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Mechanical material characterization of an embedded Carbon nanotube in polymer matrix by employing an equivalent fiber

ABSTRACT

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Effective elastic properties for carbon nanotube reinforced composites are obtained through a variety of micromechanics techniques. An embedded carbon nanotube in a polymer matrix and its surrounding interphase is replaced with an equivalent fiber for predicting the mechanical properties of the carbon nanotube/polymer composite. The effects of an interphase layer between the nanotubes and the polymer matrix as result of effective interphase layer is investigated. A modeling analysis investigating the effect of the aspect ratio on the tubes reinforcement mechanism has been carried out. The variations of mechanical properties with tube reduce, interphase thickness and waviness is investigated. Furthermore in this work, the classical theory concerning the mechanical efficiency of a matrix embedding finite length fibers has been modified by introducing the tube-to-tube Random Contact which explicitly accounts for the progressive reduction of the tubes effective aspect ratio as the filler content increases.

Keywords: *Equivalent fiber; Effective interphase model; Waviness; Aspect ratio; Mechanical properties.*

INTRODUCTION

Nanocomposites have attracted considerable attention in both academia and industry, mainly due to their extraordinary mechanical, thermal and electrical properties and even more important, a significant increase in fracture toughness [1-5]. Also the orientation of the nanotubes plays an important role in the mechanical reinforcement [6-8]. Several investigations have shown that the addition of small amounts of carbon nanotube can considerably improve the mechanical, electrical and thermal properties of polymeric composites [9-12]. It is indeed this combination of mechanical and electrical properties of individual nanotubes that makes them the ideal reinforcing agents in a number of applications.

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Different factors affecting the performance of carbon nanotube reinforced composites (CNTR) can be categorized as: nanotube type [13], size [14], shape [14], volume fraction [6,11], degree of dispersion [15], characteristics of polymer matrix and interactions between filler and matrix at their interface [16].

Computational approach can play a significant role in the development of the CNT-based composites by providing simulation results to help on the understanding, analysis and design of such nanocomposites. Tsai et al [17] used the Mori-Tanaka approach to show the effect of inclusion waviness and its distribution on the effective composite stiffness. They considered different waviness conditions: uniform waviness with variable inclusion orientation or aspect ratio, uniform aspect ratio and variable waviness and they understood that the inclusion waviness have a great effect on the tensile moduli and shear modulus for unidirectional composites. Shokrieh and Rafiee [18,19] studied the longitudinal behavior of a carbon nanotube in a polymeric matrix using a non-linear analysis on a full 3D multi-scale finite element model consisting of carbon nanotube, non-bonded interphase region and surrounding polymer. The bonding between carbon nanotube and its surrounding polymer was simulated as Van der Waals interactions. Their finite element analysis results show that the rule of mixture for conventional composites overestimates the result and cannot capture the scale difference between micro- and nano-scale. However they developed an equivalent fiber to overcome this difficulty and corresponding longitudinal, transverse and shear moduli were calculated. Developed equivalent fiber consisting of carbon nanotube and inter-phase region can be appropriately used in micromechanical equations.

Montazeri *et.al* [20] showed that modified Halpin-Tsai equation with exponential Aspect ratio can be used to model the experimental result of MWNT composite samples. They also demonstrated that reduction in Aspect ratio (L/d) and nanotube length cause a decrease in aggregation and Above 1.5 wt.%, nanotubes agglomerate causing a reduction in Young's modulus values. Thus, it is important to determine the effect Aspect ratio and arrangement of CNTs on the effective properties of CNTRC. The reinforcement effect of CNTs with different aspect

ratio in an epoxy matrix has been carried out by martone *et al* [21]. They showed that progressive reduction of the tubes effective aspect ratio occurs because of the increasing connectedness between tubes upon an increase of their concentration. Also they investigated on the effect of nanotube curvature on the average contacts number between tubes by means of the waviness that accounts for the deviation from the straight particles assumption.

The main purpose of this research is to investigate the effective moduli of the CNT reinforced polymer composite, with emphasis on the influence of CNT waviness and CNT-matrix interphase on the stiffening of the composite. The effective material properties of the fiber-reinforced composites are estimated using rule of mixture. With the knowledge that load transfer between the nanotube and polymeric phases is less than perfect we employ an equivalent fiber to consider the size-dependent material properties. The embedded wavy CNT in a polymeric resin and its surrounding interphase matrix convert into an equivalent fiber, which can be used in micromechanical analysis of CNT reinforced plastic composites.

