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Micromechanics modelling of the effective thermoelastic response of nano-tailored composites

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ABSTRACT

Owing to their remarkable thermoelastic and scale-dependent physical properties, carbon nanotubes (CNTs) have emerged as promising reinforcements to enhance the thermomechanical response of nano-tailored composite materials. Two fundamental aspects influencing the thermoelastic response of a nano-tailored composite are investigated herein; namely, CNT waviness and the existence of an interphase between a CNT and the polymer matrix. We propose a systematic micromechanical modelling scheme in conjunction with a new interphase model to determine the coefficients of thermal expansion (CTEs) of a nano-tailored composite. The proposed modelling approach has been applied to a case study involving the need to determine the effective CTEs of a novel nano-tailored composite—*fuzzy carbon fiber heat exchanger*. The results reveal that (i) the interphase between a CNT and the surrounding polymer matrix plays a crucial role in the modelling of the thermoelastic properties of the CNT-based composite, (ii) planar orientation of CNT waviness has a significant influence on the effective CTEs of the hybrid nano-tailored composite, and (iii) for the particular planar orientation of CNT waviness and the value of CNT wave frequency, the effective CTEs of the hybrid nano-tailored composite become zero, making the nanocomposite a "super-insulator".

1. Introduction

The quest for utilizing the remarkable mechanical and thermal properties of CNTs (Ruoff and Lorents, 1995; Treacy et al., 1996; Bandow, 1997; Yosida, 2000; Maniwa et al., 2001; Kwon et al., 2004; Shen and Li, 2004; Tsai et al., 2010) has led to the emergence of a new area of research that involves the development of nano-tailored composites (Odegard et al., 2003; Pipes and Hubert, 2003; Seidel and Lagoudas, 2006; Veedu et al., 2006; Hammerand et al., 2007; Kirtania and Chakraborty, 2009; Kulkarni et al., 2010; Meguid et al., 2010; Shokrieh and Rafiee, 2010; Tsai et al., 2010; Wernik and Meguid, 2010; Wernik et al., 2012; Jam et al., 2013). These studies revealed that the addition of a small fraction of CNTs into a polymer matrix introduces significant improvement in the multifunctional properties of micro- and nano-hybrid nanocomposites. More success can be achieved in improving the multifunctional properties of the hybrid nano-tailored composites by growing CNTs on the surfaces of substrates and advanced fibers. Dense aligned arrays of CNTs are specially promising for a number of applications as this morphology organizes CNTs thereby enabling enhanced utilization of their remarkable properties (Veedu et al., 2006; Garcia et al., 2008; Kulkarni et al., 2010; Ray and Kundalwal, 2013). Recently, a "fuzzy fiber" concept has been utilized by Kundalwal et al. (2014) to propose a two-layered fuzzy carbon fiber heat exchanger (FFHE) in which CNTs are radially grown on the outer circumferential surface of the hollow cylindrical carbon fiber (HCF). Their study revealed that the effective thermal conductivities of the FFHE are significantly improved by several orders of magnitude at low CNT volume fractions over those of the bare HCF heat exchanger (that is, without CNTs). Thus, the current status of progress in research on CNT-reinforced composites brings to light that the hybrid CNT-based nano-tailored composites can be the promising candidate material for developing multifunctional nanocomposite architectures those found a wide range of engineering applications in microelectronics, aerospace and automobile sectors.

The performance of a nanocomposite material is critically controlled by the interfacial bonding between a CNT and the surrounding matrix material. Using Raman scattering and X-ray

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diffraction, Chang et al. (2000) showed that there is no chemical bonding exists between a CNT and the surrounding polymer matrix. In this case, only non-bonded electrostatic and van der Waals (vdW) interactions are considered between a CNT and the surrounding polymer matrix (Lordi and Yao, 2000; McCarthy et al., 2000; Liao and Li, 2001). Electrostatic interactions can be neglected in comparison to vdW interactions, due to the fact that vdW interactions contribute more significantly in three higher orders of magnitude than electrostatic energy (Liao and Li, 2001; Gou et al., 2004; Wei, 2006). In order to estimate the effective thermoelastic properties of the CNT-reinforced composite, the consideration of vdW interactions between a CNT and the surrounding polymer matrix, is an important issue. In several research studies (Ji et al., 2010; Odegard et al., 2003; Shen and Li, 2005; Seidel and Lagoudas, 2006; Hammerand et al., 2007; Montazeri and Naghdabadi, 2010; Shokrieh and Rafiee, 2010; Tsai et al., 2010; Li et al., 2011; Jam et al., 2013), an equivalent solid continuum interphase is considered between a CNT and the polymer matrix which characterizes vdW interactions. There are two main approaches in developing models to determine the effective properties of the nanocomposite; namely, two- and three-phase models, without and with considering the CNT/matrix interphase. Ji et al. (2010) have compared the results of several analytical two-phase models with those of experimental results and found that there is no good agreement exists between analytical and experimental results if the interphase is neglected. On the other hand, the predictions by three-phase models are found to be in more agreement with experimental results than those of two-phase models (Wise and Hinkley, 2001; Ray and Garnich, 2004; Lurie et al., 2005; Nie and Basaran, 2005; Wan et al., 2005). This is due to the fact that a thin interphase usually possesses higher elastic properties than those of the surrounding polymer matrix owing to the restricted mobility of polymer chains (Donnet and Vidal, 1986; Theocaris, 1987; Shen and Li, 2005). Accordingly, our work considers the effect of the CNT/polymer matrix interphase upon the effective CTEs of the CNT-reinforced composite. To the best of authors' knowledge, there are no CTE data currently available for the CNT/polymer matrix interphase. Therefore, in this study, we have endeavoured to develop an interphase model for estimating the thermoelastic properties of the interphase.

