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Multiscale prediction of thermal conductivity for nanocomposites containing crumpled carbon nanofillers with interfacial characteristics

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ABSTRACT

The importance of the thermal conductivity of engineering plastics reinforced with nanofillers is increasing in various industries, and the need for a model with which to make reliable predictions continues. We propose a micromechanics-based multiscale model that considers multi-shaped nanofillers to predict the thermal conductivity of composites. The distribution of each phase is assumed to be probabilistically distributed, and the Kapitza resistance at the interface between the filler and matrix was calculated by means of a molecular dynamics simulation. A polybutylene terephthalate (PBT) composite system embedded with multi-walled carbon nanotubes (MWCNTs) was used in a specific simulation. Composites containing MWCNTs of different lengths were also fabricated to obtain appropriate experimental results for the verification of the proposed model. Fourier-transform infrared (FT-IR) spectroscopy, Raman spectroscopy, and field-emission scanning microscopy (FE-SEM) were carried out to confirm that the selected materials could suitably be compared. Finally, the proposed model was applied to the finite element method to examine the heat flux of the composites according to the constitutive properties, and their results were compared to the experimental results.

1. Introduction

It is well known that the physical properties of conventional plastics can be improved by incorporating nanofillers into the polymer material [1]. Specifically, heat is easily released to the outside when the thermal conductivity of a material is increased; thus, these materials can be used as substrates and as protective coverings for electronic devices, automobiles, and airplanes. Conversely, when the thermal conductivity of the material is lowered, it can serve as a nonflammable material because this process makes the material resistant to flame. Hence, if we can reliably predict the thermal conductivity of polymer-based composite materials, which currently play important roles in industry, the impact will be substantial and will ultimately lead to reductions in the manufacturing time and in the cost of the related parts. Many researchers agreed that the most essential factor when attempting to predict the thermal conductivity of nanocomposites is the correlation between the nanofillers and matrix. However, theoretical modeling has yet to be fully established. In this study, the interface and filler shape are considered as the most important factors in an analysis of a composite material, and in relation to this, a micromechanics-based multiscale methodology is proposed.

Micromechanics was originally developed to predict the mechanical behavior of a composite material [2]; however, a theoretical approach in mechanics can be modified to determine the thermal properties of a composite based on the relationship below [3]:

$$\sigma = \mathbf{C}^* \cdot \varepsilon \leftrightarrow q = -\mathbf{K}^* \cdot \nabla T \quad (1)$$

where σ, $\mathbf{C}^*$, and ε denote the stress, effective stiffness, and strain, respectively; and q, $\mathbf{K}^*$, and ∇T correspondingly denote the heat flux, effective thermal conductivity, and thermal gradient. The micromechanics-based method has proven to be effective for predicting the behaviors of multi-phase composites over the last twenty years [4–6], and recent works also prove that it can be applied to determine the effective thermal conductivity [1,7]. Many researchers have proposed multiscale strategies to evaluate the thermal conductivity of carbon nanofiller-reinforced composites

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[8–10]. In the present study, the crumpled nanofillers were assumed to be probabilistically distributed, and the interfacial Kapitza resistance between the filler and the matrix was calculated in a molecular dynamics (MD) simulation. The established model was then applied to the finite element method (FEM) to examine heat flux of composites according to the constitutive properties.

In order to carry out the specific simulations in this study, it was necessary to use a relatively typical composite system. Polybutylene terephthalate (PBT) plastic is a crystalline resin with excellent heat resistance among various engineering plastics, and it was selected as the matrix material in this study. In addition, multi-walled carbon nanotubes (MWCNTs) are among the most commonly studied nanofillers to improve the thermal conductivity of composites. Hence, composites containing MWCNTs of different lengths and contents were considered here, and such specimens were fabricated for the verification of the proposed model. Fourier-transform infrared (FT-IR) spectroscopy, Raman spectroscopy, and field-emission scanning microscopy (FE-SEM) analyses were utilized here to confirm the feasibility of comparing the selected materials.

2. Theory

2.1. Micromechanics-based model for multi-phase nanocomposites

In this section, we consider multi-phase composite systems (see Fig. 1) consisting of a polymer matrix (phase 0) and a perfectly expanded nanofiller (phase 1). During the process in which the fillers are mixed with the matrix, some of the fillers will bend slightly (phase 2) and others will bend severely (phase 3). Some of them will be bent greatly and will exist as a spherical agglomeration, typically in the shape of a sphere (phase 4). Hence, a total of five different phases are present in a single composite material, and the effective thermal conductivity of the composites containing unidirectionally aligned and variously crumpled fillers can be expressed in terms of micromechanics by the following equation,

$$\mathbf{K}^{*} = \mathbf{K}_0 \cdot \left[\mathbf{I} + \sum_{r=0}^{4} \left\{ \phi_r (\mathbf{S}_r + \mathbf{A}_r)^{-1} \cdot \left[\mathbf{I} - \phi_r \mathbf{S}_r \cdot (\mathbf{S}_r + \mathbf{A}_r)^{-1} \right]^{-1} \right\} \right] \tag{2}$$

where $\mathbf{A}_r = (\mathbf{K}_r - \mathbf{K}_0)^{-1} \cdot \mathbf{K}_0$; $\mathbf{K}_r$ and ϕ_r correspondingly denote the thermal conductivity and volume fraction of the r-phase, and $\mathbf{I}$ refers to an identical tensor.