EXPERIMENTAL

Effective wall thickness

The exact dimensions of SWNTs at the equilibrium state are still a matter under investigation. To calculate the Young's modulus of a carbon nanotube, one needs to know the wall thickness of the tube. The values of the wall thickness as suggested by available literature, varied significantly from 0.067 nm [22, 23] to 0.34 nm [18, 19] and 0.68 nm [24]. However, as reported recently the effective thickness of SWCNTs cannot be greater than or equal to the theoretical diameter of a carbon atom (0.142 nm) [25]. Note that the paper used the value 0.067 nm as the effective thickness while most other references use 0.34 nm (interlayer spacing of graphite) instead. Some researchers think that there is no need to clarify the effective wall thickness of CNTs, because one may use other parameters in a specific application, e.g., using bending stiffness. The author believes that the effective wall thickness is the most fundamental mechanics quantities for

modeling using the well-established continuum mechanics theory.

Equivalent solid cylinder

Numerous micromechanical models have been successfully used to predict the macroscopic behavior of fiber-reinforced composites. But in the past few years, the demand for the development of faster methods to compute the mechanical properties of nanostructures has been increasing. Also, in polymer nanocomposites, the polymer molecules and nanotube have the equivalent size and the polymer–nanotube interactions are highly dependent on the local molecular structure and bonding at the interface. Therefore, the structures of nanotubes and polymer chains cannot be captured as continuous phase at nano scales, in order to overcome these difficulties; the equivalent solid cylinder is used [17-19].

It should be noticed that the original attributes of cylindrical hollow structure of CNTs cannot satisfy the stated requirement; therefore, it is necessary to have an equivalent solid cylinder so that the mechanical properties of the atomistic CNT structure can be properly interpreted in the continuum solid model and precisely transformed into the CNTs nanocomposites. It is interesting to note that the radius of the equivalent solid cylinder is equal to the distance measured from the center of a CNT to the center of atom, as shown in Figure 1. In this study, only armchair type single-walled CNTs, i.e., (10, 10), were selected for the demonstration.

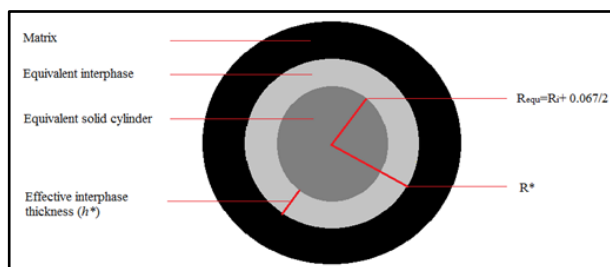


Fig. 1. Equivalent solid cylinder

Effective interphase model

When the hollow molecular structure of a CNT was converted into a solid cylinder through the theory of elasticity concept as presented in the early section, the mechanical behavior of CNT

nanocomposites can be predicted using the Mori-Tanaka approach. In the Mori-Tanaka approach, it is always assumed that the reinforcements are perfectly bounded with the surrounding polymeric matrix. However, in CNT-reinforced nanocomposites, the interfacial bonding is not perfect, but it is dominated by the non-bonded interaction that consists of the electrostatic and van der Waals (vdW) interactions. Electrostatic interactions can be neglected in comparison with vdW interactions, since vdW contributes more significantly in three higher orders of magnitude than electrostatic energy [26]. Moreover, the extent of atomistic interaction between the CNTs and surrounding matrix may have an influence on the mechanical responses of the nanocomposites.

The van der Waals forces between any two carbon atoms can be described by the Lennard–Jones model [26]. The vdW force is a non-linear force and it can be neglected when the interatomic distance is equal or greater than 0.7 nm as it is shown in Figure 2. The Lennard–Jones potential equation is given below:

$$F_{vdw} = 4 \frac{\epsilon}{r} \left[-12 \left(\frac{\sigma}{r} \right)^{12} + 6 \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

In Eq. (18) the terms σ (in nm) and ϵ (in kcal/mol) are defined as the Lennard-Jones parameters and 0.34 nm and 0.0566 kcal/mol, respectively [26]. They are material specific and determine the nature and strength of the interaction. The term r corresponds to the distance between the interacting particles.

