Composites Science and Technology 106 (2015) 156–162

Contents lists available at ScienceDirect

Composites Science and Technology

journal homepage: www.elsevier.com/locate/compscitech

Prediction and experimental validation of electrical percolation by applying a modified micromechanics model considering multiple heterogeneous inclusions

Seong Yun Kim, Ye Ji Noh, Jaesang Yu *

Carbon Convergence Materials Research Center, Institute of Advanced Composite Materials, Korea Institute of Science and Technology (KIST), Chudong-ro 92, Bongdong-eup, Wanju-gun, Jeollabukdo 565-905, Republic of Korea

ARTICLE INFO

Article history:
Received 4 August 2014
Received in revised form 19 November 2014
Accepted 21 November 2014
Available online 26 November 2014

Keywords:
A. Polymer matrix composites (PMCs)
A. Carbon nanotubes
B. Electrical properties
C. Modeling

ABSTRACT

Classical micromechanics modeling cannot capture the effect of percolation threshold at a low volume fraction of conductive fillers, even though multiple heterogeneities are considered in the modeling to investigate the effect of reinforcement dispersion, electrical tunneling behavior, and conductive networks. In this study, an analytical homogenization approach for composites containing multiple heterogeneities with conductive coated layers was developed in order to predict the percolation threshold effect, the tunneling effect using hard/soft core concept, and the effective electrical conductivity of polymer matrix composites (PMCs) containing randomly oriented ellipsoidal inclusions coated by conductive layers. The electrical conductivities of polymerized cyclic butylene terephthalate (pCBT)-based composites containing nanofillers such as carbon blacks (CBs), graphene nanoplatelets (GNPs), and carbon nanotubes (CNTs) were prepared by the recently developed composite manufacturing processing using solvent-free powder mixing and in-situ polymerization for inducing uniform dispersion of nanofillers of various shapes and dimensions within a polymer matrix. When comparing the experimentally measured electrical conductivities of those composites with the predicted values obtained from the developed micromechanics models, it is confirmed that the developed approach successfully captures the percolation threshold and the tunneling effect of reinforcements on the effective electrical conductivities of composites containing various shapes of reinforcements.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

PMCs containing conductive reinforcements, such as CNTs, carbon nanofibers, disk-shaped graphites, and metal spheres, are of interests due to their electrical, thermal, and mechanical properties for various potential applications of sensors, electronic packaging, and high-charge conductive storage [1]. With small volume contents of conductive reinforcements, the electrical and thermal properties of PMCs are drastically increased to several orders of magnitude. This phenomenon is caused by the fact that the percolation threshold issues and connected networks of conductive reinforcements occur to increase the electrical and thermal conductivities. Here, complex networks and Bethe lattice are called upon to build the percolation threshold [1–5]. The effective conductivities of PMCs are determined by many factors such as volume fractions, inter-particle interaction, and shape and orientation of the reinforcements. The percolation threshold behavior, however, is very complex, and it is not simple to predict the effective conductivities of PMCs due to the composite's microstructures. Thus, the study of the percolation threshold and/or relationship between the connected networks and composite properties is important to determine the overall conductivity of the PMCs. Specifically, the electrical percolation threshold depends not only on reinforcement geometry, but also on parameters of reinforcement interactions such as tunneling distance and effect, which is that all objects are electrically connected.

Many studies have been performed to investigate the effect of the percolation threshold of reinforcements in a polymer matrix on the effective electrical conductivity [1–5]. Monte Carlo and other numerical methods are commonly used to compute the effective conductivities [6–9]. Balberg and Binenbaum [9] used Monte Carlo simulations to investigate the average critical number of bonds for sphere and cylinder reinforcement systems with the conductive inner hard core and non-conductive outer soft core. This result as achieved by Monte Carlo simulation was proved by Ogale and Wang [10] with the experimentally obtained values of

* Corresponding author. Tel.: +82 63 219 8156; fax: +82 63 219 8239.
E-mail address: jamesyu@kist.re.kr (J. Yu).

http://dx.doi.org/10.1016/j.compscitech.2014.11.015
0266-3538/© 2014 Elsevier Ltd. All rights reserved.

the percolation threshold. These simulations, however, were limited to systems in which the reinforcement aspect ratios were short, from 10 to 30, because of the extremely high computational expense. Pan et al. [1] developed the analytic approach to investigate the effect of percolation threshold on the electrical conductivity of a two-phase composite containing randomly oriented ellipsoidal inclusions. The simple analytic method was appealing to predict an electrical conductivity without heavy computations, but this method was not able to capture the sharp increase of conductivity at low volume fractions of reinforcements. Other studies related to analytic approaches were also performed, but were limited to the case for the two-phase composites, which contains only single heterogeneity without any coated layers in a matrix.

