} = \frac{5 - 4\nu^p}{8(1 - \nu^p)}, \quad S_{2211} = S_{3311} = \frac{\nu^p}{2(1 - \nu^p)},$$
 
$$S_{2233} = S_{3322} = \frac{4\nu^p - 1}{8(1 - \nu^p)}, \quad S_{1122} = S_{1133} = 0, \qquad S_{1313} = S_{1212} = 1/4, \qquad S_{2323} = \frac{3 - 4\nu^p}{8(1 - \nu^p)}.$$

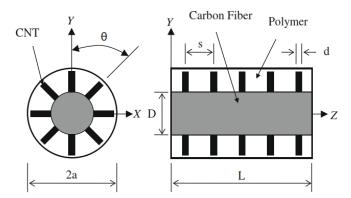
Finally, the effective thermal expansion coefficient vector  $\{\alpha\}$  of the SFFRC can be derived as [Laws 1973]

$$\{\alpha\} = \{\alpha^{\text{SCFF}}\} + ([C]^{-1} - [C^{\text{SCFF}}]^{-1})([C^{\text{SCFF}}]^{-1} - [C^p]^{-1})^{-1}(\{\alpha^{\text{SCFF}}\} - \{\alpha^p\}). \tag{20}$$

### 4. Results and discussion

In order to verify the validity of the MT model derived herein, the predictions of the MT model are first compared with the existing experimental and numerical results. Then the effective thermoelastic properties of the SFFRC containing wavy CNTs are determined by employing the MT model.

**4.1.** Comparison with experimental and numerical results. Recently, Kulkarni et al. [2010] experimentally and numerically investigated the elastic response of a nanoreinforced laminated composite (NRLC). The NRLC is made of CNT-reinforced polymer nanocomposite and carbon fiber. The cross sections of such NRLC are schematically shown in Figure 8. The geometry of the NRLC shown in Figure 8 is similar to that of the SCFF shown in Figure 3 if straight CNTs are considered. Thus, to confirm the modeling of the SCFF in the present study, we compare the results predicted by Kulkarni et al. [2010] for the NRLC with those predicted by the MT model for the SCFF with straight CNTs. It may be observed from Table 1 that the predicted value of the transverse Young's modulus  $(E_x)$  of the SCFF computed by the MT model matches closely with that of the experimental value predicted by Kulkarni et al. [2010]. The experimental value of  $E_x$  is lower than the theoretical prediction; this may be attributed to the fact that CNTs are not perfectly radially grown and straight, and hence the radial stiffening of the NRLC decreases [ibid.]. Further possible reasons for the disparity between the analytical and experimental results include lattice defects within CNTs [Ivanov et al. 2006; Yu et al. 2006] and the formation of voids in CNTreinforced composites [Grunlan et al. 2006; Borca-Tasciuc et al. 2007]. Also, the value of  $E_x$  predicted by the MT model utilized herein is much closer to the experimental value than that of the numerical value predicted by Kulkarni et al. [2010]. This is attributed to the fact that the appropriate transformation and homogenization procedures given by (9) and (10) have been employed in the present study, whereas they did not consider such transformation and homogenization procedures in their numerical modeling. These comparisons are significant since the prediction of the transverse Young's modulus of the SCFF provides a critical check on the validity of the MT model. Thus it can be inferred from the comparisons shown in Table 1 that the MT model can be reasonably applied to predict the elastic properties of the SFFRC and its phases.



**Figure 8.** Transverse and longitudinal cross sections of the NRLC (adapted with permission from [Kulkarni et al. 2010]).

| NRLC*       |            |               |          |  |  |
|-------------|------------|---------------|----------|--|--|
|             | Numerical* | Experimental* | MT model |  |  |
| $E_x$ (GPa) | 13.93      | 10.02         | 11.91    |  |  |
| $\nu_{xy}$  | 0.34       | _             | 0.38     |  |  |
| $\nu_{zx}$  | 0.16       | _             | 0.18     |  |  |

**Table 1.** Comparisons of the effective engineering constants of NRLC, 2% CNT and 41% IM7 carbon fiber, with those of SCFF containing straight CNTs.  $E_x$  is the transverse Young's modulus of the NRLC,  $v_{zx}$  and  $v_{xy}$  are the axial and transverse Poisson's ratios of the NRLC, respectively, and \* indicates data from [Kulkarni et al. 2010].