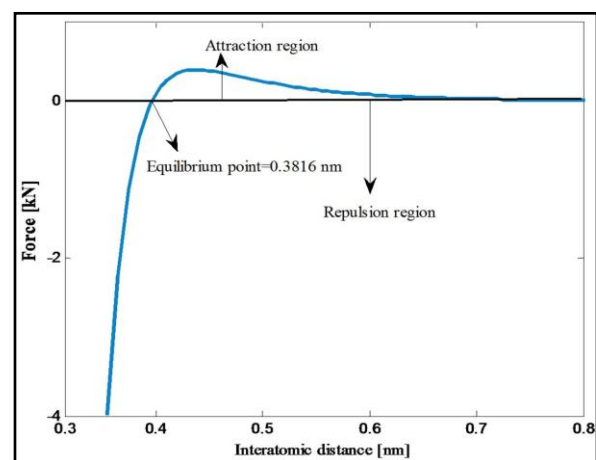


Fig. 2. Variation of the Lennard-Jones force with inter-atomic distance of carbon atoms

The maximum attraction force between atoms occurs in a peak at 0.425 nm interatomic distances, and then decreases with increasing bond length. The repulsive force between atoms increases rapidly when the bond length is shorten from the equilibrium position ($e_{\text{equilibrium}}=0.3816$ nm).

In order to fully realize the mechanical properties of CNT-reinforced composites, it is essential to understand the nature of load transfer in the interfacial region between the reinforcement and the matrix. In the present paper, the atomistic interaction between the CNTs and the polyimide matrix was characterized through the effective interphase. A homogeneous isotropic interphase medium of the same shape as the SWNT is inserted between the SWNT and matrix.

To obtain the Young modulus of effective interphase, the RVE is loaded with a uniformly distributed load (negative pressure) p in the lateral (radial) direction as shown in Figure 3. If the representative thickness of nanotube layer is equal to 0.067 nm, the stiffness of the effective interphase (K^*) can be obtained as follows:

$$F(0.17-0.067/2)=7.3744 \times 10^{-6} \quad \text{and}$$

$$\delta r = e_{\text{equilibrium}} - (0.17 - 0.067/2) = 0.2451 \text{ nm}$$

$$K_{\text{Lennard-Jones}} = F / \delta r = 30087 \text{ N/m} \quad (2)$$

The displacements corresponding to these conditions can be determined by the usual methods of integrating the strain-displacement relations. For this case, the result is:

$$u(R_{cn}) = \frac{1+\nu^*}{E^*} \left(-\frac{(R_{cn}-h^*)^2 R_{cn} P^*}{R_{cn}^2 - (R_{cn}-h^*)^2} - \frac{(1-2\nu^* R_{cn}^3 P^*)}{R_{cn}^2 - (R_{cn}-h^*)^2} \right) \quad (3)$$

Where E^* is the Young modulus and ν^* the Poisson ratio of effective interphase.

Also

$$F = P^*(2\pi R_{cn})L_{cn}, \quad K^* = \frac{F}{u(R_{cn})}$$

$$K^* = \frac{E^*}{1+\nu^*} (2\pi L_{cn}) \left(\frac{R_{cn}^2 - (R_{cn}-h^*)^2}{(R_{cn}-h^*)^2 + (1-2\nu^*)R_{cn}^2} \right) \quad (4)$$

Combining Eq. (19) with Eq. (21) results in ($K^*=K_{\text{Leonard-Jons}}$):

$$E^* = (1+\nu^*) \frac{(R_{cn}-h^*) + (1-2\nu^*)R_{cn}^2}{R_{cn}^2 - (R_{cn}-h^*)^2} \left(\frac{30087}{2\pi L_{cn}} \right) \quad (5)$$

The Young modulus of SWCNT and its interphase can be estimated by the macroscopic rule-of-mixtures. This rule reads as:

$$E_L = (E_z)_{\text{equ}} \left(\frac{R_{\text{equ}}}{R_{cn}} \right) + E^* \left(1 - \left(\frac{R_{\text{equ}}}{R_{cn}} \right) \right) \quad (6)$$

$$E_T = \frac{E^* (E_x)_{\text{equ}}}{E^* \left(\frac{R_{\text{equ}}}{R_{cn}} \right)^2 + (E_x)_{\text{equ}} \left(1 - \left(\frac{R_{\text{equ}}}{R_{cn}} \right)^2 \right)} \quad (7)$$

