Research Article

Małgorzata Chwał* and Aleksander Muc

FEM micromechanical modeling of nanocomposites with carbon nanotubes

<https://doi.org/10.1515/rams-2021-0027>

received December 17, 2020; accepted March 11, 2021

Abstract: Mechanical properties of carbon nanotube (CNT)-based nanocomposites are broadly discussed in the literature. The influence of CNT arrangements on the elastic properties of nanocomposites based on the finite-element method (FEM) and representative volume element (RVE) approach is presented here. This study is an application of RVE modeling in the characterization of elastic behavior of CNT polymer nanocomposites. Our main contribution is the analysis of the impact of a nanotube arrangement on the elastic properties of nanocomposite to comprehensively determine the material constants. While most of the articles are focused on one distribution, not all material constants are determined. Our FEM analysis is compared with micromechanical models and other results from the literature. The current work shows that nanotube arrangements lead to different results of elastic properties. The analytical micromechanical models are consistent with the numerical results only for axial Young's modulus and Poisson's ratio, whereas other elastic constants are lower than the numerical predictions. The results of these studies indicate that FEM can predict nanocomposite mechanical properties with good accuracy. This article is helpful and useful to comprehensively understand the influence of CNT arrangements on the elastic properties of nanocomposites.

Keywords: nanocomposites, carbon nanotubes, homogenization, mechanical properties, FEM

1 Introduction

Since the originating work [1], specific attention, both academic and industrial, has been focused on the application of carbon nanotubes (CNTs). Due to unique properties, it is believed that few weight percentages of CNTs can significantly improve the mechanical properties of nanocomposites. Several studies containing experiments [2] and theoretical methods [3–12] have been utilized to find effective mechanical properties of CNTs. CNTs are widely used as a reinforcing phase in polymeric [13,14], ceramic [15], and metallic matrix composites [16]. However, most of them are polymeric-based composites. Recently, researchers are extensively focused on CNT/epoxy nanocomposites because of their broad applications in the electronics, aeronautics, and automotive industries. However, the increase in high-performance materials by the integration of CNTs into polymeric matrices is challenging because thermodynamic and kinetic barriers make difficult the effective dispersion of nanotubes [17].

The properties of CNT-based nanocomposite are discussed both based on experimental tests and theoretical descriptions [18–21]. To name a few, the experimental analysis of CNT polymer nanocomposites was presented by Garcia et al. [22], Yeh et al. [23], or Mikhalech et al. [24]. However, experiments at the nano-level are of high costs. On the other hand, analytical computations can be challenging to formulate or sometimes excessively complex to solve. So to accurately characterize nanocomposites, numerical modeling is indisputably necessary to support analytical computations and experimental attempts. Researchers suggest various numerical modeling approaches to estimate the mechanical properties of CNT nanocomposites, for instance, molecular dynamics (MD), equivalent continuum models, and finite-element method (FEM). Griebel and Hamaekers [25] studied a short single-walled CNT (SWCNT) and an infinite SWCNT embedded in a polyethylene matrix based on MD. Their results showed good agreement with the rule of mixture (ROM) in the case of the infinite CNT and with an extended ROMs in the case of the short CNT. Arash et al. [26] used MD to determine the

* **Corresponding author: Małgorzata Chwał**, Chair of Machine Design and Composite Structures, Faculty of Mechanical Engineering, Cracow University of Technology, 31-155 Cracow, Poland, e-mail: malgorzata.chwal@pk.edu.pl

Aleksander Muc: Chair of Machine Design and Composite Structures, Faculty of Mechanical Engineering, Cracow University of Technology, 31-155 Cracow, Poland, e-mail: olekmuc@mech.pk.edu.pl