Herein, the crumpled filler was regarded as a simple spheroidal inclusion, which is relatively easy to express mathematically. Assuming that the shape of the spheroidal filler differs depending on the degree of bending (Fig. 1), it can be applied to a micromechanical formulation with the help of Eshelby's tensor. The spheroidically shaped Eshelby's tensor $\mathbf{S}$ is defined as follows [3]:

$$(S_{11})_r = (S_{22})_r = q_r/2, \quad (S_{33})_r = 1 - q_r, \quad (r = 1,\ 2,\ 3) \tag{3}$$

with

$$q_r = \frac{\alpha_r}{(\alpha_r^2 - 1)^{1.5}} \left\{ \alpha_r \left(\alpha_r^2 - 1 \right)^{0.5} - \cosh^{-1} \alpha_r \right\} \tag{4}$$

In Eq. (5), α_r is the aspect ratio of the filler corresponding to the r-

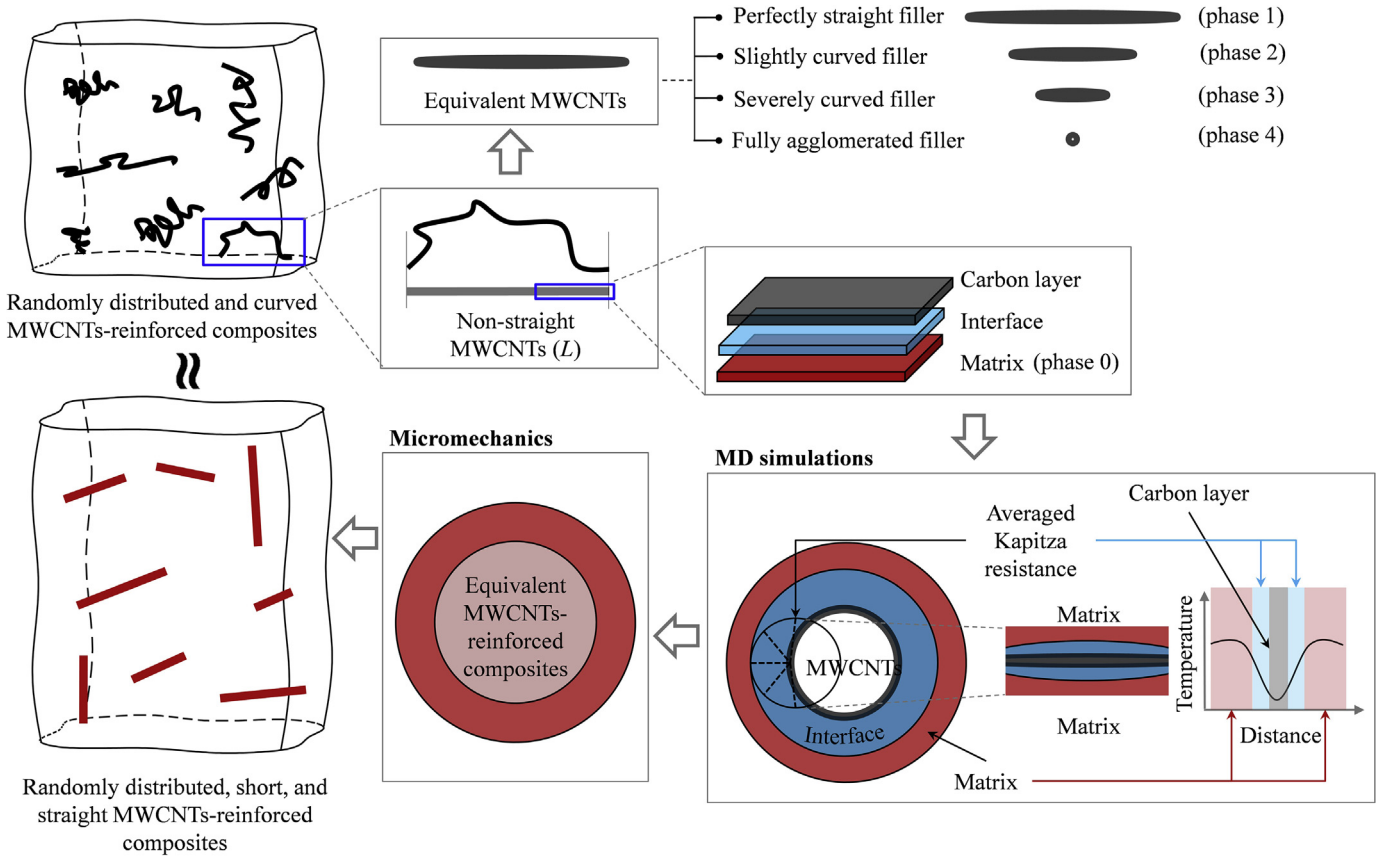

Fig. 1. A schematic diagram of the considered multi-phase composite system in the present study: the proposed two-step multiscale modeling composed of micromechanics and MD simulation.

phase. In this paper, it is assumed that the aspect ratio of the fillers in each phase is defined as

$$\alpha_r = \begin{cases} L/d, & (r = 1) \\ \ln(\alpha_{r-1}), & (r = 2 \text{ and } 3) \end{cases} \tag{5}$$

where L and d denote the length and diameter (or thickness) of the filler, respectively. When the filler is completely agglomerated and has a spherical shape, $\mathbf{S}_4$ can simply be expressed as $(S_{11})_4=(S_{22})_4=(S_{33})_4=1/3$.

