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A numerical study to investigate the effect of carbon nanotube (CNT) entanglement on the electrical behavior of nanocomposites

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ABSTRACT

Due to their outstanding electrical and mechanical properties, carbon nanotubes (CNT) have been utilized as popular reinforcing elements for composite materials (Ajayan and Tour, 2007). However, the higher stiffness and aspect ratio (length-to-width ratio) characteristics of CNT lead to entanglement of the tubes, and often interferes with development of CNT conductive networks (Shi et al., 2004). In the present study, a micromechanical model based on Weng (2010) and Yang et al. (2014) is introduced and proposed to estimate the effect of CNT entanglement on the electrical performance of nanocomposites. A series of numerical studies for CNT-reinforced composites is carried out, and the influences of the degree of entanglement on the overall electrical properties of composites are discussed. In addition, the predictive capability of the proposed method is demonstrated via comparisons with experimental data.

1. INTRODUCTION

Composites containing carbon nanotube (CNT) can be suitable candidates for the use in various engineering applications, including structural self-sensing, thermal interfacing, and electromagnetic shielding (Chung, 2012). Especially for excellent electrical conductivity per unit weight, these materials have a high potential to play an important role in the future (Ebert et al., 2011).

A significant issue concerning such CNT embedded within a matrix is curviness nature and their agglomeration (Ahmad et al., 2006); however, the classical micromechanics-based models (Weng, 2010; Pan et al., 2014) tend to neglect these

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issues for simplification of the calculation. In this paper, a recent work done by the authors (Yang et al., 2014) is summarized, and the effects of CNT agglomeration on the electrical behavior of nanocomposites are discussed. Based on the proposed method, the influence of the aspect ratio of CNTs is also examined via numerical simulations.

2. MODELING OF COMPOSITES REINFORCED WITH AGGLOMERATED CNT

The micromechanics-based model developed by Castañeda and Willis (1995) is considered here to predict the effective electrical conductivity of composites. Following Castañeda and Willis (1995) and Weng (2010), the electrical conductivity of the aligned CNT-reinforced nanocomposites can be estimated as (Castañeda and Willis, 1995; Weng, 2010)

$$\mathbf{L}^{*}_{Aligned} = \mathbf{L}_0 + \left[\mathbf{I} - \sum_{q=1}^{n}\left(\phi_q \mathbf{T}\cdot\mathbf{S}\cdot\mathbf{L}_0\right)^{-1}\right]^{-1} \cdot \left[\sum_{q=1}^{n}\left(\phi_q \mathbf{T}\right)^{-1}\right] \tag{1}$$

where ϕ_r and L_q denote the volume fraction and the electrical conductivity of the q-phase; **I** signify the identical tensor and the component **T** is defined in Pan et al. (2011). **S** denotes the Eshelby tensor, which is given in Landau et al. (1984) and Pan et al. (2011). In addition, the effective electrical conductivity of nanocomposites containing 3D randomly oriented CNT can be written as (Weng, 2010)

$$\mathbf{L}^{*}_{3D} = \mathbf{L}_0 + \left[\mathbf{I} - \sum_{q=1}^{n}\left(\phi_q \breve{\mathbf{T}}\cdot\mathbf{L}_0\right)^{-1}\right]^{-1} \cdot \left[\sum_{q=1}^{n}\left(\phi_q \breve{\mathbf{T}}\right)^{-1}\right] \tag{2}$$

where the component $\breve{\mathbf{T}}$ is given in Weng (2010).

3. NUMERICAL SIMULATIONS

Numerical simulations based on the aforementioned computational model are conducted to investigate the effect of the nanotube agglomeration on the electrical behavior of CNT-reinforced alumina composites (Ahmad, et al., 2006). The relations between aspect ratio of CNT and electrical conductivity of nanocomposites are illustrated in Figure 1, indicating that the percolation threshold of nanocomposites is rapidly initiated with lengthy CNTs. In addition, Figure 1 shows that the agglomeration of CNT is quite influential on the overall electrical properties of nanocomposites. Detailed results of the numerical simulations will be given in the presentation.

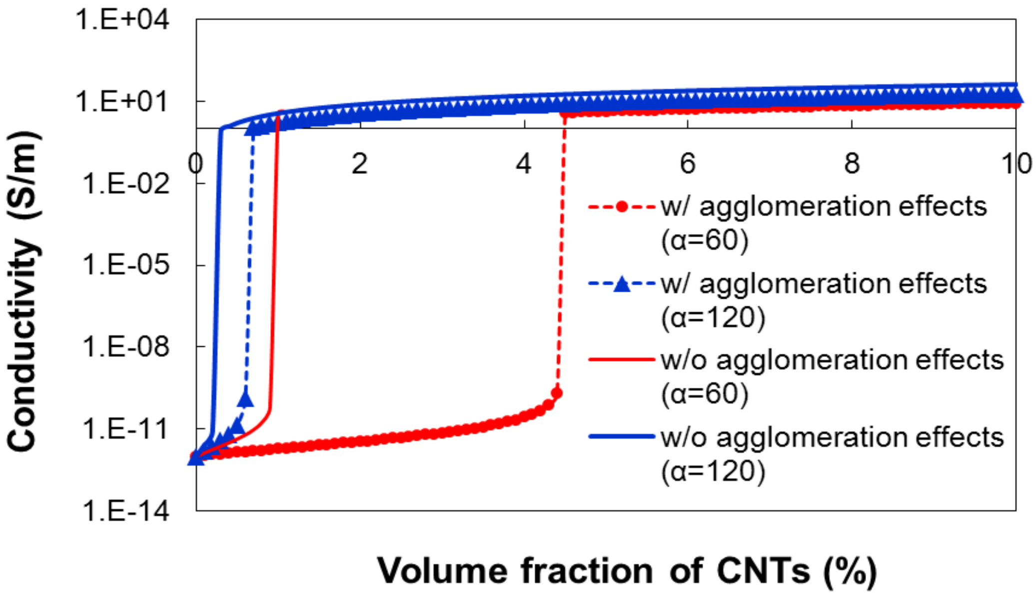

Figure 1. The predicted electrical conductivity of the nanocomposites with respect to the aspect ratio (α) and agglomeration of CNT

4. SUMMARIES

This work examines the influence of CNT agglomeration on the electrical behavior of composites containing CNTs. The present approach is derived by incorporating the micromechanics-based model (Weng, 2010) into the computational algorithm (Yang et al., 2014). Within the present study, the influence of the aspect ratio of CNT is examined via numerical simulations. The results indicate that the percolation threshold of nanocomposites is rapidly initiated with lengthy CNTs.

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