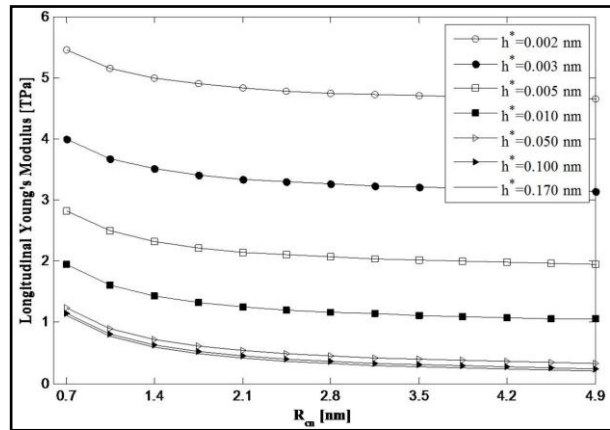


Fig. 3. Variations of Longitudinal Young's Modulus with reduce

Where E_L and E_T are longitudinal modulus, and transverse modulus of equivalent fiber with considering effective interphase. Using the results obtained in previous sections, the investigated CNT

and its inter-phase can be converted into an equivalent long fiber.

Young's modulus of developed equivalent fiber representing the CNT and its inter-phase material are summarized in Table 1 in comparison with reported results by literature values (where available).

Table 1. Comparison of results of our current investigation for (10, 10) SWCNT ($L_{cn}=9.26$ nm, $R_{cn}=0.68$ nm) with literature ($R_{equ}=0.68$ nm)

Researcher	Effective Wall thickness (nm)	Effective interphase thickness, h^* (nm)	Young modulus (Tpa)
Current work	0.067	0.0020	5.456
	0.067	0.0025	4.578
Yakobson et al. (1996)[24]	0.066	-	5.5
Xiaohu Yao et al (2008)[25]	0.066	-	5.5
	0.075	-	4.74

Figure 3 shows variations the longitudinal Young modulus versus reduce (R_{cn}) of the equivalent fiber for different value interphase thickness, h^* , ranging from 0.002 nm all the way to 0.17 nm. As noticed the Young modulus decreases rapidly with increasing R_{cn} for different value of h^* and then remains almost unaltered for $R_{cn} > 2.8$ nm. It can be concluded that for different values of equivalent fiber reduce, R_{cn} increasing the value of h^* decreases the Young modulus. This indicates that the effective moduli of the SWCNT are sensitive to the existence of interphase and its mechanical properties.

The equivalent fiber for SWCNT with chiral index of (10, 10) is a solid cylinder with diameter of 1.36nm. Mechanical properties of an equivalent fiber are listed in Table 2. It should be mentioned that Poly $\{(m\text{-phenylenevinylene})\text{-co-}[(2,5\text{-dioctoxy-}p\text{-phenyle) vinylene}]\}$, referred as (PmPV), is selected as a matrix material [11]. The relevant material properties for the constituent materials are as follows:

$$E_M = 2.1GPa, v_M = 0.34, \rho_M = 1150Kg/m^3, PmPV$$

Table 2. Material properties of equivalent fiber

Mechanical properties	Equivalent fiber
Longitudinal Young's modulus	5.456 (Tpa)
Poisson's ratio	0.175

Aspect ratio

In this section we will discuss about the results in the literature on mechanical properties of polymer nanotube composites. The rule of mixture equation assumes that the filler are straight and uniform dispersion of the filler in the polymer matrix. Also it can't consider the length of filler therefore it can be modified by incorporating efficiency parameter (η^*) to account for the aspect ratio (AR) and waviness (w) of nanotube. The effective mechanical properties of the composite are obtained based on a micromechanical model according to [21]:

$$E = V_{cn} E_{\eta^*} + V_m E^m \quad (8)$$

$$E_{\eta^*} = \eta^* E_{cn}$$

$$\eta^* = 1 - \frac{\tanh(K \cdot AR / (1 + \langle c \rangle))}{K \cdot AR / (1 + \langle c \rangle)}$$

$$K = \sqrt{\frac{-2}{1 + v_m} \frac{E_{cn} \ln(V_{cn})}{E_m}}$$

Where E_{cn} , E_{η^*} and $\langle c \rangle$ are elasticity modulus, effective reinforcement modulus and the average number of contacts per particle, respectively, of the carbon nanotube and E^m and $G^m \left(G^m = \frac{E^m}{2(1+v^m)} \right)$ are corresponding properties for the matrix.