The bending level of fillers can vary depending on the combination of the constituent materials or on the method used to fabricate the specimen. It is nearly impossible to determine the degree of bending quantitatively; thus, a probabilistic method is applied in the present study. Weibull's probabilistic function [11] has been used to solve various engineering problems as an effective means of expressing the occurrence of certain phenomena. The distribution of the fillers corresponding to each phase in this study is described by modifying Weibull's model, as follows [12]

$$\begin{aligned} &\phi_1 = \phi - \overline{\phi}_2, \quad \phi_2 = \overline{\phi}_2 - \overline{\phi}_3, \quad \phi_3 = \overline{\phi}_3 - \phi_4, \\ &\phi_4 = \overline{\phi}_3[1 - \exp\{-(S_0)^M\}], \\ &\overline{\phi}_3 = \overline{\phi}_2[1 - \exp\{-(S_0)^M\}], \\ &\overline{\phi}_2 = \phi[1 - \exp\{-(S_0)^M\}] \end{aligned} \tag{6}$$

where S_0 and M are probability constants that determine the filler bending distribution. Lastly, the following orientation averaging process is applied to determine the effective thermal conductivity of composites reinforced with randomly oriented fillers [13],

$$\overline{\mathbf{K}^*} = \frac{1}{4\pi} \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} \mathbf{K}^* \cdot \mathbf{Q} \cdot \mathbf{Q} \sin\theta \mathrm{d}\theta \mathrm{d}\varphi \tag{7}$$

where $\mathbf{Q}$ represents the rotation matrix, which can be expressed as follows [14]

$$\mathbf{Q} = \begin{bmatrix} \cos(\varphi) & -\sin(\varphi) & 0 \\ \cos(\theta)\sin(\varphi) & \cos(\theta)\cos(\varphi) & -\sin(\theta) \\ \sin(\theta)\sin(\varphi) & \cos(\varphi)\sin(\theta) & \cos(\theta) \end{bmatrix} \tag{8}$$

The interface between the matrix and the fillers is also an important aspect to consider when predicting realistic properties of complex composite systems. In order to consider the influence of the interface on composites, the thermal conductivity of filler in the r-phase is defined as [15]: $\mathbf{K}_r^i=(\mathbf{K}_r L)/(2\mathbf{K}_r R_{\mathrm{Kap}} + L)$, where $\mathbf{K}_r^i$ is the thermal conductivity of the r-phase considering the interface effect and R_{kap} signifies the Kapitza resistance, which is calculated through MD simulations.

2.2. MD simulations

An atomistic MD simulation is carried out to determine the reliable value of the Kapitza resistance, R_{kap}. As a typical system, we consider the PBT composite here, where a carbon layer is embedded in the matrix. In order to investigate the difference between an ordinary polymer and a composite, the two systems shown in Fig. 2 were subjected to calculations in the present MD simulations. The simulation cells consist of a single linear PBT chain composed of 136 repeating-unit monomers ($M_{\mathrm{w}} \approx 30$ kDa) and carbon layer (3.3 nm^2).

The Forcite module of Materials Studio 2017 is used for the MD simulation and the COMPASS II force field (FF) is adopted to describe the interatomic potential. The carbon layer is inserted into the PBT matrix in a Grand Canonical Monte Carlo (GCMC) simulation, and a dynamics simulation (NPT) is carried out in the isothermal-isobaric ensemble at 1 atm and 298 K for 10–100 ns until the volume of the atomistic system converges to the equilibrium quantity [16,17]. A dynamics simulation (NVT) in the canonical ensemble is then conducted at 298 K for 30–200 ns while fixing the volume of the cell at the converged value from NPT simulation.