mechanical properties of RVEs made of the short or the infinite CNTs embedded in the polymer matrix taking into account the interphase. Al-Ostaz et al. [27] applied MD to calculate the elastic properties of SWCNT-enhanced composites considering matrix, CNT, and interphase. They analyzed cases of aligned and randomly distributed SWCNTs. Anjana et al. [28] studied the effects of the volume fraction and aspect ratio on the mechanical properties of SWCNT nanocomposites using also MD. In the literature, different homogenization techniques are proposed to predict the mechanical properties of the CNT-reinforced polymer composite. Selmi et al. [29] presented a comparative study of several micromechanical models to evaluate the elastic properties of SWCNT-reinforced polymers. Among others, the stiffness enhancement of the epoxy matrix containing SWNTs was investigated for randomly oriented and fully aligned reinforcements. Fisher et al. [30] analyzed the effects of nanotube waviness on the modulus of CNT-reinforced polymers using a combined finite element and micromechanical approach. Tsai et al. [31] combined the micromechanical modeling and physical experiments to predict the modulus of CNT-reinforced nanocomposite. Hassanzadeh-Aghdam et al. [32] described the effective elastic properties of regular and random arrangements of CNTs in the polymer nanocomposites based on representative volume element (RVE). The applied RVE consisted of three phases containing CNT, polymer matrix, and interphase formed due to van der Waals forces between the CNT and the polymer. FEM is the alternative method of predicting the elastic properties of CNT-based nanocomposites which combine easy realization and cost efficiency. Liu and Chen [33,34] used RVE and FEM to estimate the elastic properties of the CNT-reinforced polymer nanocomposites. Chwał [35] and Chwał and Muc [36] applied a similar approach with various boundary conditions to calculate the mechanical properties of SWCNT-polymer nanocomposite. Zuberi and Esat [37] investigated the mechanical properties of the SWCNT-reinforced epoxy nanocomposite through FEM. Meguid et al. [38] calculated the effective properties of CNT-reinforced epoxies with the help of an atomistic-continuum (AC) model. Shokrih et al. [39] and Spanos et al. [40] joined FEM with micromechanical modeling to simulate the mechanical behavior of CNT-based nanocomposites. Malague et al. [41] proposed a procedure to assess size effects in SWCNT-polymer nanocomposites using the atomistic simulations and equivalent continuum model with a large number of CNTs. Alian et al. [42] also used multiscale modeling of CNT-epoxy nanocomposites. Alasvand Zarasvand and Golestanian [43] conducted experimental, numerical, and micromechanical studies to determine the nonlinear behavior of CNT-reinforced polymer.

Kassa and Arumugam [44] applied the combined numerical approach and experimental verification for the prediction of the elastic behavior of CNT-reinforced polymer nanocomposites.

According to the literature review, it is observed that the influence of different parameters including CNT wall number, length, aspect ratio, waviness, alignment, distribution, van der Waals forces, interphases, and matrix modulus on nanocomposite mechanical properties has been studied. The alignment of CNTs is a significant structural parameter that affects the elastic properties of CNT-based nanocomposites. Therefore, the main goal of this investigation is to determine the elastic properties of CNT-epoxy nanocomposites considering the arrangements of nanoreinforcement. Our main input is the analysis of the effect of a nanotube arrangement on the elastic properties of nanocomposite to comprehensively determine the material constants. According to our knowledge, most of the studies are focused on one distribution or not all material constants are determined. Our predictions are also compared to other modeling techniques or experimental data. Here we focus on nanocomposites having the two most common distributions of reinforcement, namely, square and hexagonal. Since the global mechanical response of the CNT nanocomposite is expected, the continuum mechanics approach is adequate. This work involves the numerical homogenization procedure of RVE and the FEM. Theoretical models describing effective mechanical properties of CNT-based nanocomposites are still a current issue.

2 Materials and methods

The current analysis considers the influence of reinforcement distributions in the representative subregion on the effective elastic properties of the nanocomposite. According to the experimental observations, in CNT-polymer nanocomposite the reinforcement distribution is usually unknown. These nanocomposites cannot offer high mechanical properties. On the other hand, theoretical computations indicate an excellent increase in the mechanical properties even for a small amount of CNT in nanocomposites. Sometimes the theoretical predictions and experimental data can be in error by orders of magnitude [31]. However, some techniques can be applied to align the nanotube distributions in a polymeric matrix. Here to estimate the influence of CNT arrangement on the elastic properties of nanocomposite, some idealization of the CNT distribution in the matrix is assumed. There are many ways to idealize the

cross section of a composite. We focus on nanocomposites having the two most common distributions of reinforcement considered in microcomposites, namely, square and hexagonal [45–47] (Figure 1). Based on the work by Hill [48], for perfectly distributed fibers due to symmetry and periodicity, one representative array can be selected to analyze the composite at the microscale. Thus, from the whole specimen, a representative subregion called RVE is selected (Figure 1). Moreover, this RVE as a volume of material statistically characterizes a homogeneous material. For these arrangements, the transversely isotropic material with aligned and uniformly distributed long CNTs is adopted in this work. Here we assume the isotropic planes (2 and 3) are perpendicular to the axial direction (1) of the CNTs (Figure 1).

Since the purpose of the analysis is to evaluate the material constants for nanocomposite, the prepared model should be able to simulate the stress–strain behavior. For finite element-based simulation, the RVE is selected from nanocomposite with long SWCNTs, aligned and uniformly distributed in the epoxy matrix. We have decided to consider CNT as a long fiber instead of a short one according to the experimental results presented in the work of Garcia et al. [22]. They have concluded that nanocomposites having highly aligned CNTs should be considered as a typical long-fiber composite.