|                 | $E_{yy}$ (GPa)        |        | $E_{xx}$ (GPa) |       |  |
|-----------------|-----------------------|--------|----------------|-------|--|
| $w = A/\lambda$ | FE Model <sup>#</sup> | MT     | FE Model#      | MT    |  |
| 0               | 18                    | 17.800 | 4.577          | 4.448 |  |
| 0.005           | 17.920                | 17.790 | 4.574          | 4.448 |  |
| 0.010           | 17.780                | 17.800 | 4.570          | 4.446 |  |
| 0.015           | 17.690                | 17.750 | 4.566          | 4.445 |  |
| 0.020           | 17.570                | 17.720 | 4.563          | 4.442 |  |
| 0.025           | 17.480                | 17.680 | 4.561          | 4.440 |  |
| 0.030           | 17.130                | 17.630 | 4.559          | 4.435 |  |

**Table 2.** Comparisons of the engineering constants of unwound PMNC material with sinusoidally wavy CNTs, where  $^{\#}$  indicates data from [Farsadi et al. 2013], with  $E^n = 1030 \,\text{GPa}$ ,  $\nu^n = 0.063$ ,  $E^p = 3.8 \,\text{GPa}$ ,  $\nu^p = 0.4$ , and CNT volume fraction  $\nu_n = 0.014$ ; w is the waviness ratio, A and  $\lambda$  are the amplitude and the wavelength of the sinusoidally wavy CNT,  $E^n$  and  $E^p$  are the Young's moduli of the CNT and polymer matrix, respectively,  $E_{yy}$  and  $E_{xx}$  are the axial and transverse Young's moduli of unwound PMNC containing sinusoidally wavy CNTs, respectively, and  $\nu^n$  and  $\nu^p$  are the Poisson's ratios of the CNT and polymer matrix, respectively.

Next, the engineering constants of unwound PMNC containing sinusoidally wavy CNTs determined by the MT model are compared with those of the similar nanocomposite containing sinusoidally wavy CNTs studied by Farsadi et al. [2013]. Table 2 illustrates these comparisons. The two sets of results predicted by the FE and MT models are in excellent agreement, validating the MT model used in this study. The CTEs of unwound PMNC containing straight CNTs determined by the MT model are also compared with those of the similar CNT-reinforced composite studied by Kirtania and Chakraborty [2009], as shown in Table 3. For the effective values of CTEs of the CNT-reinforced composite, the two sets of results predicted by the FE and MT models are in excellent agreement, validating the MT model used here. It may also be observed from Tables 2 and 3 that the analytical MT model presented in this study requires much less computational time than the FE model. Thus one may use the analytical MT model for intuitive predictions of the effective thermoelastic properties of any novel advanced composites.

|       | $\alpha_1(\times 10^-)$ | $^{-6}  \mathrm{K}^{-1})$ | $\alpha_2(\times 10^{-6} \mathrm{K}^{-1})$ |         |  |
|-------|-------------------------|---------------------------|--|---------|--|
| $v_n$ | FE Model <sup>\$</sup>  | MT                        | FE Model <sup>\$</sup>                     | MT      |  |
| 0.5   | 25.2030                 | 24.4850                   | 69.7540                                    | 69.9030 |  |
| 1     | 15.3020                 | 15.0720                   | 72.8670                                    | 72.8790 |  |
| 3     | 5.0978                  | 5.1820                    | 74.7155                                    | 74.5120 |  |
| 5.45  | 2.2670                  | 2.2978                    | 73.5434                                    | 73.1220 |  |
| 7.9   | 1.0643                  | 1.1170                    | 71.7165                                    | 71.1300 |  |
| 10.3  | 0.4253                  | 0.4847                    | 69.7879                                    | 69.0140 |  |
| 15.77 | -0.3201                 | -0.2560                   | 65.1728                                    | 64.0370 |  |

Table 3. Comparisons of the CTEs of unwound PMNC material with straight CNTs, where \$\\$ indicates data from [Kirtania and Chakraborty 2009], with  $E^n = 1000 \, \text{GPa}$ ,  $v^n = 0.2$ ,  $E^p = 3.89$  GPa,  $v^p = 0.37$ ,  $\alpha^n = -1.5 \times 10^{-6}$  K<sup>-1</sup>, and  $\alpha^p = 58 \times 10^{-6}$  K<sup>-1</sup>;  $\alpha_1$  and  $\alpha_2$  are the axial and transverse CTEs of unwound PMNC with straight CNTs, respectively, and  $\alpha^n$  and  $\alpha^p$  are the CTEs of the CNT and polymer matrix, respectively.