It should be noticed that the average number of contacts $\langle c \rangle$ for tubes is dependent on their aspect ratio:

$$\langle c \rangle = w \cdot V_{cn} \cdot \left(4 + \frac{3AR^2}{3AR + 2} \right) \quad (9)$$

Where, the waviness w has been introduced in order to account for the carbon nanotubes and curvature within the real composite. Accordingly to literature, the variation of the excluded volume due to nanotubes curvature has been here accounted for by introducing the waviness parameter, w .

Figure 4 shows the model calculations of the nanocomposite modulus, E , compared to experimental data from different literature sources. The model is able to be fitted to the experimental data in all the cases investigated for very different aspect ratios CNTs. Our results are in agreement with an argument proposed by Martone [21].

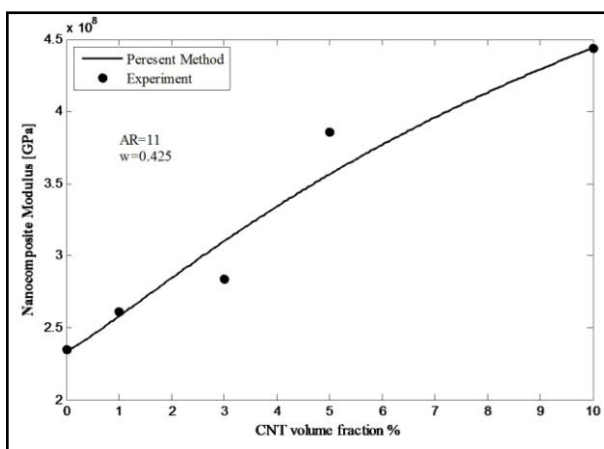


Fig. 4. Comparison of the Young's moduli of CNT-reinforced composite at different volume fraction of CNT with the experimental data

The results shown in Table 3 reveal that the modulus of elasticity of long as well as short wavy CNTs is lesser than that of straight one. Also, it is very clear from the results that with increase in waviness index, stiffness of nanocomposite decreases. Also, when modulus values of long and short CNTs is compared for the same waviness index; better reinforcement is found in the case of long CNT with reference to short one.

Figure 5 shows the effect of nanotube waviness and the fraction of a nanotube on the value of the effective fiber modulus. Results shown in Figure 5 indicate that the highest stiffness is observed in the case of straight CNT ($w=0.1$). As waviness index increases, values of Young's modulus of nanocomposites decrease. It is seen that for $V_{cn}=0.1$ when $w<0.4$, the effective moduli of the composite decrease drastically with the increase of

w . When $w>0.4$, the variation is not significant. Therefore, for the considered material, the reinforcing efficiency of the CNTs is very sensitive to the waviness when it is less than about 0.4. Our results are in agreement with an argument proposed by Shao et al [26].

Table 3. Variation of the effective reinforcement modulus for different CNT waviness and aspect ratio ($V_{cn}=0.05$)

AR	$w=0$	$w=0.5$	$w=1$	$w=5$
50	7.9137e11	1.6932e11	7.0115e10	4.6551e9
100	2.0878e12	2.7995e11	9.8542e10	5.3134e9
500	4.7041e12	4.6591e11	1.3569e11	5.9452e9
1000	5.0801e12	5.0108e11	1.4176e11	6.0320e9
5000	5.3808e12	5.3203e11	1.4690e11	6.1028e9

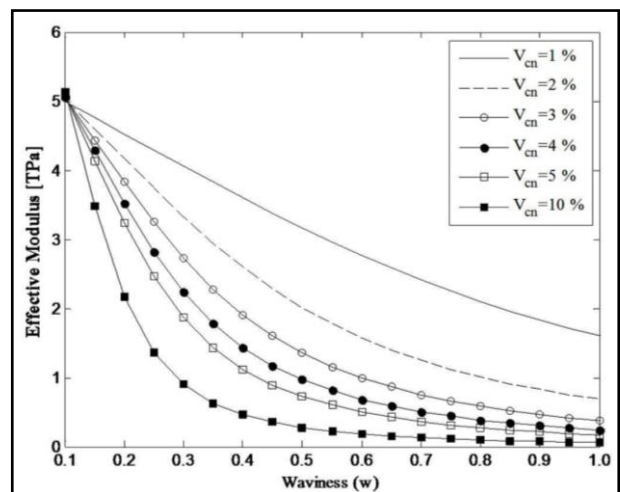


Fig. 5. Predictions of effective reinforcement modulus for nanotubes with AR=1000

Figure 6 shows the effect of increasing the nanotube volume fraction on the composite's Young's modulus. At low volume fractions of nanotube the effect of increasing the waviness of the nanocomposite modulus seems to be minor. As the volume fraction increase, the increase of waviness starts to show significant effect even at low level of waviness. The interesting and new results show that effective Young's modulus of composite with straight CNT ($w=0$) is compared with wavy one, better reinforcement is found for straight CNTs, but for wavy CNT, effective Young's modulus

decreases with increasing the volume fraction which shows an opposite trend compared to straight CNTs.