The aligned long CNT–polymer nanocomposite consists of three phases, namely, polymer matrix, cylindrical CNTs, and circular cavities (Figure 2). A similar model was proposed by Selmi et al. [29]. We do not take into account interphase, assuming perfect bonds between CNTs and epoxy. It is beyond the scope of this article and will be addressed in a future study. In the case of a

square array, the nanotube is in the RVE center. Whereas for a hexagonal array, RVE has modified sides, i.e., with one nanotube at its center and a quarter of a nanotube at each corner (Figure 3).

Here both the CNTs and the polymeric matrix are assumed as an isotropic, homogenous, and linearly elastic material. The typical material data for SWCNT and epoxy resin [36] have been used in the finite element analysis (FEA; Table 1).

To compute the effective elastic properties of CNT–epoxy nanocomposite, the 3-D RVE was built. The full RVEs for square and hexagonal arrangements are presented in Figure 3. The following notations have been applied for RVE: a_1 – the length (along the axis of CNT), a_2 – the width, a_3 – the high of RVE, R_i – the inner radius, and t – the thickness of CNT. Due to the symmetry of the reinforced RVEs, a quarter of the RVEs was modeled in the ABAQUS package (Figure 2). Mostly the volume fraction of CNTs in nanocomposites is low [20]. At a higher CNT fraction, the mechanical properties of the nanocomposite were observed to deteriorate due to the formation of CNT agglomerates, which act as stress concentrators. In this work, we use the low-volume fraction of CNT, i.e., only 2.75% vol. Therefore, we consider the cylindrical CNT which has an outer diameter of 10 nm and thickness of 0.3 nm. The calculated CNT volume fraction considers only the area occupied by the cylindrical nanotube without considering the inner cavity.

After the geometrical calculations, the numerical FE model of RVEs was built. The details of the models are listed in Table 2. The general structural analysis was conducted.

Numerical RVEs were built using eight-node linear hexahedron finite elements. A double layer of the elements on the CNT model was generated (Figure 4).

Figure 1: The idealization of CNTs' distribution in nanocomposite and representative volume element (RVE) for (a) square and (b) hexagonal distribution.

Figure 2: Magnification of the cylindrical CNT embedded in the one-fourth RVE for 2.75% vol of CNTs for (a) square and (b) hexagonal distribution.

Figure 3: Representative volume element: (a) square array and (b) hexagonal array.

The displacements and tractions applied at the boundaries of the nanocomposite RVE are presented as [45]:

$$u_i(S) = \varepsilon_{ij} x_j \quad (1)$$

$$T_i(S) = \sigma_{ij} n_j \quad (2)$$

where S – the bounding surface, x_j – the surface coordinate, and n_j – the component of the normal vector to S . The applications of appropriate displacement u_i give uniform stresses σ_{ij} used for calculating nanocomposite material constant.

In the micromechanical analysis, the geometry of fiber arrangement in the matrix is an essential condition to develop a material model for the analysis. In the present study, it is assumed that the fibers and the matrix are

the only two phases in the composite, the fibers and matrix are perfectly bonded, the fibers are continuous and parallel with a cylindrical cross section and have a uniform diameter along its length, and the fibers and matrix comply with Hooke's law. The effective Hooke's law for a composite is defined as:

$$\bar{\sigma}_{ij} = [C^*] \bar{\varepsilon}_{ij} \quad (3)$$

where the overbar denotes the average over the unit cell and $\bar{\sigma}_{ij}$ and $\bar{\varepsilon}_{ij}$ are the average stress and strain tensor, respectively, $[C^*]$ is the effective elastic moduli in which a total number of independent components is controlled by the prescribed symmetry, $i, j = 1, 2, 3$. The stress-strain

Table 1: Material data

	Young's modulus (GPa)	Poisson's ratio
Carbon nanotube	1,000	0.3
Epoxy resin	3.2	0.3

Table 2: Numerical model details

Parameter	Square array	Hexagonal array
RVE dimensions: $2a_1 \times 2a_2 \times 2a_3$ (nm)	$100 \times 20 \times 20$	$100 \times 20 \times 40$
Total number of FE	30,880	36,160
Element type	8-nodes linear hexahedrons

Figure 4: A numerical model of the full RVE for (a) square and (b) hexagonal distribution of CNTs.

relation (3) for a transversely isotropic material, with an x_2 – x_3 plane of isotropy, is given by:

$$\bar{\sigma}_{11} = C_{11}^* \bar{\epsilon}_{11} + C_{12}^* (\bar{\epsilon}_{22} + \bar{\epsilon}_{33}) \quad (4)$$

$$\bar{\sigma}_{22} = C_{12}^* \bar{\epsilon}_{11} + C_{22}^* \bar{\epsilon}_{22} + C_{23}^* \bar{\epsilon}_{33} \quad (5) \quad \text{where}$$

$$\bar{\sigma}_{33} = C_{12}^* \bar{\epsilon}_{11} + C_{23}^* \bar{\epsilon}_{22} + C_{22}^* \bar{\epsilon}_{33} \quad (6)$$