With respect to reality, composites materials contain multiple heterogeneities such as well-dispersed reinforcements, agglomerated reinforcements, interphase between fillers and a matrix, and defects. In order to capture the real behavior of composites on estimating the effective properties, these multiple heterogeneities should be considered to investigate the effect of reinforcement dispersion, electrical tunneling behavior, and conductive networks. Classical micromechanics modeling, unfortunately, cannot capture the effect of percolation threshold at a low volume fraction of conductive fillers due to the fact that this methodology assumes that every independent filler is well distributed and dispersed in a matrix. In this study, an analytical homogenization approach for composites containing multiple heterogeneities with conductive coated layers is developed to predict the percolation threshold effect, the tunneling effect using hard/soft core concept originally developed by Berhan and Sastry [8], and the effective electrical conductivity of PMCs containing randomly oriented ellipsoidal inclusions coated by conductive layers. Here, various ellipsoidal inclusions can be selected, such as prolate and oblate spheroid, disk, and sphere with controlling ellipsoid's dimensions. The parametric studies are performed to investigate the tunneling effect of conductive interphase on the effective composite electrical conductivities. In addition, various reinforcement shapes such as prolate and oblate spheroids, and sphere cases were used to predict the percolation threshold behavior on the effective electrical conductivities. These results obtained from the analytic approach developed in this study are compared with the experimentally measured data.

2. Modeling approach

The double inclusion method developed by Hori and Nemat-Nasser was originally established for the estimate of effective elastic moduli of composites containing an isolated inclusion embedded into a sub-domain. Consider an ellipsoidal inclusion V, which includes another ellipsoidal inclusion Ω in it and is embedded in an unbounded region of elasticity $\boldsymbol{L}_{ijkl}$ as shown in Fig. 1a. The double inclusion method can be generalized to a multi-inclusion method, in which each heterogeneity is coated by an arbitrary number of layers, as shown in Fig. 1b. The multi-inclusion method can also be generalized to a multi-phase composite model, in which composites contain multiple heterogeneities such as well-dispersed and/or agglomerated reinforcements and defects in a matrix.

2.1. Modified Mori–Tanaka method (M-MTM) for estimating the effective electrical conductivity

The mean electric field gradient in the matrix is assumed to have been perturbed by the presence of other heterogeneities. The continuum averaged electric flux vector (J) and electric field gradient ($\nabla\phi$) are used in the MTM to predict the effective electrical conductivity tensor for the composite. The mathematical relationships used to determine the electrical conductivity in a conductor are similar in functional form to those used to develop the micromechanics models for thermal conductivity for steady state heat flux [11]. The electrical flow in a composite may be characterized in terms of the far-field applied electric flux vector (J), i.e.,

$$J = -\bar{\boldsymbol{\sigma}} \cdot \nabla\phi, \tag{1}$$

where $\bar{\boldsymbol{\sigma}}$ is the effective second-rank electrical conductivity tensor and $\nabla\phi$ is the electrical field gradient which can be expressed in terms of the electrical potential, ϕ. Similar to the classical Eshelby solution for linear elasticity [12–14], where the strain field inside each heterogeneity is constant, the resulting electric field gradient inside each heterogeneity is constant when calculating effective electrical conductivities.