Carbon nanotube waviness is inherent to the fabrication process of CNT-reinforced polymer composites. Scanning electron microscopy (SEM) images shown in Refs. (Berhan et al., 2004; Yamamoto et al., 2009; Vo et al., 2012) clearly demonstrate that CNTs remain highly curved when they are either embedded in the polymer matrix or grown on the circumferential surface of the fiber. Several research studies reported that CNT waviness influences the effective thermoelastic properties of micro- and nano-hybrid nanocomposites; see, e.g., Refs. (Fisher et al., 2002; Berhan et al., 2004; Tsai et al., 2011; Farsadi et al., 2012; Handlin et al., 2013; Kundalwal and Ray, 2013, 2014). It is therefore the objective of this work to develop a novel micromechanics approach for determining the effective CTE of hybrid nano-tailored composite to account for the influence of the CNT/polymer matrix interphase and CNT waviness. The developed micromechanical modelling approach is applied to a case study involving the need to determine the effective CTEs of a novel FFHE made of nanocomposite.

2. The interphase model

The thermoelastic properties of the interphase can be determined by a general function that varies in the radial direction (Jasiuk and Kouider, 1993; Chouchaoui and Benzeggagh, 1997; Wacker et al., 1998; Ji et al., 2010; Shen and Li, 2005). The variation in the thermoelastic properties of the interphase is assumed to satisfy the following conditions,

$$\left[C^{i}\right]\Big|_{r=r_n} = [C^{n}]|_{r=r_n},\ \left[C^{i}\right]\Big|_{r=r_i} = [C^{p}]|_{r=r_i},\ \left\{\alpha^{i}\right\}\Big|_{r=r_n} = \{\alpha^{n}\}|_{r=r_n} \ \text{and} \ \left\{\alpha^{i}\right\}\Big|_{r=r_i} = \{\alpha^{p}\}|_{r=r_i} \tag{1}$$

The general form of tensors appearing in Eq. (1) are given by

$$\left[C^{k}\right] = \begin{bmatrix} C^{k}_{11} & C^{k}_{12} & C^{k}_{13} & 0 & 0 & 0 \\ C^{k}_{12} & C^{k}_{22} & C^{k}_{23} & 0 & 0 & 0 \\ C^{k}_{13} & C^{k}_{23} & C^{k}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C^{k}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C^{k}_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C^{k}_{66} \end{bmatrix} \ \text{and} \quad \left\{\alpha^{k}\right\} = \begin{Bmatrix} \alpha^{k}_{1} \\ \alpha^{k}_{2} \\ \alpha^{k}_{3} \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{1a}$$

where $[C^k]$ and $\{\alpha^k\}$ are the elastic coefficient matrix and the thermal expansion coefficient vector of the kth phase. In Eq. (1), the respective superscripts n, i and p denote the CNT fiber, interphase and polymer matrix. Furthermore, r_n is the CNT radius and r_i is the outer radius of the interphase, as depicted in Fig. 1.

In order to determine the elastic properties of the interphase, several models have been implemented in earlier studies (Chouchaoui and Benzeggagh, 1997; Wacker et al., 1998; Ji et al., 2010; Shen and Li, 2005). None of these models devoted attention to model the CTE of the interphase layer. Based on the earlier research work of Chouchaoui and Benzeggah (1997) on the prediction of the elastic properties of the interphase, we implement a

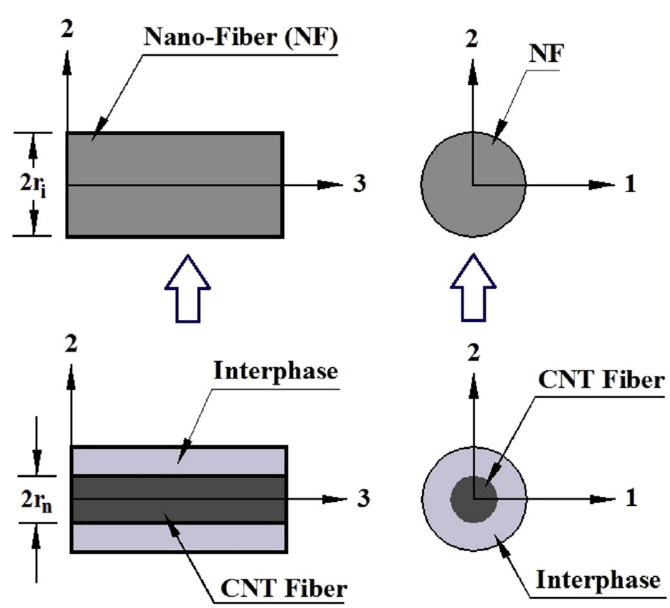

Fig. 1. Transverse and longitudinal cross sections of the RVE containing the CNT fiber and the interphase, and that of the RVE of the equivalent nano-fiber.