$$\bar{\sigma}_{12} = 2C_{44}^* \bar{\epsilon}_{12} \quad (7)$$

$$\bar{\sigma}_{13} = 2C_{44}^* \bar{\epsilon}_{13} \quad (8)$$

$$\bar{\sigma}_{23} = (C_{22}^* - C_{23}^*) \bar{\epsilon}_{23} \quad (9)$$

The transversely isotropic material is characterized by a set of five equations having five effective independent stiffness moduli C_{11}^* , C_{12}^* , C_{22}^* , C_{23}^* , and C_{44}^* . The effective elastic moduli can be expressed in terms of five independent engineering constants, such as the axial and transverse Young's moduli E_A^* and E_T^* , the axial and transverse Poisson's ratios ν_A^* and ν_T^* , and the axial shear modulus G_A^* as follows [49]:

$$C_{11}^* = E_A^* + 4\chi\nu_A^{*2} \quad (10)$$

$$C_{12}^* = 2\chi\nu_A^* \quad (11)$$

$$C_{22}^* = \chi + \frac{0.5E_T^*}{1 + \nu_T^*} \quad (12)$$

$$C_{23}^* = \chi - \frac{0.5E_A^*}{1 + \nu_T^*} \quad (13)$$

$$C_{44}^* = G_A^* \quad (14)$$

$$\chi = \frac{0.25E_A^*}{0.5(1 - \nu_T^*)\left(\frac{E_A^*}{E_T^*}\right) - \nu_A^{*2}} \quad (15)$$

Effective elastic properties of the transverse isotropic CNT–polymer nanocomposite were estimated through a series of numerical simulations (Table 3). Involving the symmetry of RVE, the displacements were applied on the characteristic faces of one-fourth RVE, namely, $x_1 = 0$, $x_1 = a_1$, $x_2 = 0$, $x_2 = a_2$, $x_3 = 0$, and $x_3 = a_3$ (Figure 3). The displacements in x_1 , x_2 , and x_3 directions are denoted as u_1 , u_2 , and u_3 , respectively. The assumed small displacement is symbolized as e .

The effective properties are computed according to the following relations:

- For load acting in axial direction – the axial modulus and Poisson's ratio are:

$$E_A^* = \frac{\bar{\sigma}_{11}}{\bar{\epsilon}_{11}} \quad (16)$$

$$\nu_A^* = -\frac{\bar{\epsilon}_{22}}{\bar{\epsilon}_{11}} \quad (17)$$

Table 3: Boundary conditions

Engineering constant		Boundary conditions					
		x_1 -axis		x_2 -axis		x_3 -axis	
		$x_1 = 0$	$x_1 = a_1$	$x_2 = 0$	$x_2 = a_2$	$x_3 = 0$	$x_3 = a_3$
Axial elongation	E_A and ν_A	$u_1 = 0$	$u_1 = e$	$u_2 = 0$		$u_3 = 0$	
Transverse elongation	E_T and ν_T	$u_1 = 0$		$u_2 = 0$	$u_2 = e$	$u_3 = 0$	
Axial shear	G_A	$u_2 = 0$	$u_2 = e$	$u_1 = 0$	$u_1 = 0$	$u_3 = 0$	$u_3 = 0$
		$u_3 = 0$	$u_3 = 0$	$u_3 = 0$	$u_3 = 0$		

- For load acting in transverse direction – the transverse modulus and Poisson's ratio are:

$$E_T^* = \frac{\bar{\sigma}_{22}}{\bar{\varepsilon}_{22}} \quad (18)$$

$$\nu_T^* = -\frac{\bar{\varepsilon}_{33}}{\bar{\varepsilon}_{22}} \quad (19)$$

- For axial shear loading – the axial shear modulus is:

$$G_A^* = \frac{\bar{\sigma}_{12}}{2\bar{\varepsilon}_{12}} \quad (20)$$

The average stresses and strains were numerically calculated using the volume averaging method:

$$\bar{\sigma}_{ij} = \frac{1}{V} \int \sigma_{ij} dV = \frac{1}{V} \sum_{k=1}^N \sigma_{ij}^k V^k \quad (21)$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V} \int \varepsilon_{ij} dV = \frac{1}{V} \sum_{k=1}^N \varepsilon_{ij}^k V^k \quad (22)$$

where N – the total number of integration points, σ_{ij}^k – the stress component, and ε_{ij}^k – the strain component at integration points k in volume V^k .

3 Comparative analysis and discussion

The results of the effective engineering constants of CNT–polymer nanocomposites are listed in Figure 5. The numerical values are compared with micromechanical models such as the Vanin model [50], the Chamis model [51], and the Halpin–Tsai model [52] in the case of long CNTs embedded in the epoxy matrix. In micromechanical computations, we used data presented in Tables 1 and 2. Moreover, to discuss FEM results, some literature findings are placed in Figure 5 regarding other modeling techniques such as the AC and MD. Among others, only some works have been selected, which consider polymeric matrix reinforced with a small amount of SWCNTs. Being aware that theoretical predictions, in general, overestimate experimental findings, we also verified the results with the experimental ones from the literature, e.g., ref. [22].

