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Evaluation and modelling of electrically conductive polymer nanocomposites with carbon nanotube networks

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ABSTRACT

Superior electrical, thermal, and mechanical properties of carbon nanotubes (CNTs) have made them effective filler for multifunctional polymer nanocomposites (PNCs). In particular, electrically conductive PNCs filled with CNTs have been researched extensively. These studies aimed to increase the PNCs' electrical conductivity (σ) and to minimize the percolation thresholds (ϕ_c). In this work, we have developed an improved model to describe the CNT networks and thereby evaluate the PNCs' ϕ_c and σ. The new model accounts for the electrical conductance contributed by the continued CNT network across the boundary of adjacent representative volume elements. It more realistically represents the interconnectivity among CNTs and enhances the evaluation of the structure-to-property relationship of PNCs' σ.

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1. Introduction

Possessing superior electrical, thermal, and mechanical properties, carbon nanotubes (CNTs) [1–5] are considered powerful and effective filler for tailoring the multifunctional properties of polymer nanocomposites (PNCs) [6]. In particular, due to their exceptionally high intrinsic electrical conductivity and high aspect ratio, it is possible to embed only a small amount of CNTs in a polymer matrix to achieve significant enhancement in the PNC's electrical conductivity (σ). Small CNT loadings also allow PNCs to maintain the favorable properties of polymers, including low density, high chemical resistance, and good processability. Accordingly, PNCs filled with CNTs have received much attention for their many potential applications, such as field emission [7], lightning strike protection [8], highly sensitive strain sensors [9–11], and electromagnetic-wave interference materials [12].

The insulator-to-conductor transition of PNCs through the addition of conductive fillers can be modelled by the percolation theory [13]. According to the theory, there exists a critical concentration of CNTs over which further increase in CNT loading would make the PNC become electrically conductive. This critical concentration, namely percolation threshold (ϕ_c), signals the formation of the first conductive path bridging the two terminals of the polymer matrix. This theory is mathematically represented by Equation (1).

$$\sigma = \sigma_0(\phi - \phi_c)^t \text{ for } \quad \phi > \phi_c \tag{1}$$

where σ_0 is a physical parameter commonly attributed to the intrinsic conductivity of CNTs; and t is the critical exponent, which is known to be dominated by the dimensionality of the system.

The ϕ_c of PNCs filled with CNTs have been reported to range from 0.0025 wt.% [14] to 10.5 wt.% [15]. Upon further increase in CNT loading in a polymer matrix over ϕ_c, PNC's σ will gradually increase and reach a maximum plateau. While extensive research has focused on minimizing ϕ_c [16], maximizing PNC's σ has been another objective in the development of CNT–filled PNCs. To the best of the authors' knowledge, the highest σ reported (i.e., approximately 3000 S/m) was achieved by Kim *at al.* with a PMMA-MWCNT nanocomposite [12].

Extensive experimental studies have shown that PNCs' ϕ_c and σ depend on many factors including the dispersion, alignment and aspect ratio of CNTs. Aguilar et al. reported a decrease in PNCs' ϕ_c due to lightly agglomerated dispersion state of CNTs [17]. Variation in the dependence of PNCs' ϕ_c on CNTs' degree of alignment in PNCs with different CNT contents was reported by Du et al. [18]. Using CNTs with higher aspect ratios, significant enhancement in PNC's σ was achieved by Yao et al. [19].

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In addition to experimental studies, fundamental understanding of the conductive percolation mechanism has been established through several theoretical and numerical studies. A number of these studies modelled interconnecting CNTs as random resistor networks embedded in a polymer matrix. The random CNT resistor network model has been progressively developed from two-dimensional (2D) [20] to multi-layered 2D [21] to three-dimensional (3D) [22,23] scale. In the 3D model, a representative volume element (RVE) is assumed to be periodically repeated to represent the PNC. Hu et al. [22] considered the CNTs extruding through the RVE's boundary surface to be part of the adjacent RVE by cutting the extruding portion and relocating it onto the opposite boundary surface. However, such approach overlooks the interconnectivity of CNTs across the boundary surface and requires a RVE of large volume in order to achieve numerical convergence. In this context, Bao et al. [23] extended the modelling scheme by considering periodically connective paths on opposite surfaces of RVE. Nevertheless, there are still some possible cases of interconnecting CNTs across the boundary surfaces of adjacent RVEs that are disregarded under this approach. Furthermore, the "cut-and-relocate" approach, which adopted in both studies to handle CNTs extruding out of the RVE, would lead to immediate increase in the number of CNTs in contact with the two terminals, and thereby generated unnecessary bias on the random distribution of CNTs in the polymer matrix.