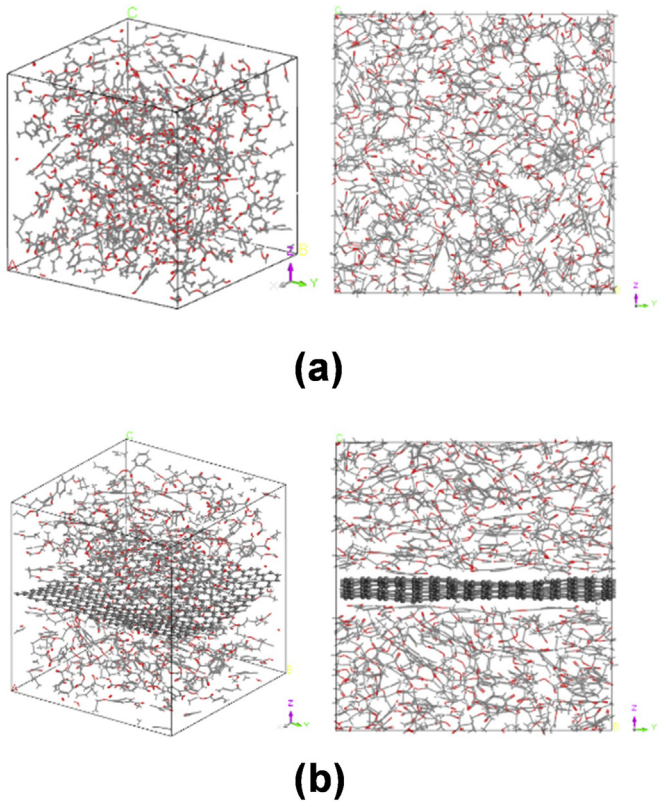

Fig. 2. The final snapshot after the whole MD procedure of the (a) PBT matrix ($M_w \approx 30$ kDa) and (b) PBT nanocomposites with carbon layer (3.3 nm^2).

The thermal properties of the polymer and composite are calculated based on the reverse non-equilibrium molecular dynamics (RNEMD) method [18]. The optimal atomistic structure is required for the simulation, and we applied the final 1 ns NVT simulation trajectories to the RNEMD method. Using the RNEMD method, the simulation cell is divided into 20 layers, after which different velocities are assigned to the molecules. The thermal characteristics are predicted by analyzing the changes occurring thereon. The predicted temperature gradient and heat flux of the two atomistic systems are used to calculate the value of R_{kap} [19,20] according to $R_{\mathrm{Kap}} = \Delta T/J$, where ΔT and J correspond to the temperature drop and associated heat flux across the interface.

3. Experiment

3.1. Materials and fabrications

In the present study, polybutyleneterephthalate (PBT) resin (LUPOX GP1000M, LG chemistry co., Korea) was utilized as the matrix. The density, melting point, and melt flow rate of the matrix measured on the basis of ASTM D792, ASTM D3418, and ASTM D1238 were 1.29 g/cc, 223 °C, and 34 g/min, respectively. Two different lengths of MWCNT (Jeio Co., Korea) were used as a filler material to improve the thermal conductivity. The lengths of the short MWCNT (Jeno tube 9) and the long MWCNT (Jeno tube 8)

Table 1
Physical properties of utilized materials in the present study.

		Density (g/cc)	Diameter (nm)	Length (μm)
PBT matrix		1.29	–	–
MWCNT	short	2.10	7–10	10–50
	long			100–200

were 10–50 μm and 100–200 μm, respectively, and the diameters of both types were similar at, 7–10 nm. The physical properties of materials utilized in the present study are listed in Table 1.

The manufacturing process of the composite specimens is presented in Fig. 3. MWCNT fillers were incorporated into the PBT resin at a target ratio (Table 2) and mixed using a Haake Rheomix internal mixer (HAAKE™ Rheomix 600R OS Mixer, Thermo scientific Inc., Marietta, GA, USA) at a screw speed of 60 rpm for 30 min at 250 °C. Pressure of 20 MPa for 20 min at 250 °C using a heating press (D3P-30J, Daheung Science, Incheon, Korea) was then applied to the mixture. The composites were poured into 2.5 cm^2 square mold which was 2 mm thick, and then cooled to room temperature with cooling water.

3.2. Characteristics

A FT-IR spectroscopy (Nicolet 6700, Thermo Scientific, USA) analysis was conducted to confirm the surface chemistry of the MWCNTs, which may affect the properties of the interface with the PBT resin. The measurement was carried out in the range of 500–4000 cm^{-1} and at a resolution of 16 cm^{-1}. In addition, the Raman spectra (LabRAM HR 800, HORIBA Jobin Yvon, Japan) were analyzed to evaluate the structural defects of the two types of MWCNTs. The Raman spectra analysis was conducted using a 514-nm Ar-ion laser. In order to observe the degree of MWCNT dispersion in the composites, the MWCNT/PBT composites were frozen with liquid nitrogen and then crushed. The crushed samples were surface-coated with platinum using a sputter coating machine (Ion Sputter E-1030, Hitachi High Technologies, Japan) for 120 s in a vacuum state. The dispersibility and surface morphology were observed through FE-SEM (Nova NanoSEM 450, FEI Corp., USA) while applying voltage of 10 kV in a nitrogen stream.

The thermal conductivity of the composite specimens was measured using a thermal conductivity measuring instrument (TPS 2500 S, Hot Disk ab, Sweden) at room temperature and normal pressure according to ISO 22007-2. The sensor belonging to the instrument consists of a double spiral of thin nickel wire and operates as a heat source. The sensor supplies a constant power (P) to induce a temperature rise (ΔT), and the corresponding temperature is measured by converting the sensor resistance change. The thermal conductivity of the specimens was determined by solving the Fourier equation based on the supplied P and measured ΔT values.