**4.2.** Analytical modeling results. Armchair SWCNTs, carbon fiber, and polymer matrices are considered for evaluating the numerical results. Their material properties are taken from [Villeneuve et al. 1993; Peters 1998; Honjo 2007; Kwon et al. 2004; Shen and Li 2004] and are listed in Table 4. Since the investigations of earlier researchers [Yosida 2000; Maniwa et al. 2001; Jiang et al. 2004; Kwon et al. 2004; Jiang et al. 2009] have shown strong temperature dependence in the CTEs of CNTs, the variation in CTEs of the armchair (10, 10) CNT with temperature deviation is considered here. However, the elastic properties of CNTs, carbon fiber, and polymer are reported to be marginally dependent on the temperature deviation [Shen 2001]. Hence, the temperature dependence of the elastic properties of the constituent phases of the SFFRC is neglected. The relationships between the axial  $(\alpha_3^n)$  and transverse  $(\alpha_1^n)$  CTEs of the armchair (10, 10) CNT and the temperature deviation ( $\Delta T$ ) are given by [Kwon et al. 2004]:

$$\alpha_1^n = \alpha_2^n = 3.7601 \times 10^{-10} \Delta T^2 - 3.2189 \times 10^{-7} \Delta T - 3.2429 \times 10^{-8} \text{ K}^{-1},$$

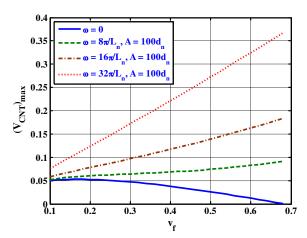
$$\alpha_3^n = 6.4851 \times 10^{-11} \Delta T^2 - 5.8038 \times 10^{-8} \Delta T + 9.0295 \times 10^{-8} \text{ K}^{-1}.$$
(21)

$$\alpha_3^n = 6.4851 \times 10^{-11} \Delta T^2 - 5.8038 \times 10^{-8} \Delta T + 9.0295 \times 10^{-8} \,\mathrm{K}^{-1}.$$
 (22)

For the SFFRC, the hexagonal packing array of the SCFFs is considered for evaluating the numerical results. The maximum value of the CNT volume fraction in the SFFRC can be determined based on the

| Material                    | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{23}$ | $C_{33}$ | $C_{66}$ | $\alpha_1$ | $\alpha_2$ |                 |
|-----------------------------|----------|----------|----------|----------|----------|----------|------------|------------|-----------------|
| $(10, 10) \text{ CNT}^a$    | 288      | 254      | 87.8     | 87.8     | 1088     | 17       | b          | b          | $d_n = 0.00136$ |
| Carbon fiber <sup>c,d</sup> | 236.4    | 10.6     | 10.6     | 10.7     | 24.8     | 25       | 1.1        | 6.8        | 2a = 10         |
| Polymer <sup>e</sup>        | 4.09     | 1.55     | 1.55     | 1.55     | 4.09     | 1.27     | 66         | 66         |                 |

**Table 4.** Material properties of the constituent phases of the SFFRC, where <sup>a</sup> indicates data from [Shen and Li 2004], <sup>c</sup> [Honjo 2007], <sup>d</sup> [Villeneuve et al. 1993], and <sup>e</sup> [Peters 1998]. The values of  $\alpha_1$  and  $\alpha_2$  of the armchair (10, 10) CNT marked with <sup>b</sup> are from [Kwon et al. 2004] and are given in the text. Values of C are in units of GPa,  $\alpha$  in  $10^{-6} \,\mathrm{K}^{-1}$ , and  $d_n$  and a in  $\mu \mathrm{m}$ .