For axial Young's modulus E_A^* and axial Poisson's ratio ν_A^* , the FEA results are almost identical for square and hexagonal arrays. These values are also the same as the predictions from the rule of mixture – see the Vanin model, the Chamis model, and also the Halpin–Tsai model

(Figure 5). To make a comparison/verification of our computations, different analyses of comparable materials have been chosen from the literature. We decided to compare our findings with other simulations or experimental results, which related to a polymeric nanocomposite reinforced with a small amount of SWCNTs. The AC model presented by Alian et al. [42] indicates about 36% lower values of E_A^* for (5,5) SWCNT concentration of 3% vol. in the epoxy matrix. Anjana et al. [28] also showed lower values (33%) for axial modulus according to MD simulations. Griebel and Hamaekers [25] obtained values 20% lower for (10,10) SWCNT/PE nanocomposite based on MD. However, Al-Ostaz et al. [27] reported much higher MD values for E_A^* (92.18 GPa) than our predictions. Generally, for comparable nanocomposite, i.e., the small diameter CNTs and polymeric matrix, AC models and MD simulations give lower E_A^* than that of our FEM predictions. What is surprising, the MD results of almost the same material (SWCNT/PE) presented in works [25] and [27] show a huge discrepancy in the axial Young's modulus. In paper [27], E_A^* is about 92 GPa; whereas in the work [28], E_A^* is about 25 GPa. However, Sharma et al. [14] informed that the macroscopic ROM, which takes into account only the CNT's volume fraction in determining the composite modulus, appears to break down for CNT/polymer composites where there are strong interfacial interactions. They have obtained higher values of E_A^* and E_T^* from MD simulations than from ROM. Other elastic moduli, the transverse Young's modulus E_T^* , the axial shear modulus G_A^* , and the transverse Poisson's ratio ν_T^* , represent the main challenge for researchers. So a lot of analytical models are proposed, and also MD and FEA are used. Here the predicted values of E_T^* from FEM are higher than the micromechanical predictions but lower than the results from AC model [42].

All micromechanical relations and models involving continuum assumption result in higher values of E_T^* than MD results from the work [28]. The current FE model also leads to the relatively high value of the axial shear modulus G_A^* which is not predicted by the micromechanical models. This inconsistency needs further consideration from the authors. The lower discrepancy is observed for the transverse shear modulus G_T^* . The transverse Poisson's ratio ν_T^* calculated numerically for the square and hexagonal arrays shows higher values than computed according to micromechanical models. There is a lack of data from other models (Figure 5). This discrepancy also needs further consideration from the authors. The experimental results for CNT–epoxy nanocomposites still inform much about lower elastic properties. For example, according to the work by Garcia et al. [22], the axial

Figure 5: Comparison of the effective elastic properties of CNT–polymer nanocomposite according to different models (EA, axial Young’s modulus; ET, transverse Young’s modulus; GA, axial Kirchhoff’s modulus; and GT, transverse Kirchhoff’s modulus; vA, axial Poisson’s ratio, vT, transverse Poisson’s ratio).

Young’s modulus is almost three times lower than our FEM results. In general, the modeling predictions indicate higher values of effective engineering constants mostly because of assumed idealizations.

To assess the influence of the CNT’s addition on the mechanical properties of nanocomposite, the results for the square and hexagonal arrays are normalized with pure matrix moduli. The normalized values for the axial (E_A^*/E_m) and transverse (E_T^*/E_m) Young’s modulus, and the axial (G_A^*/G_m) and transverse shear modulus (G_T^*/G_m) are shown in Figure 6.

The applied matrix properties are as follows: $E_m = 3.2$ GPa and $G_m = 1.231$ GPa. The theoretical predictions

confirm the increase in mechanical properties for the polymeric nanocomposite with the addition of CNTs. Improvement in mechanical properties is visible in the axial and the transverse direction; however, the highest increase is for the axial Young’s modulus – more than ninefold regardless of the CNT arrays in the composite. The current FEA also revealed more than threefold increase in the axial shear modulus. However, this result is not confirmed in micromechanical calculations, so the authors will consider further analysis. The normalized transverse moduli rise but not as impressive as in the axial direction. The transverse stiffness modulus grows about 22–30%, whereas the transverse shear modulus

Figure 6: Comparison of the normalized moduli of the CNT/polymer nanocomposites.

increases about 10% for the hexagonal array and only 1% for the square array.

