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Transversely isotropic properties of carbon nanotube/polymer composites

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ABSTRACT

The effective elastic moduli for carbon nanotube-based nanocomposites are derived and investigated. The conducted analyses based on the numerical homogenization procedure employ a spatial periodically arranged in a square array representative volume element and the finite element method. The transversely isotropic material having aligned and uniformly distributed long carbon nanotubes is considered. The perfect bonding between the carbon nanotubes and the matrix are assumed. Related to the transversely isotropic nanocomposite the five elastic material constants are needed to completely describe the elastic behavior. Based on the calculated material constants for the nanocomposite, the results are given and compared with the other values presented in the literature. In general, the increase of the effective material constants normalized by the matrix modulus is observed in comparison with pure polymeric matrix.

1. Introduction

The special attention is focused on the application of carbon nanotubes (CNTs) as a polymeric composite reinforcement because of their exceptional properties especially mechanical and electrical that combine with the very low density and the high aspect ratio [1–6]. The problem of the CNT/polymer nanocomposites is widely discussed in the review papers, e.g., [7–9]. Related to advanced nanocomposites, the numerical computations are undisputable important due to the fact that the experimental costs are very high. The numerical simulations can help to understand behavior of the material and give the basic knowledge further used in a design of such nanocomposites. Introducing the continuum mechanics assumption, the discrete atomistic structure may be neglected, homogenizing the behavior of molecules and atoms components. Validity of the above assumptions relating the applicability of the continuum-based theories vs. the physical models constitutes still an open problem.

Different trends and methods are observed in modeling 3D nanocomposites. First of all it is worth to mention that Odegard et al. [10] have applied the energy method to analyze the effective properties of the transversely isotropic nanofiber modeled as a space set of trusses describing a single-walled CNT, an interphase and a polymer. Ashrafi and Hubert [11] have used this method to predict the effective properties of the single-walled CNT (SWCNT) twisted arrays. In both cases, the effective values were used in the micromechanical analysis of the nanocomposites based on the traditional Mori-Tanaka homogenization method. Recently, in homogenization theories some innovative methods are proposed, see e.g., the papers of Barretta et al. [12] and Greco and Luciano [13]. Liu and Chen [14,15] have used the 3-D stress–strain relations concerning the normal stresses and strains to evaluate the effective properties of the CNT-based composites using the representative volume element (RVE) and the finite element method (FEM). They have computed four constants out of five required constants essential to model the elastic behavior of the transversely isotropic composite material. Three (and two, resp.) load cases were used to obtain the four independent material properties for the cylindrical RVE [14] and the square RVE [15], respectively. Similar approach was used by Hernandez–Perez and Aviles [16] to study the influence of interface on the effective mechanical properties of CNT-based nanocomposites. Recently, the mechanical properties of CNT-reinforced epoxy composite were also presented in the work of Zuberi and Esat [17]. Currently, in the modeling of carbon nanotubes the nonlocal approaches based on the Erigen's pioneered works [18,19] are considered, see e.g., the papers of Peddieson et al. [20] or Barretta et al. [21–24].

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The consistent description of the elastic properties for CNT is available in the literature (see e.g., Refs [25,26]) but there is still lack of complete numerical evaluation of the effective material constants for the CNT-based nanocomposites [10,11,14–16].

In the present paper we focused on the numerical description of the CNT-based polymeric nanocomposites to obtain the complete elastic behavior for the proposed material model. The present work is the extension of our previous studies [27,28]. The computations of the effective material properties for the CNT-reinforced nanocomposites are joined with the global mechanical response of the RVE therefore the continuum mechanics approach seems to be acceptable for such an analysis.

1.1. Continuum mechanics theoretical background

The Hook law for a composite material can be written as follows:

$$\overline{\sigma}_\alpha = C^*_{\alpha\beta}\overline{\varepsilon}_\beta \tag{1}$$

where $\overline{\sigma}_\alpha$ and $\overline{\varepsilon}_\beta$ are the average stresses and strains over the volume of the RVE, respectively, $C^*_{\alpha\beta}$ are the effective elastic moduli [29] whose total number of independent components is controlled by the prescribed symmetry (α, β = 1..6 – see Ref. [30]). Assuming a composite material with unidirectional parallel fiber reinforcement, the transverse isotropy mechanical model is used, where the isotropic plane (2–3) is perpendicular to the longitudinal direction (1) of the fibers. Thus, from the whole specimen a square representative subregion (RVE) can be selected in the form shown in Fig. 1.