**Figure 9.** Variation of the maximum CNT volume fraction with the carbon fiber volume fraction in the SFFRC.

surface to surface distance at the roots of the two adjacent CNTs (0.0017  $\mu$ m), the CNT diameter ( $d_n$ ), and the running length of the sinusoidally wavy CNT ( $L_{nr}$ ) as [Kundalwal and Ray 2013]

$$(V_{\text{CNT}})_{\text{max}} = \frac{\pi d_n^2 L_{nr}}{d(d_n + 0.0017)^2} v_f,$$
(23)

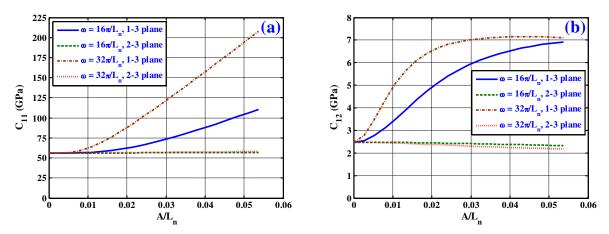
where  $d_n$  is the diameter of the CNT in  $\mu$ m. The derivation of (23) can be found in [Kundalwal and Ray 2013]. It is evident from (2) and (23) that an increase in the amplitude of the CNT increases the running length of the CNT which eventually increases the maximum CNT volume fraction  $(V_{\text{CNT}})_{\text{max}}$  in the SFFRC. Figure 9 illustrates the variation of the maximum value of the CNT volume fraction in the SFFRC with the carbon fiber volume fraction  $(v_f)$  while the values of the wave frequency  $(\omega)$  vary from  $\omega = 8\pi/L_n$  to  $\omega = 32\pi/L_n$ . As expected, the maximum value of the CNT volume fraction in the SFFRC increases with the increase in the values of  $v_f$  and  $\omega$ . To investigate the effect of wavy CNTs on the thermoelastic properties of the SFFRC, the value of  $\omega$  is varied while keeping the value of  $v_f$  as 0.3, and adopting the following values of the other geometrical parameters of the RVE of the SFFRC:

- diameter of the armchair (10, 10) SWCNT  $d_n = 0.00136 \,\mu\mathrm{m}$  [Shen and Li 2004],
- radius of the carbon fiber  $a = 5 \mu m$ ,
- radius of the RVE of the SFFRC  $R = 8.2888 \,\mu\text{m}$ ,
- radius of the SCFF  $b = 7.5353 \,\mu\text{m}$ ,
- half-length of the carbon fiber  $L_f = 100 \,\mu\text{m}$ ,
- half-length of the RVE of the SFFRC  $L = 110 \,\mu\text{m}$ ,
- length of the straight CNT  $L_n = 2.5353 \,\mu\text{m}$ ,
- maximum amplitude of the wavy CNT  $A = 100d_n \mu m$ ,
- maximum waviness factor  $A/L_n = 0.0536 \,\mu\text{m}$ .

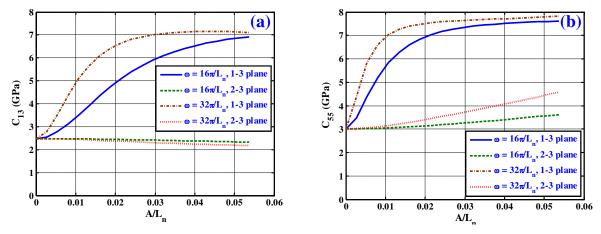
First, the effective thermoelastic coefficients of the PMNC for different values of  $\omega$  of the CNT are computed by employing the MT model. The estimated effective thermoelastic properties of the PMNC

are then used to compute the effective thermoelastic properties of a SCFF in which the carbon fiber is the reinforcement and the matrix phase is the PMNC material. However, for the sake of brevity, the effective thermoelastic properties of the PMNC and SCFF are not presented here. Unless otherwise mentioned, the two fixed values of  $\omega$  ( $\omega = 16\pi/L_n$  and  $\omega = 32\pi/L_n$ ) are considered for evaluating the results.