4. Results and discussion

4.1. Theoretical results

The results of a parametric analysis based on the proposed model are presented in Figs. 4 and 5. The material and model parameters adopted in the simulations were as follows: $K_0 = 0.2976$ W/m·K, $K_1 = 1950$ W/m·K, $d = 8.5$ nm, $L = 30$ μm, $R_{kap} = 1E\text{-}8$ m^2K/W, $S_0 = 5$, and $M = 0.5$. First, the effect of the filler orientation on the thermal conductivity of the composites was predicted, as can be observed in Fig. 4(a). The predicted thermal conductivity of the composite with aligned filler materials exhibits much higher values compared to that with randomly oriented filler materials. In addition, with the same amount of filler, longer filler materials appear to improve the effective thermal conductivity of the composites (Fig. 4(b)). The simulated thermal conductivity of the composites according to the model constants (S_0 and M) are shown in Fig. 5(a) and (b). It was found that the thermal conductivity of the composites decreases exponentially with an increase of both model constants. However, when S_0 and M exceed 5 and 0.5, respectively, the thermal conductivity of the composites converges to the matrix level.

Fig. 6 shows the temperature distribution in the PBT matrix and in the carbon layer-embedded PBT composites. On the same

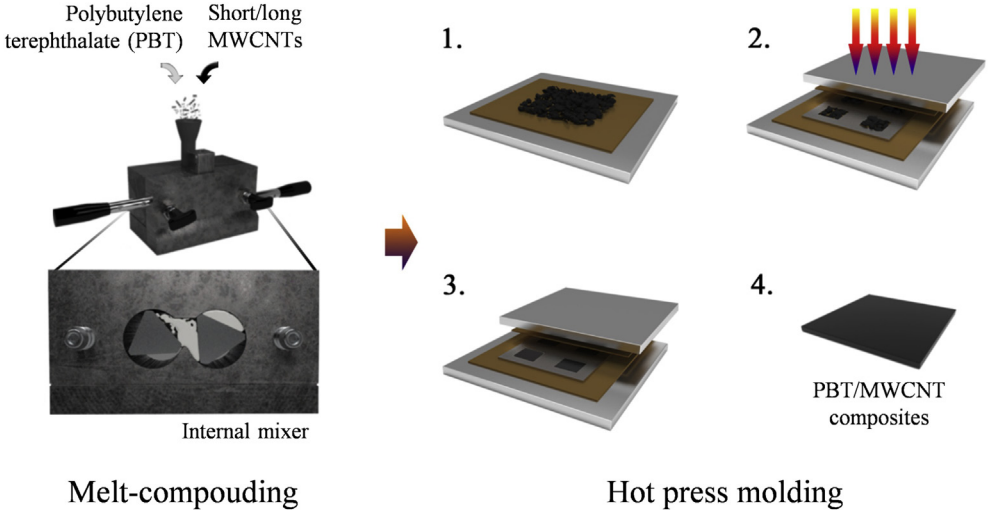

Fig. 3. Manufacturing process of composite specimens composed of PBT resin with highly dispersed MWCNT fillers.

Table 2
Material constituents of composites containing short and long MWCNTs.

Filler contents		Thermal conductivity	
weight fraction (%)	volume fraction (%)	short MWCNT (W/m·K)	long MWCNT (W/m·K)
0.00	0.00	0.298	0.298
0.50	0.31	0.327	0.332
1.00	0.62	0.353	0.358
3.00	1.89	0.451	0.484
5.00	3.13	0.547	0.600
10.00	6.39	0.646	0.811
12.00	7.73	0.860	1.032
15.00	9.78	1.050	1.375
20.00	13.31	1.170	1.652

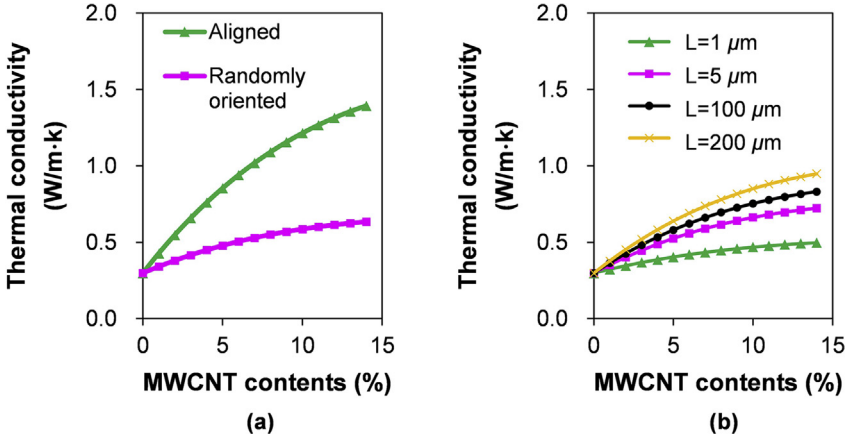

Fig. 4. The present predicted thermal conductivity of (a) aligned/3D randomly oriented and (b) different length (1–200 μm) of MWCNTs-reinforced nanocomposites.