The stress–strain relation (1) for a transversely isotropic body may be written in the form:

$$\begin{Bmatrix} \overline{\sigma}_1 \\ \overline{\sigma}_2 \\ \overline{\sigma}_3 \\ \overline{\sigma}_4 \\ \overline{\sigma}_5 \\ \overline{\sigma}_6 \end{Bmatrix} = \begin{bmatrix} C^*_{11} & C^*_{12} & C^*_{12} & 0 & 0 & 0 \\ C^*_{12} & C^*_{22} & C^*_{23} & 0 & 0 & 0 \\ C^*_{12} & C^*_{23} & C^*_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}\left(C^*_{22} - C^*_{23}\right) & 0 & 0 \\ 0 & 0 & 0 & 0 & C^*_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & C^*_{66} \end{bmatrix} \begin{Bmatrix} \overline{\varepsilon}_1 \\ \overline{\varepsilon}_2 \\ \overline{\varepsilon}_3 \\ \overline{\gamma}_4 \\ \overline{\gamma}_5 \\ \overline{\gamma}_6 \end{Bmatrix} \tag{2}$$

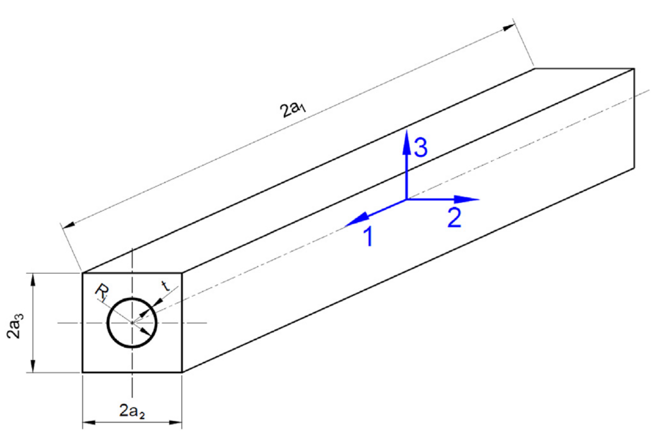

Fig. 1. Representative volume element (RVE) of carbon nanotube based nanocomposite.

where the typical six-by-six (Kelvin-Voigt) matrix notation has been applied. The transversely isotropic material is described by the set of five equations (the fifth and the sixth equation are equal – see Eq. (2)) having five effective independent stiffness moduli such as: C^*_{11}, C^*_{22}, C^*_{12}, C^*_{23}, and C^*_{66}. The effective elastic moduli can be used to compute the five elastic properties of the homogenized nanocomposite material properties, such as the longitudinal and transversal Young's moduli E^*_{11} and E^*_{22}, the longitudinal and transversal Poisson's ratios ν^*_{12} and ν^*_{23}, and the longitudinal shear modulus G^*_{12} as follows:

$$\begin{aligned} E^*_{11} &= C^*_{11} - \frac{2C^{*2}_{12}}{C^*_{22} + C^*_{23}} \\ \nu^*_{12} &= \frac{C^*_{12}}{C^*_{22} + C^*_{23}} \\ E^*_{22} &= \frac{\left[C^*_{11}\left(C^*_{22} + C^*_{23}\right) - 2C^{*2}_{12}\right]\left(C^*_{22} - C^*_{23}\right)}{C^*_{11}C^*_{22} - 2C^*_{12}} \\ \nu^*_{23} &= \frac{C^*_{11}C^*_{23} - C^{*2}_{12}}{C^*_{11}C^*_{22} - C^{*2}_{12}} \\ G^*_{12} &= G^*_{13} = C^*_{66} \end{aligned} \tag{3}$$

The last missing shear modulus in the transversal direction G^*_{23} may be calculated in the following way:

$$G^*_{23} = C^*_{44} = \frac{1}{2}\left(C^*_{22} - C^*_{23}\right) \tag{4}$$

In 1885 H. Helmholtz proved that the infinitesimal displacement of the deformable body can be expressed as the sum of three components: the translational displacement u^0_i, the rigid body displacement and the displacement due to pure elastic deformations ε^0_{ij}. Assuming that the rigid body deformations are negligibly small the displacements components can be written as follows:

$$u_i = u^0_i + \varepsilon^0_{ij}x_j, \mathrm{i}, \mathrm{j} = 1, 2, 3 \tag{5}$$

For the assumed RVE the six components of the strains ε^0_{ij} are approximated in the following manner:

$$\begin{aligned} u_i(a_1, x_2, x_3) - u_i(-a_1, x_2, x_3) &= 2a_1\varepsilon^0_{i1} \\ u_i(x_1, a_2, x_3) - u_i(x_1, -a_2, x_3) &= 2a_2\varepsilon^0_{i2} \\ u_i(x_1, x_2, a_3) - u_i(x_1, x_2, -a_3) &= 2a_3\varepsilon^0_{i3} \end{aligned} \tag{6}$$

where

$$\begin{aligned} -a_1 &\le x_1 \le a_1 \\ -a_2 &\le x_2 \le a_2 \\ -a_3 &\le x_3 \le a_3 \end{aligned} \tag{7}$$

The $2a_j\varepsilon^0_{ij}$ is the applied displacement used to enforced a strain ε^0_{ij} over a distance $2a_j$ (Fig. 1) and the u_i are assumed to be the boundary displacements. The volume average strain is equal the applied strain $\overline{\varepsilon}_\beta = \varepsilon^0_{ij}$.

To calculate the five unknown elastic moduli the set of five relations derived from Eq. (2) should be solved. Thus, the components of the effective elastic matrix are determining solving different elastic models of RVE subjected to the appropriate boundary conditions defined in (6) where only one component of the applied strain ε^0_{ij} is different from zero for each of the loading problems. In order to make the computations easier the unit value of applied stain $\varepsilon^0_{ij} = 1$ was chosen. As a result, using the boundary conditions