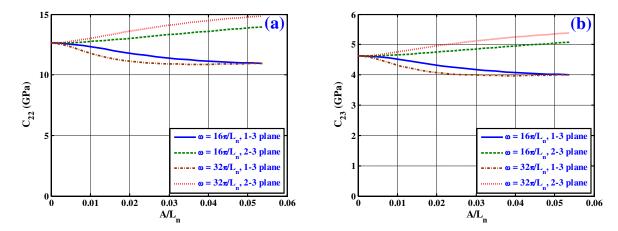
Figure 10 illustrates the variation of the effective elastic coefficients  $C_{11}$  and  $C_{12}$  of the SFFRC with waviness factor  $A/L_n$ . It may be observed from Figure 10(a) that the effective values of  $C_{11}$  of the SFFRC are not affected by variations of the amplitude of the wavy CNTs in the 2-3 plane. When the wavy CNTs are coplanar with the 1-3 plane, increase in the values of  $A/L_n$  and  $\omega$  significantly increases  $C_{11}$ . Figure 10(b) reveals that the waviness of the CNTs causes a significant increase in the value of  $C_{12}$  when the wavy CNTs are coplanar with the 1-3 plane. Figure 11 demonstrates the variation of the values of  $C_{13}$  and  $C_{55}$  of the SFFRC with the waviness factor. Since the SFFRC is transversely isotropic material, the values of  $C_{13}$  are found to be identical to those of  $C_{12}$ , as shown in Figures 10(b)



**Figure 10.** Variation of the effective elastic coefficients (a)  $C_{11}$  and (b)  $C_{12}$  of the SF-FRC with waviness factor ( $v_f = 0.3$ , ( $V_{\text{CNT}}$ )<sub>max</sub>).



**Figure 11.** Variation of the effective elastic coefficients (a)  $C_{13}$  and (b)  $C_{55}$  of the SF-FRC with waviness factor ( $v_f = 0.3$ , ( $V_{\text{CNT}}$ )<sub>max</sub>).

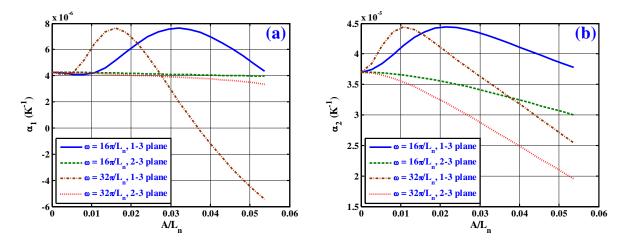


**Figure 12.** Variation of the effective elastic coefficients (a)  $C_{22}$  and (b)  $C_{23}$  of the SF-FRC with waviness factor ( $v_f = 0.3$ , ( $V_{\text{CNT}}$ )<sub>max</sub>).

and 11(a). It may be observed from Figure 11(b) that the value of  $C_{55}$  of the SFFRC initially increases significantly, and then stabilizes for higher values of  $A/L_n$ , when the wavy CNTs are coplanar with the 1-3 plane. Figure 12(a) reveals that increase in the value of  $A/L_n$  decreases  $C_{22}$  when the CNT waviness is coplanar with the 1-3 plane, whereas the value of  $C_{22}$  increases for higher values of  $A/L_n$  when the CNT waviness is coplanar with the 2-3 plane. A similar trend is obtained for the value of  $C_{23}$ , as shown in Figure 12(b). Although not presented here, the same is true for the effective elastic coefficient  $C_{44}$ .

It may be noted from Figures 10–12 that if the wavy CNTs are coplanar with the 1-3 plane then the axial elastic coefficients of the SFFRC are significantly improved over their values with straight CNTs ( $\omega=0$ ) for higher values of  $A/L_n$  and  $\omega$ . When the wavy CNTs are coplanar with the longitudinal plane (1-3 or 1'-3' plane) of the carbon fiber, as shown in Figure 2, the amplitudes of the CNT waves becomes parallel to the 1-axis, which results in the aligning of the projections of parts of the CNT lengths with the 1-axis leading to axial stiffening of the PMNC. The greater the value of  $\omega$ , the more such projections will occur, and hence the effective axial elastic coefficients ( $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ ,  $C_{55}$ , and  $C_{66}$ ) of the SFFRC increase with an increase in the value of  $\omega$ . On the other hand, if the wavy CNTs are coplanar with the transverse plane (2-3 or 2'-3' plane) of the carbon fiber, then the transverse elastic coefficients ( $C_{22}$ ,  $C_{23}$ ,  $C_{33}$ , and  $C_{44}$ ) of the SFFRC increase from their values with straight CNTs ( $\omega=0$ ). The reverse is true when the wavy CNTs are coplanar with the 1-3 (1'-3') plane.