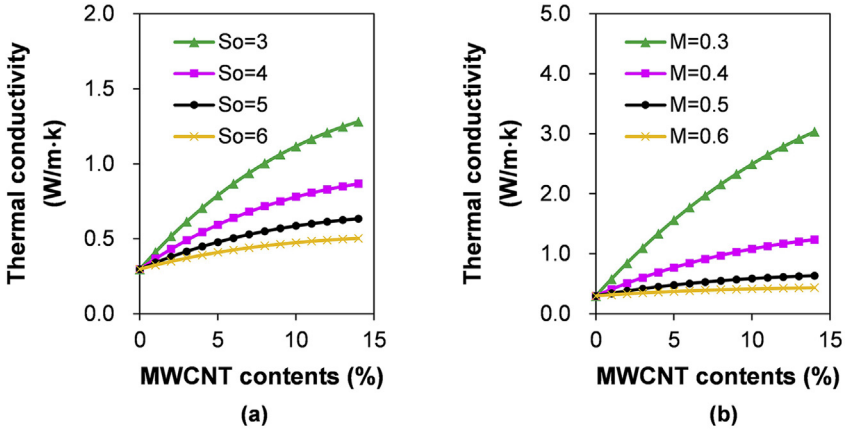

Fig. 5. Influences of the model constants on the overall thermal conductivity of nanocomposites: (a) S_0 and (b) M.

temperature scale, a clear difference between the two systems can be recognized. Specifically, the interfacial layer is distinctly defined in the composites. The values of $\overline{\mathbf{K}^*}$ and R_{Kap} for each system were calculated based on the results presented in Fig. 7. The thermal conductivity of the PBT polymer was calculated and found to be 0.244 W/m·K, similar to the values in the literature [21,22], confirming the validity of the present MD simulation. R_{Kap} was calculated from the temperature gradient and estimated to be 0.204×10^{-8} m^2 K/W. The calculated value of R_{Kap} is also similar to previously measured and simulated values [23,24], and this value was applied in the remaining analyses here.

4.2. Experimental results

The FT-IR spectroscopy results are shown in Fig. 8(a). It can be observed that the major peaks were similar, with an O-H peak of 3430 cm^{-1} and a C-H peak of 2915 cm^{-1}, indicating that the two types of MWCNTs have similar surface properties. It can therefore be concluded that the interfacial characteristics according to the MWCNT length have little effect on the composites and that the same interface constant is applicable in the simulation. The Raman analysis results in Fig. 8(b) show the D peak at 1338 cm^{-1}, the G peak at 1580 cm^{-1}, and the 2D peak at 2670 cm^{-1}. The D peak stems

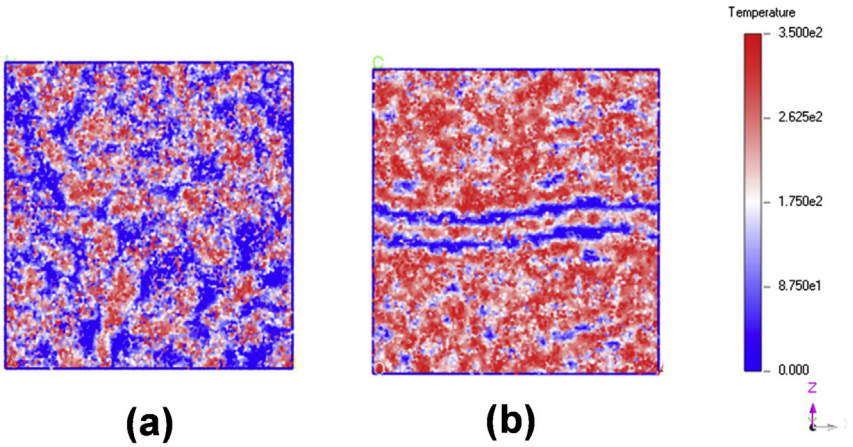

Fig. 6. The distribution of the temperatures in (a) PBT matrix and (b) carbon layer-embedded PBT composites.

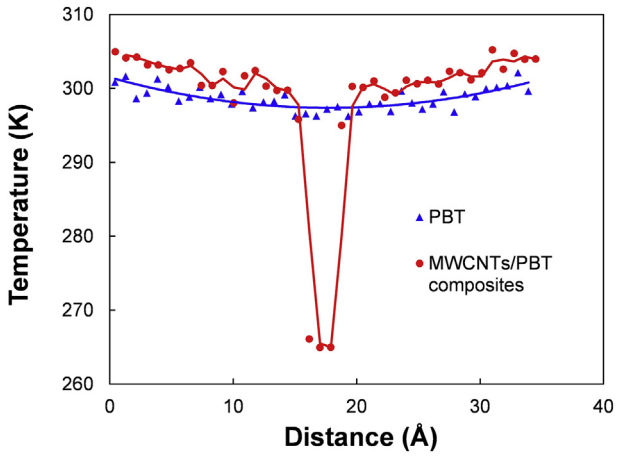

Fig. 7. The calculated temperatures of the PBT matrix and composites from MD simulations with respect to depth of atomistic structures.

from the amorphous structure and the defects, and the intensity of the peak is pronounced when the defects of the MWCNTs and the sp3 bonds increase. In addition, the G peak is generated by the in-plane phonon mode and is common to graphite materials. The defect level of the MWCNTs can be evaluated by the ratio of the intensities of the D and G peaks (ID/IG ratio). The ID/IG ratios of the long and short MWCNTs were found to be 1.38 and 1.13, respectively, and the degree of defects in the long MWCNTs was slightly greater. However, the effect of the difference in the filler defects on the thermal conductivity is expected to be negligible given that the gap between the two values is quite small.