Along with periodicity, dimensions of the RVE have been identified as a critical factor in ensuring accuracy and efficiency of the simulation. There have been some discussions on the appropriate dimensions of RVE to model the electrical properties of PNCs [23]. In particular, most numerical studies based on 3D models utilize cubic RVEs to capture isotropic percolation of CNTs inside the polymer matrix [22,23]. However, Shklovskii et al. [24] theoretically analyzed two-component systems containing metallic and dielectric regions of isotropic geometry and established that the macroscopic conductivity of such a network could be anisotropic. Percolative conductive systems with high aspect ratio fillers such as CNTs are more likely to be anisotropic. Such concept of anisotropic percolation behaviors for CNT-filled PNCs was experimentally supported by Fu et al. [25]. Their study demonstrated the influence of the test sample's thickness, across which σ was measured, on ϕ_c of MWCNT-low density polyethylene (LDPE) nanocomposites. Experimental results showed that the PNC's ϕ_c increased with the sample's thickness. Such observation was rationalized in terms of the probability of CNTs to construct a conductive pathway across opposite surfaces separated by different length scales.

In this study, we have devised a more realistic and efficient modelling tool to account for the interconnectivity of the CNT network across boundary surfaces of adjacent RVEs. In the proposed model, the omission of the "cut-and-relocate" approach, typically used in simulating PNC's σ and ϕ_c, will eliminate the unnecessary bias caused by the immediate increase in the number of CNTs penetrating the RVE's two terminals. Furthermore, the concept of anisotropic percolation behavior was further explored by comparing the variation of simulated PNC's ϕ_c with the change in RVEs' dimensions in different directions (i.e., both parallel and perpendicular to the direction of electrical current flow). The aforementioned fundamental improvements in the proposed model will facilitate the identification of structure-to-property relationship of electrically conductive CNT. In addition, our simulation results showed that the new model allowed further reduction of the RVE's dimensions, and thereby lowered the computation cost of the Monte Carlo simulation without compromising the accuracy of the simulation. By applying the new model to predict PNCs' ϕ_c and σ, the simulation results were compared to experimental data reported in literature [26–28] and also to results from previous numerical studies [22,23]. Furthermore, the effect of preferential alignment of CNTs in PNCs with different CNT loadings was investigated using the new modelling scheme.

2. Theoretical framework

In the simulation model, electrically conductive PNCs can be represented by a cuboid RVE of $L_x \times L_y \times L_z$ embedded with a random distribution of CNTs. A schematic of the cuboid RVE is shown in Fig. 1. Electric current is considered to propagate from the left boundary surface (i.e., high voltage electrode) to the right boundary surface (i.e., low voltage electrode).

2.1. Cuboid representative volume element (RVE) of electrically conductive PNCs

Each CNT is considered as a rigid rod and is represented by a line segment starting from $(x_{i,1}, y_{i,1}, z_{i,1})$ and ending at $(x_{i,2}, y_{i,2}, z_{i,2})$. In order to model the random distribution of CNTs, the coordinates of the starting and ending points are generated by Equations (2) and (3), respectively.

$$x_{i,1} = L_x \cdot rand \tag{2a}$$

$$y_{i,1} = L_y \cdot rand \tag{2b}$$

$$z_{i,1} = L_z \cdot rand \tag{2c}$$

where *rand* is a uniformly distributed random number in [0,1].

$$x_{i,2} = x_{i,1} + L_{CNT} \cos \varphi_i sin\theta_i \tag{3a}$$

$$y_{i,2} = y_{i,1} + L_{CNT} \sin \varphi_i sin\theta_i \tag{3b}$$

$$z_{i,2} = z_{i,1} + L_{CNT} \cos \theta_i \tag{3c}$$

where L_{CNT} is the average length of the CNT; φ_i is the azimuthal angle; and θ_i is the polar angle.

The orientation of CNT_i is defined by the azimuthal and polar angles, which can be generated by Equations (4a) and (4b).

$$\varphi_i = 2\pi \cdot rand \tag{4a}$$

$$\cos \theta_i = (1 - cos\theta_{max}) \times rand + cos\theta_{max} \tag{4b}$$

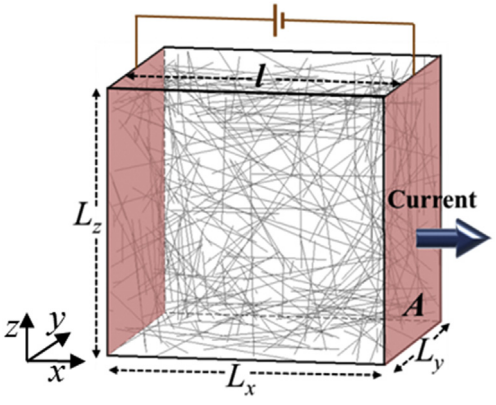

Fig. 1. A schematic of CNTs randomly dispersed in a representative volume element.

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