The current values are comparable with FEM results in the work by Liu and Chen [33]. They observed a 10-fold increase in E_A^* for the 5% vol. of CNTs in the nanocomposite. However, they reported more than threefold rise in the transverse Young's modulus, which is not confirmed by the present analysis. The discrepancy in the transverse properties of nanocomposites may suggest that the transverse moduli are more sensitive to fluctuations in volume fractions of CNTs than the axial ones. As presented in the work [34], the impact of volume fraction on the transverse properties is less prominent in nanocomposites having stiffer matrices than the polymeric ones. The normalized E_A^* according to the AC models is lower than the current FE predictions, in which CNT is modeled as the hollow cylinder. The normalized E_A^* is about 28% [42] and 58% [40] lower than our FEM values. However, MD results [25,27] show much higher values. According to Griebel and Hamaekers [25], 6% vol. of CNTs showed a 38-fold increase in normalized E_A^* . Moreover, Al-Ostaz et al. [27] presented a 75-fold rise in E_A^* ; whereas the current work indicates a 9-fold rise. The experimental values listed in the article by Garcia et al. [22] for highly aligned CNT-polymer nanocomposites also indicated a high increase in the axial Young's modulus (more than threefold). From these FEM analyses and literature comparison, it is not possible to judge which predictions are better.

4 Conclusions

The FE modeling was carried out for two different CNT arrangements, namely, square and hexagonal. By applying various boundary conditions on RVE, the effective material properties were calculated. Our findings are compared with micromechanical results. Besides, some literature results are also presented and discussed. Numerical results showed a high increase in the elastic properties; however, during modeling of the nanocomposite, a lot of assumption is made, which are mostly a great challenge to realize during the sample preparations such as, e.g., perfect alignment and strong interphase. Some findings are not confirmed both in the micromechanical modeling and in the literature review, and it needs further consideration. We have also analyzed results from different techniques applied in nanocomposite modeling. However, at this point, it is not possible to judge which predictions are better. It is still worthwhile to note the discrepancy between the FEM models and

experimental observations. The comparison of results with the experimental ones revealed that CNT/polymer nanocomposites are efficient in load carrying; however, experiments do not fulfill theoretical predictions. However, the nanocomposite FEM modeling is very important and can lead to potentially valuable research. The modeling results are in the current interest of searching a method to gain the theoretical predictions of CNT's dispersion and distribution in the polymeric matrix and functionalization of CNT.

Funding information: The paper publication has received funding from Cracow University of Technology.

Author contributions: M. Chwał: Conceptualization, Methodology, Investigation, Visualization, Writing- Original Draft
A. Muc: Conceptualization.

Conflict of interest: Authors state no conflict of interest.

References

- 1 Iijima, S. Helical microtubules of graphitic carbon. *Nature*, Vol. 354, 1991, pp. 56–58.
- 2 Treacy, M. M. J., T. W. Ebbesen, and J. M. Gibson. Exceptionally high Young's modulus observed for individual carbon nanotubes. *Nature*, Vol. 381, 1996, pp. 678–680.
- 3 Odegard, G. M., T. Gates, L. M. Nicholson, and K. E. Wise. Equivalent-continuum modeling of nano-structured materials. *Composites Science and Technology*, Vol. 62, 2002, pp. 1869–1880.
- 4 Li, C. and T. W. Chou. A structural mechanics approach for the analysis of carbon nanotubes. *International Journal of Solids and Structures*, Vol. 40, 2003, pp. 2487–2499.
- 5 Muc, A. and M. Jamróz. Homogenization models for carbon nanotubes. *Mechanics of Composite Materials*, Vol. 40, 2004, pp. 101–106.
- 6 Tserpes, K. I. and P. Papanikos. Finite element modeling of single-walled carbon nanotubes. *Composites Part B: Engineering*, Vol. 36, 2005, pp. 468–477.
- 7 Hu, N., H. Fukunaga, C. Lu, M. Kameyama, and B. Yan. Prediction of elastic properties of carbon nanotube reinforced composites. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, Vol. 461, 2005, pp. 1685–1710.
- 8 Meo, M. and M. A. Rossi. Molecular-mechanics based finite element model for strength prediction of single wall carbon nanotubes. *Materials Science and Engineering A*, Vol. 454–455, 2007, pp. 170–177.
- 9 Shokrieh, M. M. and R. Rafiee. Prediction of Young's modulus of graphene sheets and carbon nanotubes using nanoscale continuum mechanics approach. *Materials & Design*, Vol. 31, 2010, pp. 790–795.
- 10 Wernik, J. M. and S. A. Meguid. Atomistic-based continuum modeling of the nonlinear behavior of carbon nanotubes. *Acta Mechanica*, Vol. 212, 2010, pp. 167–179.