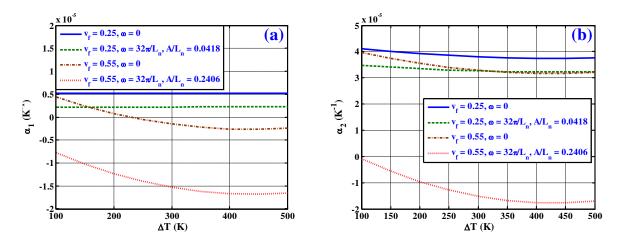
Figure 13 illustrates the variation in the axial ( $\alpha_1$ ) and transverse ( $\alpha_2$ ) CTEs of the SFFRC with the waviness factor. It may be observed from Figure 13(a) that the values of  $\alpha_1$  of the SFFRC are not affected by variations in the amplitude of the wavy CNTs in the 2-3 plane, whereas the value of  $\alpha_1$  initially increases and then significantly decreases for higher values of  $A/L_n$  and  $\omega$  when the CNT waviness is coplanar with the 1-3 plane. It is also important to note from Figure 13(a) that the effective value of  $\alpha_1$  is zero for  $A/L_n$  and  $\omega$  as 0.037 and  $32\pi/L_n$ , respectively, when the wavy CNTs are coplanar with the 1-3 plane. Figure 13(b) reveals that the waviness of the CNTs improves the effective values  $\alpha_2$  of the SFFRC when the wavy CNTs are coplanar with the 2-3 plane, compared to those of the SFFRC with straight CNTs ( $\omega = 0$ ). Although not presented here, the computed effective values of  $\alpha_3$  are found to match identically with those of  $\alpha_2$ , corroborating the fact that the SFFRC is transversely isotropic material.



**Figure 13.** Variation of the effective (a) axial  $(\alpha_1)$  and (b) transverse  $(\alpha_2)$  CTEs of the FFRC with waviness factor  $(\Delta T = 300 \ K, v_f = 0.3, (V_{\text{CNT}})_{\text{max}})$ .

Note from (20) that the CTEs of the SFFRC are dependent on the elastic coefficients of the SFFRC. Hence, with the increase in the value of  $A/L_n$  up to  $\sim 0.013$ , the axial elastic coefficients of the unwound PMNC are increased which eventually influences the effective CTEs of the unwound PMNC when the CNT waviness is coplanar with the 1-3 plane. Therefore, the effective CTEs ( $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$ ) of the FFRC are initially increased for lower values of  $A/L_n$ . For  $A/L_n \ge 0.013$ , the effective CTEs ( $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$ ) of the SFFRC with wavy CNTs coplanar with the 1-3 plane start to decrease. This is attributed to the fact that the negative axial and transverse CTEs  $(\alpha_1^n \text{ and } \alpha_3^n)$  of the radially grown wavy CNTs on the circumferential surfaces of the carbon fibers significantly suppress the positive CTE  $(\alpha^p = 66 \times 10^{-6} \, \mathrm{K}^{-1})$  of the polymer matrix, which eventually lowers the effective values of  $\alpha_1$  of the SFFRC. This effect becomes more pronounced for higher values of  $A/L_n$  and  $\omega$  because the CNT volume fraction in the SFFRC increases with  $A/L_n$  and  $\omega$ , as depicted in Figure 9. From Figures 10–13 it is important to note that the axial thermoelastic coefficients significantly improve for higher values of  $A/L_n$  and  $\omega$  when the CNT waviness is coplanar with the 1-3 plane. The effect of wavy CNTs coplanar with the 2-3 plane on the axial thermoelastic coefficients of the SFFRC is not as pronounced. On the other hand, marginal improvement in the transverse thermoelastic coefficients of the SFFRC is observed when the CNT waviness is coplanar with the 2-3 plane. Hence, for investigating the effect of temperature deviation on the effective thermal expansion coefficients of the SFFRC, the wavy CNTs are considered to be coplanar with the 1-3 plane when the values of  $\omega$  and A are  $32\pi/L_n$  and  $0.136 \,\mu$ m, respectively.