The MTM may be extended to the case for composites containing multiple distinct heterogeneities (fibers, spheres, platelets, voids, etc.) using the multi-inclusion and multi-phase composite models [15]. Yu et al. [11,16–19] used this approach for determining elastic moduli and thermal conductivities of a variety of nanocomposites. Suppose that the matrix contains m distinct types of ellipsoidal heterogeneities (p = 1, 2,. . ., m) each consisting of n_p layers (α_p = 1, 2,..., n_p; p = 1, 2,. . ., m). Each type of heterogeneity has distinct electrical properties, shape, and orientation distribution. The overall effective electrical conductivity tensor, $\bar{\boldsymbol{\sigma}}$, for a composite containing m distinct types of heterogeneities (p = 1, 2,. . ., m) each having an arbitrary number of layers (n_p) in a matrix (0) can be expressed as

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}_M \cdot \left\{ \boldsymbol{I} + \sum_{p=1}^{m} \left[\sum_{\alpha_p=1}^{n_p} c_{(p)_{\alpha_p}} (\boldsymbol{S}_{(p)} - \boldsymbol{I}) \cdot \left(\boldsymbol{A}_{(p)}^{(\alpha_p)} - \boldsymbol{S}_{(p)} \right)^{-1} \right] \right\} \cdot \left\{ \boldsymbol{I} + \sum_{p=1}^{m} \left[\sum_{\alpha_p=1}^{n_p} c_{(p)_{\alpha_p}} \boldsymbol{S}_{(p)} \cdot \left(\boldsymbol{A}_{(p)}^{(\alpha_p)} - \boldsymbol{S}_{(p)} \right)^{-1} \right] \right\}^{-1} \tag{2}$$

Here

$$\boldsymbol{A}_{(p)}^{(\alpha_p)} = \left(\boldsymbol{\sigma}_M - \boldsymbol{\sigma}_{(p)}^{(\alpha_p)} \right)^{-1} \cdot \boldsymbol{\sigma}_M \tag{3}$$

is the second-rank electrical field concentration tensor for the α_pth layer of the pth heterogeneity (α_p = 1,2,. . ., n_p, p = 1,2,. . ., m). Further, $\boldsymbol{\sigma}_{(p)}^{(\alpha_p)}$ is the second-rank electrical conductivity tensor for the α_pth layer of the pth heterogeneity, $\boldsymbol{c}_{(p)_{\alpha_p}}$ is the volume fraction of the α_p-th layer of the pth heterogeneity, and $\boldsymbol{S}_{(p)}$ is the well-known second-rank Eshelby tensor common to the pth heterogeneity and all layers of the pth heterogeneity and $\boldsymbol{I}$ is the second-rank identity tensor. Here a "·" is used to denote the tensor single dot product. The Eshelby tensor ($\boldsymbol{S}_{(p)}$) accounts for the influence of the aspect ratio/geometry of the heterogeneity on the local electrical field. For an ellipsoidal inclusion with a symmetric axis 1, its non-zero components are expressed as

$$\boldsymbol{S}_{(p)_{22}} = \boldsymbol{S}_{(p)_{33}} = \begin{cases} \frac{\alpha}{2(\alpha^2-1)^{(3/2)}} \left[\alpha(\alpha^2 - 1)^{(1/2)} - \cosh^{-1}\alpha \right], & \alpha > 1 \\ \frac{\alpha}{2(\alpha^2-1)^{(3/2)}} \left[\cos^{-1}\alpha - \alpha(1 - \alpha^2)^{(1/2)} \right], & \alpha < 1 \end{cases}, \tag{4}$$

where α is the aspect ratio (ellipsoid's length-to-diameter ratio) and $\boldsymbol{S}_{(p)11}$ = 1–2 $\boldsymbol{S}_{(p)22}$. For a sphere and a long prolate ellipsoid, it reduces to $\boldsymbol{S}_{(p)11} = \boldsymbol{S}_{(p)22} = \boldsymbol{S}_{(p)33}$ = 1/3, and $\boldsymbol{S}_{(p)11}$ = 0, $\boldsymbol{S}_{(p)22} = \boldsymbol{S}_{(p)33}$ = 1/2, respectively. In addition, for a thin oblate ellipsoid, it reduces to $\boldsymbol{S}_{(p)11}$ = 1, $\boldsymbol{S}_{(p)22} = \boldsymbol{S}_{(p)33}$ = 0. If $i \neq j$, $\boldsymbol{S}_{(p)ij}$ = 0.

Download English Version:

https://daneshyari.com/en/article/7215619

Download Persian Version:

https://daneshyari.com/article/7215619

Daneshyari.com