- 11 Dominguez-Rodriguez, G., A. Tapia, and F. Aviles. An assessment of finite element analysis to predict the elastic modulus and Poisson's ratio of singlewall carbon nanotubes. *Computational Materials Science*, Vol. 82, 2014, pp. 257–263.
- 12 Chwał, M. and A. Muc. Modeling of atomic interactions in carbon nanotubes. *IOP Conference Series: Materials Science and Engineering*, Vol. 744, 2020, pp. 1–5.
- 13 Moumen, A. E., M. Tarfaoui, and K. Lafdi. Computational homogenization of mechanical properties for laminate composites reinforced with thin film made of carbon nanotubes. *Applied Composite Materials*, Vol. 25, 2017, pp. 1–20.
- 14 Sharma, S., R. Chandra, P. Kumar, and N. Kumar. Molecular dynamics simulation of polymer/carbon nanotube composites. *Acta Mechanica Sinica*, Vol. 28, 2015, pp. 409–419.
- 15 Poh, L., C. Della, S. Ying, C. Goh, and Y. Li. Micromechanics model for predicting effective elastic moduli of porous ceramic matrices with randomly oriented carbon nanotube reinforcements. *AIP Advances*, Vol. 5, 2015, id. 097153.
- 16 Aristizabal, K., A. Katzensteiner, A. Bachmaier, F. Mucklich, and S. Suarez. On the reinforcement homogenization in CNT/metal matrix composites during severe plastic deformation. *Materials Characterization*, Vol. 136, 2018, pp. 375–381.
- 17 Hameed, N., N. V. Salim, T. L. Hanley, M. Sona, B. L. Fox, and Q. Guo. Individual dispersion of carbon nanotubes in epoxy via a novel dispersion–curing approach using ionic liquids. *Physical Chemistry Chemical Physics: PCCP*, Vol. 15, 2013, pp. 11696–11703.
- 18 Jojibabu, P., Y. X. Zhang, and B. Gangadhara Prusty. A review of research advances in epoxy-based nanocomposites as adhesive materials. *International Journal of Adhesion and Adhesives*, Vol. 96, 2020, id. 102454.
- 19 Chwał, M. and A. Muc. Design of reinforcement in nano and microcomposites. *Materials*, Vol. 12, 2019, id. 1474.
- 20 Rafiee, R., Ed., *Carbon nanotube-reinforced polymers. From nanoscale to macroscale*, Elsevier, Amsterdam, Netherlands, 2018.
- 21 Martone, A., G. Faiella, V. Antonucci, M. Giordano, and M. Zarrelli. The effect of the aspect ratio of carbon nanotubes on their effective reinforcement modulus in an epoxy matrix. *Composites Science and Technology*, Vol. 71, 2011, pp. 1117–1123.
- 22 Garcia, E. J., A. J. Hart, B. L. Wardle, and A. H. Slocum. Fabrication and nanocompression testing of aligned carbon-nanotube–polymer nanocomposites. *Advanced Materials*, Vol. 19, 2007, pp. 2151–2156.
- 23 Yeh, M. K., T. H. Hsieh, and N. H. Tai. Fabrication and mechanical properties of multiwalled carbon nanotubes/epoxy nanocomposites. *Materials Science and Engineering A*, Vol. 483–484, 2008, pp. 289–292.
- 24 Mikhalech, A., T. Gspann, and A. Windle. Aligned carbon nanotube–epoxy composites: the effect of nanotube organization on strength, stiffness, and toughness. *Journal of Materials Science*, Vol. 51, 2016, pp. 10005–10025.
- 25 Griebel, M. and J. Hamaekers. Molecular dynamics simulations of the elastic moduli of polymer–carbon nanotube composites. *Computer Methods in Applied Mechanics and Engineering*, Vol. 193, 2004, pp. 1773–1788.
- 26 Arash, B., Q. Wang, and V. K. Varadan. Mechanical properties of carbon nanotube/polymer composites. *Scientific Reports*, Vol. 4, 2014, id. 6479.
- 27 Al-Ostaz, A., G. Pal, P. R. Mantena, and A. Cheng. Molecular dynamics simulation of SWCNT-polymer nanocomposite and its constituents. *Journal of Materials Science*, Vol. 43, 2008, pp. 164–173.
- 28 Anjana, R., S. Sharma, and A. Bansal. Molecular dynamics simulation of carbon nanotube reinforced polyethylene composites. *Journal of Composite Materials*, 2016, pp. 1–15.
- 29 Selmi, A., C. Friebe, I. Doghri, and H. Hassis. Prediction of the elastic properties of single walled carbon nanotube reinforced polymers: A comparative study of several micromechanical models. *Composites Science and Technology*, Vol. 67, 2007, pp. 2071–2084.
- 30 Fisher, F. T., R. D. Bradshaw, and L. C. Brinson. Effects of nanotube waviness on the modulus of nanotube-reinforced polymers. *Applied Physics Letters*, Vol. 80, 2002, pp. 4647–4649.
- 31 Tsai, C. H., C. J. Chang, K. Wang, C. Zhang, Z. Liang, and B. Wang. Predictive model for carbon nanotube–reinforced nanocomposite modulus driven by micromechanical modeling and physical experiments. *IEEE Transactions*, Vol. 44, No. 7, 2012, pp. 590–602.
- 32 Hassanzadeh-Aghdam, M. K., M. J. Mahmoodei, and R. Ansari. Micromechanical characterizing the effective elastic properties of general randomly distributed CNT–reinforced polymer nanocomposites. *Probabilistic Engineering Mechanics*, Vol. 53, 2018, pp. 39–51.
- 33 Liu, Y. J. and X. L. Chen. Evaluation of effective material properties of carbon nanotube-based composites using a nanoscale representative volume element. *Mechanics of Materials*, Vol. 35, 2003, pp. 69–81.
- 34 Chen, X. L. and Y. J. Liu. Square representative volume elements for evaluating the effective material properties of carbon nanotube-based composites. *Computational Materials Science*, Vol. 29, 2004, pp. 1–11.
- 35 Chwał, M. Numerical evaluation of effective material constants for CNT-based polymeric nanocomposites. *Advanced Materials Research*, Vol. 849, 2014, pp. 88–93.
- 36 Chwał, M. and A. Muc. Transversely isotropic properties of carbon nanotube/polymer composites. *Composites Part B: Engineering*, Vol. 88, 2016, pp. 295–300.
- 37 Zuberi, M. J. S. and V. Esat. Investigating the mechanical properties of single walled carbon nanotube reinforced epoxy composite through finite element modelling. *Composites Part B: Engineering*, Vol. 71, 2015, pp. 1–9.
- 38 Meguid, S. A., J. M. Wernik, and Z. Q. Cheng. Atomistic-based continuum representation of the effective properties of nano-reinforced epoxies. *International Journal of Solids and Structures*, Vol. 47, 2010, pp. 1723–1736.
- 39 Shokrieh, M. M., R. Mosalmani, and A. Shamaei. A combined micromechanical–numerical model to simulate shear behavior of carbon nanofiber/epoxy nanocomposites. *Journal of Materials and Design*, Vol. 67, 2015, pp. 531–537.
- 40 Spanos, K. N., S. K. Georgantzinos, and N. K. Anifantis. Investigation of stress transfer in carbon nanotube reinforced composites using a multi-scale finite element approach. *Composites Part B: Engineering*, Vol. 63, 2014, pp. 85–93.