Practically, the carbon fiber volume fraction in short fiber composites can vary, typically from 0.2 to 0.6. Hence, to analyze the effect of temperature deviation on the effective thermal expansion coefficients of the SFFRC, the two discrete values of the carbon fiber volume fraction are considered, 0.25 and 0.55. Figure 14(a) and (b) illustrate the variation of the values of  $\alpha_1$  and  $\alpha_2$  of the SFFRC, respectively, with the temperature deviation for different values of the carbon fiber volume fraction. It is important to note from these figures that the effective values of CTEs of the SFFRC decrease with the increase in the temperature deviation for higher values of  $v_f$  and  $\omega$ . It may also be observed that wavy CNTs coplanar with the 1-3 plane significantly improve the CTEs of the SFFRC over the values with straight CNTs



**Figure 14.** Variation of the effective (a) axial ( $\alpha_1$ ) and (b) transverse ( $\alpha_2$ ) CTEs of the SFFRC with temperature deviation when the wavy CNTs are coplanar with the longitudinal plane (that is, 1-3 plane) of the carbon fiber ( $A = 0.136 \,\mu\text{m}$ ).

 $(\omega=0)$ . This is attributed to the fact that as the values of  $v_f$  and  $\omega$  increase the CNT volume fraction in the SFFRC increases, as shown in Figure 9, which eventually improves the values of the CTEs of the SFFRC. It is also seen from these two plots that the CTEs of the SFFRC can be modified by changing the values of  $A/L_n$  and  $\omega$  according to the requirements of thermal management.

## 5. Conclusions

The effective thermoelastic properties of a novel short fuzzy fiber-reinforced composite (SFFRC) containing wavy carbon nanotubes (CNTs) have been investigated. An analytical micromechanics model based on the Mori–Tanaka model was utilized to predict the effective thermoelastic coefficients of this novel composite. The influence of the waviness of the CNTs on the thermoelastic coefficients of the SFFRC has been studied, considering sinusoidally wavy CNTs to be coplanar with either of two mutually orthogonal planes. The following main conclusions can be drawn from the investigations carried out here.

- (1) If the plane of the radially grown wavy CNTs is coplanar with the longitudinal plane of the carbon fiber then the axial effective thermoelastic coefficients of the SFFRC are significantly improved over those of the FFRC with either straight CNTs ( $\omega = 0$ ) or wavy CNTs coplanar with the transverse plane of the carbon fiber.
- (2) When the CNT waviness is coplanar with the transverse plane of the carbon fiber, marginal improvement has been observed in the transverse effective thermoelastic coefficients of the SFFRC.
- (3) If the CNT waviness is coplanar with the longitudinal plane of the carbon fiber then the thermoelastic response of the SFFRC significantly improves with an increase in the temperature for higher values of the carbon fiber volume fraction, waviness factor, and wave frequency of the CNT.

Therefore, the SFFRC with sinusoidally wavy CNTs studied here may be used for advanced structures that require stringent constraints on dimensional stability.

# List of abbreviations

| CNT          | Carbon nanotube                  | NRLC         | Nanoreinforced laminated composite     |
|--------------|----------------------------------|--------------|--|
| CTE          | Coefficient of thermal expansion | <b>PMNC</b>  | Polymer matrix nanocomposite           |
| CVD          | Chemical vapor deposition        | RVE          | Representative volume element          |
| FE           | Finite element                   | SCFF         | Short composite fuzzy fiber            |
| MDS          | Molecular dynamics simulation    | SEM          | Scanning electron microscopy           |
| MT           | Mori–Tanaka                      | SFFRC        | Short fuzzy fiber-reinforced composite |
| <b>MWCNT</b> | Multiwalled carbon nanotube      | <b>SWCNT</b> | Single-walled carbon nanotube          |