A SEM image of the fracture surface of the MWCNT-embedded composite fabricated by the proposed process is shown in Fig. 9 according to the weight fraction of the filler (1, 3, 10, and 20 wt%). This outcome shows that the filler incorporated into the composite shows good dispersibility throughout the fracture surface regardless of the weight fraction up to 20 wt%. Table 2 presents the measured thermal conductivity levels of the composites according to the mixing ratio (weight and volume fractions) of the MWCNTs.

The thermal conductivity of the composites was observed to increase gradually as the incorporated amount of MWCNT was increased. The different effects of the filler length on the thermal conductivity stem from the phonon scattering phenomenon. It is known that the thermal conductivity of carbon/polymer

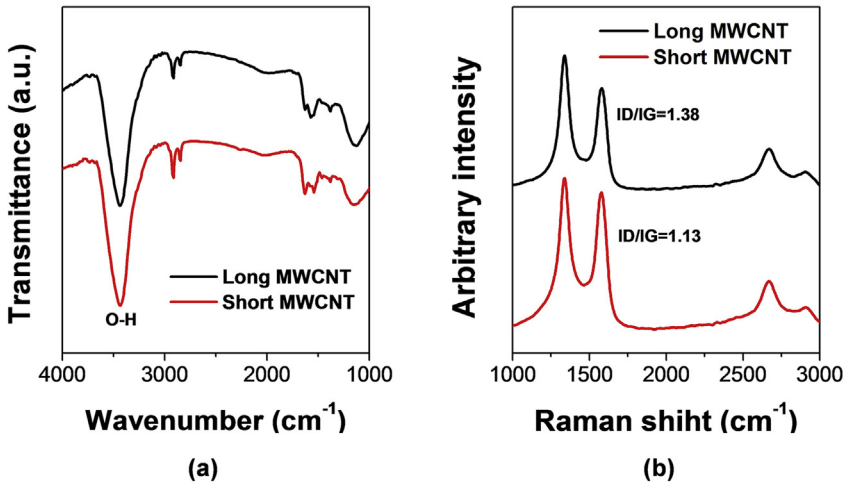

Fig. 8. Results of (a) FT-IR and (b) Raman analyzes of utilized MWCNT fillers.

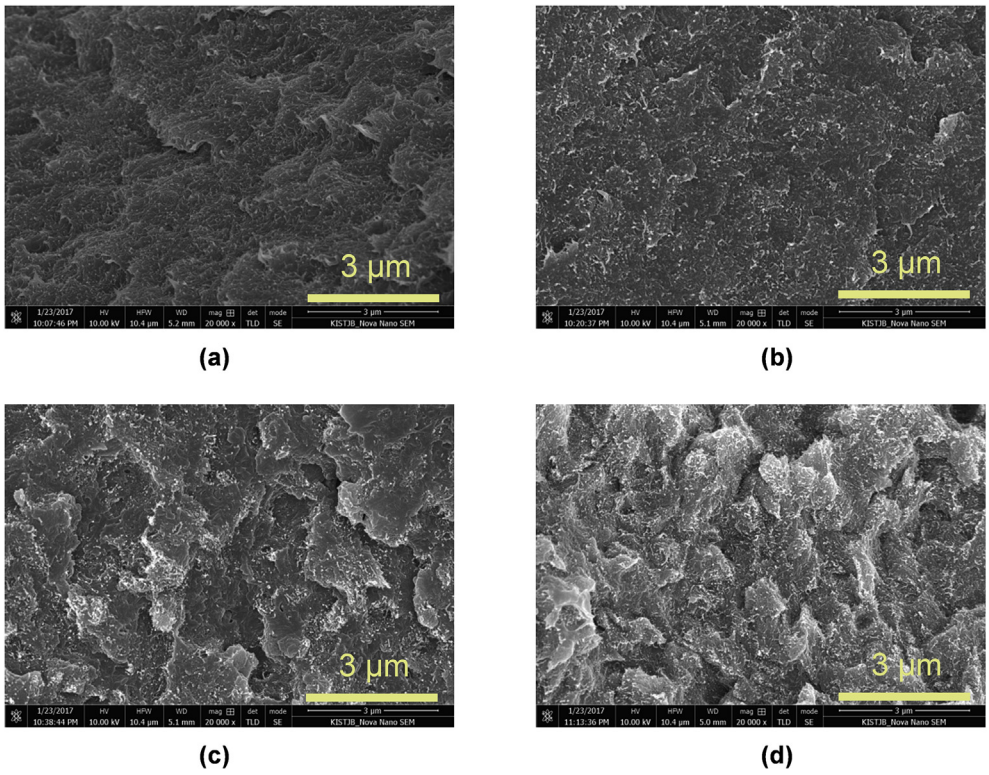

Fig. 9. SEM images of the fracture surface of composites containing (a) 1 wt%, (c) 3 wt%, (e) 10 wt%, and (f) 20 wt% of MWCNTs.