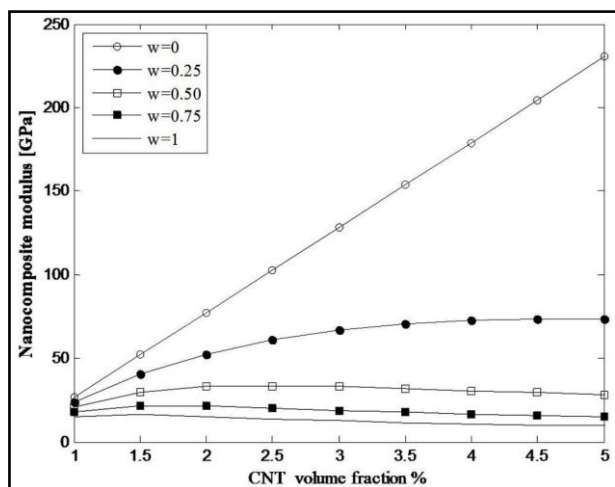


Fig. 6. The effect of nanotube volume fraction on the Young's modulus of nanocomposites for different waviness

CONCLUSIONS

Waviness of carbon nanotubes and interphase region play a critical role in determining their reinforcing efficiency in CNT-reinforced nanocomposites. The studies of these effects on the mechanical properties are of highly theoretical and technological significance for both micro-size and nano-size fibre-reinforced composites. In this study, extended rule of mixture was employed to obtain the mechanical properties of CNT embedded in a polymer matrix with vdW interphase region which is replaced with the developed equivalent fiber. The micromechanics equations cannot capture the scale difference between the nano and micro levels. In order to overcome this difficulty, a virtual equivalent fiber is applied. As noticed the Young modulus of nanotube decreases rapidly with increasing R_{cn} for different value of h^* and then remains almost unaltered for $R_{cn} > 2.8 \text{ nm}$. Results show that, by increasing the values of waviness indices, tensile strength of nanocomposites gets decreased. Also, when modulus values of long and short CNTs is compared for the same waviness index; better reinforcement is found in the case of long CNT with reference to short one. The interesting and new results show that effective Young's modulus of composite with straight CNT

($w=0$) is compared with wavy one, better reinforcement is found for straight CNTs, but for wavy CNT, effective Young's modulus decreases with increasing the volume fraction which shows an opposite trend compared to straight CNTs.

REFERENCES

- [1] Dai H., (2002), Carbon nanotubes: opportunities and challenges. *Surf. Sci.* 500: 218–241.
- [2] Kang I., Heung Y., Kim J., Lee J., Gollapudi R., Subramaniam S., Narasimhadevara S., Hurd D., Kirker G., Shanov V., Schulz M., Shi D., Boerio J., Mall S., Ruggles-Wren D., (2006), Introduction to carbon nanotube and nanofiber smart materials. *Compos. Part B.* 37: 382–394.
- [3] Lau K. T., Gu C., Hui D., (2006), A critical review on nanotube and nanotube/nanoclay related polymer composite materials. *Compos. Part B.* 37: 425–436.
- [4] Thostenson E. T., Ren Z. F., Chou T. W., (2001), Advances in the science and technology of carbon nanotubes and their composites: A review. *Compos. Sci. Technol.* 61: 899–912.
- [5] Odegard G. M., Gates T. S., Wise K. E., Park C., Siochi E. J., (2003), Constitutive modelling of nanotube-reinforced polymer composites. *Compos. Sci. Technol.* 63: 1671–87.
- [6] Griebel M., Hamaekers J., (2004), Molecular dynamic simulations of the elastic moduli of polymer-carbon nanotube composites. *Comput. Meth. Appl. Mech. Eng.* 193: 1773–1777.
- [7] Cadek M., Coleman J. N., Barron V., Hedicke K., Blau W. J., (2002), Morphological and mechanical properties of carbon-nanotube-reinforced semicrystalline and amorphous polymer