# List of symbols

|   | 2220 02 5/ 2220 022   |
|---|---|
| A   | Amplitude of the CNT ( $\mu$ m)   |
| $[\tilde{A}_1], [\tilde{A}_2], [\tilde{A}_3]$ | Matrices of the strain concentration factors  |
| a   | Radius of the carbon fiber ( $\mu$ m)   |
| b   | Radius of the SCFF ( $\mu$ m)   |
| $[\overline{C}^{	ext{NC}}]$                   | Elastic coefficient matrix of the unwound PMNC containing wavy CNTs (GPa)                                     |
| $[C^r]$                                       | Elastic coefficient matrix of the $r$ -th phase (GPa)   |
| $C_{ij}^r$                                    | Elastic coefficients of the $r$ -th phase (GPa)   |
| $d_n$   | Diameter of the CNT ( $\mu$ m)  |
| $E^n$ and $E^p$                               | Young's moduli of the CNT and polymer matrix, respectively (GPa)  |
| $E_x$   | Transverse Young's modulus of the NRLC (GPa)  |
| $E_{yy}$ and $E_{xx}$                         | Axial and transverse Young's moduli of the unwound PMNC containing sinusoidally wavy CNTs, respectively (GPa) |
| [I]   | Fourth-order identity matrix  |
| L   | Length of the RVE of the SFFRC ( $\mu$ m)   |
| $L_f$   | Half-length of the short carbon fiber embedded in the RVE of the SFFRC ( $\mu$ m)                             |
| $L_n$   | Length of straight CNT ( $\mu$ m)   |
| $L_{nr}$                                      | Running length of sinusoidally wavy CNT ( $\mu$ m)  |
| $(N_{\rm CNT})_{\rm max}$                     | Maximum number of radially grown aligned CNTs on the circumferential surface of the short carbon fiber        |
| n   | Number of waves of a sinusoidally wavy CNT along its axial direction  |
| R   | Radius of the RVE of the SFFRC ( $\mu$ m)   |
| $[S^r]$                                       | Eshelby tensor of the <i>r</i> -th domain   |
| $S_{ij}^r$                                    | Elements of the Eshelby tensor of the <i>r</i> -th domain   |
| $[T], [T_1], [T_2]$                           | Transformation matrices   |
| $(V_{\rm CNT})_{\rm max}$                     | Maximum volume fraction of the CNT in the SFFRC   |
| $v_{ m SCFF}$                                 | Volume fraction of the SCFF in the SFFRC  |
| $v_f$   | Volume fraction of the carbon fiber in the SFFRC  |
| $ar{v}_f$                                     | Volume fraction of the carbon fiber in the SCFF   |
| $v_m$   | Volume fraction of the matrix in the composite  |
| $v_n$   | Volume fraction of the CNT in the PMNC/the CNT-reinforced nanocomposite                                       |
|   |   |

| $v_{ m PMNC}$         | Volume fraction of the PMNC in the SCFF   |
|-----------------------|---|
| $v_P$                 | Volume fraction of the polymer in the PMNC  |
| $ar{v}_P$             | Volume fraction of the polymer in the SFFRC   |
| $v_{ m SCFF}$         | Volume fraction of the SCFF in the SFFRC  |
| $\{\alpha\}$          | Thermal expansion coefficient vector of the SFFRC (K <sup>-1</sup> )                                      |
| $\{\alpha^r\}$        | Thermal expansion coefficient vector of the $r$ -th phase $(K^{-1})$                                      |
| $\alpha_i^r$          | Thermal expansion coefficients of the $r$ -th phase $(K^{-1})$  |
| $\Delta T$            | Temperature deviation from the reference temperature (K)  |
| $\{\epsilon^r\}$      | Strain vector of the <i>r</i> -th phase   |
| λ                     | Wavelength of the CNT (nm)  |
| $v^n$ and $v^p$       | Poisson's ratios of the CNT and polymer matrix, respectively  |
| $v_{zx}$ and $v_{xy}$ | Axial and transverse Poisson's ratios of the unwound PMNC containing sinusoidally wavy CNTs, respectively |
| $\{\sigma^r\}$        | Stress vector of the <i>r</i> -th phase (GPa)   |
| ω                     | Wave frequency of the CNT $(\mu m^{-1})$  |

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