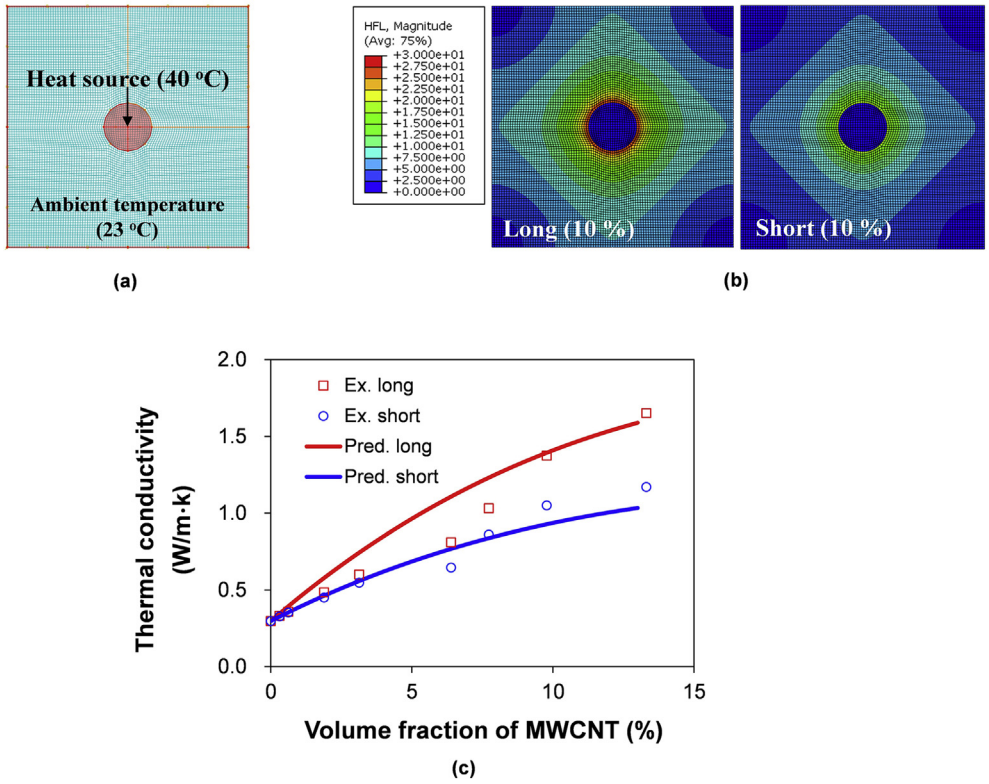

Fig. 10. (a) Layout of the FEM simulation, (b) predicted heat flux in a structure reinforced with different length of MWCNT, and (c) the comparison of thermal conductivities of nanocomposite between prediction and experimental data.

composites is mainly determined by phonon (vibration of lattice) transport between the filler materials. The interfacial thermal resistance between the filler and the matrix interferes with the transfer of phonons, which limits the enhancement of the thermal conductivity. Thus, based on the above-mentioned mechanisms, it can be concluded that composites incorporating long MWCNTs have higher thermal conductivity than that of composites with short MWCNTs.

4.3. Comparisons between the predictions and measurements

A FEM analysis was carried out to investigate the effects of the difference in the thermal conductivity on the heat flux of the composites. The layout of the FE simulation is illustrated in Fig. 10(a), and the predicted heat flux in the specimen reinforced with different lengths of MWCNTs is presented in Fig. 10(b). It can be confirmed that more heat flux occurs when the thermal conductivity of the composite is high, assuming that MWCNTs at a rate of 10% are incorporated into the PBT.

In addition, the validity of the proposed multiscale analysis method was verified in comparison with the experimental results. To confirm reliability of the proposed framework further, PBT composite specimens incorporating both short and long MWCNTs were compared. Although there was some divergence, Fig. 10(c) indicates that the predictions are in good agreement with the experimental results in all cases. The lengths of the short and long MWCNTs used here were 30 μm and 150 μm, respectively.

5. Conclusions

A multiscale analysis method combining probabilistic micromechanics, MD simulations, and FEM analyses was proposed in this study. The predictions show that the factors considered in the present study have a significant impact on the results of the proposed analysis method. Related experiments were also conducted to verify the validity of the simulation, and the process and results of the study were described. By comparing the predictions with outcomes in the literature and with experimental results, it was proved that the proposed MD and multiscale approaches are valid. For the model application, analyses of PBT composites reinforced with MWCNTs as a filler material was conducted with a target system.

It is obvious that the nanofillers can exist in a wide variety of forms inside the matrix. In this study, the nanofillers were divided into four representations: perfectly expanded, slightly bend, severely bend, and spherical agglomeration. However, it was for convenience of calculation, and should be divided into hundreds of forms in filler. The simplified method with the above assumption may lead a slight overestimation or underestimation of the material performances. Despite the limitations, the proposed methodology is expected to be applicable to various composite systems, such as metal/ceramic matrixes containing graphite/graphene filler materials, and future studies will take this direction.

Acknowledgements

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