- composites. *Appl. Phys. Lett.* 81: 5123–5125.
- [8] Thostenson E. T., Chou T. W., (2003), On the elastic properties of carbon nanotube-based composites: modelling and characterization. *J. Phys—Appl. Phys.* 36: 573–82.
- [9] Fidelus J. D., Wiesel E., Gojny F. H., Schulte K., Wagner H. D., (2005), Thermo-mechanical properties of randomly oriented carbon/epoxy nanocomposites. *Compos. Part. A.* 36: 1555–1561.
- [10] Bonnet P., Sireude D., Garnier B., Chauvet O., (2007), Thermal properties and percolation in carbon nanotube–polymer composites. *J. Appl. Phys.* 91: 2019–2030.
- [11] Han Y., Elliott J., (2007), Molecular dynamics simulations of the elastic properties of polymer/carbon nanotube composites. *Comput. Mater. Sci.* 39: 315–323.
- [12] Zhu R., Pan E., Roy A. K., (2007), Molecular dynamics study of the stress–strain behavior of carbon-nanotube reinforced Epon 862 composites. *Mater. Sci. Eng. A.* 447: 51–57.
- [13] Gojny Florian H., Wichmann H. G., Fiedler B., Schulte K., (2005), Influence of different carbon nanotubes on the mechanical properties of epoxy matrix composites – A comparative study. *Compos. Sci. Tech.* 65: 2300–2313.
- [14] Shadya E., Gowayed Y., (2010), Effect of nanotube geometry on the elastic properties of nanocomposites. *Compos. Sci. Tech.* 70: 1476–1481.
- [15] Peter W., Pius M., Ludwig K. L., Ursula Dettlaff W., Frank K., Siegmars R., Wendelin J., Stark A. B., (2007), The degree and kind of agglomeration affect carbon nanotube cytotoxicity. *Toxic. Lett.* 168: 121–131.
- [16] Karl P., Ramanan K, Peter F. G., (2007), The role of interfacial interactions in the dynamic mechanical response of functionalized SWNTEPS nanocomposites. *Polymer.* 48: 3540e3545.
- [17] Tsai J. L., Tzeng, S. H., Chiu, Y. T., (2010), Characterizing elastic properties of carbon nanotubes/polyimide nanocomposites using multi-scale simulation. *Composites: Part B.* 41: 106–115.
- [18] Shokrieh M., Roham R. M., (2010), Prediction of mechanical properties of an embedded carbon nanotube in polymer matrix based on developing an equivalent long fiber. *Mech. Res. Commun.* 37: 235–240.
- [19] Shokrieh M., Roham R. M., (2010), On the tensile behavior of an embedded carbon nanotube in polymer matrix with non-bonded interphase region. *Compos. Struct.* 92: 647–652.
- [20] Montazeri A., Javadpour j., Khavandi A., Tcharkhtchi A., Mohajeri A., (2010), Mechanical properties of multi-walled carbon nanotube/epoxy composites. *Mater. and Desig.* 31: 4202–4208.
- [21] Martone A., Faiella G., Antonucci V., Giordano M., Zarrelli M., (2011), The effect of the aspect ratio of carbon nanotubes on their effective reinforcement modulus in an epoxy matrix. *Compos. Sci. Tech.* 71: 1117–1123.
- [22] Gou J., Minaei B., Wang B., Liang Z., Zhang C., (2004), Computational and experimental study of interfacial bonding of single-walled nanotube reinforced composites. *J. Comput. Mater. Sci.* 31: 225–36.
- [23] Battezzatti L., Pisani C., Ricca F., (1975), Equilibrium conformation and surface motion of hydrocarbon molecules physisorbed on graphite. *J. Chem. Soc.*, 71: 1629–39.
- [24] Yakobson B. I., Brabec C. J., Bernholc J., (1996), Nanomechanics of carbon

nanotubes: Instabilities beyond linear response. *Phys. Rev. Lett.* 76: 2511–2514.

- [25] Yao X., Han Q., Xin H., (2008), Bending buckling behaviors of single- and multi-walled carbon nanotubes. *Comp. Mater. Sci.* 43: 579–590.
- [26] Shao L. H., Luo R. Y., Bai S. L., Wang J., (2009), Prediction of effective moduli of carbon nanotube–reinforced composites with waviness and debonding. *Compos. Struc.* 87: 274–281.

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