- 41 Malagu, M., M. Goudarzi, A. Lyulin, E. Benvenuti, and A. Simone. Diameter-dependent elastic properties of carbon nanotube-polymer composites. *Composites Part B: Engineering*, Vol. 131, 2017, pp. 260–281.
- 42 Alian, A. R., S. I. Kundalwal, and S. A. Meguid. Multiscale modeling of carbon nanotube epoxy composites. *Polymer*, Vol. 70, 2015, pp. 149–160.
- 43 Alasvand Zarasvand, K. and H. Golestanian. Determination of nonlinear behavior of multi-walled carbon nanotube reinforced polymer: Experimental, numerical, and micromechanical. *Materials & Design*, Vol. 109, 2016, pp. 314–323.
- 44 Kassa, M. K. and A. B. Arumugam. Micromechanical modeling and characterization of elastic behavior of carbon nanotube-reinforced polymer nanocomposites: A combined numerical approach and experimental verification. *Polymer Composite*, Vol. 41, 2020, pp. 3322–3339.
- 45 Hashin, Z. and B. W. Rosen. The elastic moduli of fiber-reinforced materials. *Journal of Applied Mechanics*, Vol. 31, 1964, pp. 223–232.
- 46 Vasiliev, V. V. and E. V. Morozov. *Mechanics and analysis of composite materials*, Elsevier, Amsterdam, Netherlands, 2001.
- 47 Raju, B., S. R. Hiremath, and M. D. Roy. A review of micromechanics based models for effective elastic properties of reinforced polymer matrix composites. *Composite Structures*, Vol. 204, 2018, pp. 607–619.
- 48 Hill, R. A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, Vol. 13, 1965, pp. 213–222.
- 49 Tsai, S. W. *Theory of composites design*, Think Composites, Dayton, USA, 1992.
- 50 Vanin, G. A. *Micro-mechanics of composite materials*, Kiev, Nauka Dumka, 1985.
- 51 Chamis, C. C. Mechanics of composite materials: past, present, and future. *Journal of Composites, Technology and Research*, Vol. 11, 1989, pp. 3–14.
- 52 Halpin, J. C. and J. L. Kardos. The Halpin–Tsai equations: a review. *Polymer Engineering and Science*, Vol. 16, 1976, pp. 344–352.