Composites Part B 100 (2016) 240–246

Contents lists available at ScienceDirect

Composites Part B

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

Numerical computation of electrical conductivity of carbon nanotube-filled polymers

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ARTICLE INFO

Article history:
Received 12 October 2015
Received in revised form
26 May 2016
Accepted 4 June 2016
Available online 6 June 2016

Keywords:
Polymer-matrix composites (PMCs)
Nano-structures
Electrical properties
Finite element analysis (FEA)

ABSTRACT

A Finite Element (FE) model, based on the tunneling effect, has been developed for simulating the electrical behavior of carbon nanotube-filled polymers. The geometry modeled belongs to a three-dimensional plate with an equivalent to the nanocomposite physical structure and electrical behavior evaluated using homogenization techniques. The FE model, after validated against experimental and numerical data from the literature, has been applied to conduct a parametric study on the effects of nanotube's volume fraction, electrical conductivity and aspect ratio and polymer's height of barrier. The numerical results show that with increasing the nanotube volume fraction, electrical conductivity and aspect ratio the electrical conductivity of the nanocomposite increases significantly. The height of barrier has effect only at large volume fractions where it varies conversely with electrical conductivity. The proposed FE model is simple compared to the existing numerical models, requires very low computational effort and may be potentially used for the design and optimization of multifunctional nanocomposites.

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1. Introduction

At present, carbon nanotubes (CNTs) are widely used as nano-fillers in polymers due to their excellent mechanical and electrical properties aiming to enhance the mechanical strength and electrical behavior of the parent material [1–3]. Such nanofilled materials are referred in the literature as 'multifunctional materials'. The enhanced electrical behavior of CNT/polymers is exploited for sensing damage in fiber-reinforced polymer composites [4,5], for building integrated circuits at smaller scales [6] as well as for developing conductive structural adhesives [7]. Although the design of multifunctional materials is mainly conducted using manufacturing trials and experiments, reliable modeling- and simulation-driven design tools are very attractive as they are cost- and time-effective.

A considerable number of numerical approaches have been proposed for simulating the electrical behavior of nanocomposites. Most of the approaches are based on a (three-dimensional) 3D resistor network model [7–13]. Hu et al. [7] used a 3D statistical percolation model and a 3D resistor network model to predict the electrical properties of CNT nanocomposites and the effects of critical parameters. Spinelli et al. [8] and De Vivo et al. [9] simulated CNT-based nanocomposite as a 3D material containing randomly distributed conducting cylinders. They estimated the variation of electrical conductivity of the nanocomposites structure for different volume loadings of the conducting phase through a 3D resistor network at which the tunneling effect between conducting clusters has been taken into account. Also, by using a Monte Carlo method, the electrical conductivity and the percolation thresholds of the obtained structures were analyzed as a function of geometrical and physical influencing parameters. Hu et al. [10] combined a 3D statistical resistor network model incorporating the tunneling effect between neighbouring CNTs and a fiber reorientation model. Bao et al. [11] developed an improved 3D percolation model to investigate the effect of the alignment of CNTs on the electrical conductivity of nanocomposites. In the model, both intrinsic and contact resistances were considered, and a new method of resistor network recognition that employs periodically connective paths was developed. This method leads to a reduction in the size effect of the representative cuboid in the Monte Carlo simulations.

In the present work, a simplified numerical model, compared to those described above, is proposed for simulating the electrical behavior of CNT-based nanocomposites. The model is based on the finite element (FE) method, thus incorporating many of the

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http://dx.doi.org/10.1016/j.compositesb.2016.06.048
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advantages of the method such as the low programming and computational effort and transferability between different codes. Moreover, the model may be used as a basis or as module in a multiscale approach which could be used for simulating the electrical behavior of structural parts made from CNT-based nanocomposites.

2. Theory – conduction mechanism

The transition from the insulation behavior to the conductive one is the result of electrical path formation by the filler component. CNT-reinforced polymers are characterized by the random distribution as well as the random orientation of the filler material. As a consequence, in the composite material, paths are formed by CNTs, while, due to the unavoidable distance between the CNTs, the electrical path continuity is achieved by the existence of tunneling resistance, which is the main mechanism being responsible for governing the electrical conduction in the nanocomposite. For this reason, in the model, the charge transport between two consecutive CNTs has been taken into account using the tunneling resistance R_{tunnel} derived from [12]:

$$R_{tunnel} = \frac{h^2 d}{S_{CNT} e^2 \sqrt{2m\lambda}} exp\left(\frac{4\pi d}{h}\sqrt{2m\lambda}\right) \quad (1)$$

where h is the Planck's constant, d is the distance between CNTs, e is the electron charge, m is the mass of electron and λ represents the height of barrier that takes values of a few eV. The network system, which is formed by two conductive particles (MWCNTs in this case) separated by a thin layer of insulating polymer, could be described as a system of two metallic electrodes separated by an insulating film in accordance to [12]. The equilibrium conditions require that the top of energy gap of the insulator to be positioned above the Fermi level of the MWCNTs. As a consequence, the action of the polymer is to introduce a potential barrier between the conductive particles. The electronic current can flow through the polymer region between the two MWCNTs if: (a) the electrons in the MWCNTs have enough thermal energy to surmount the potential barrier and flow in the conduction band, (b) the barrier is thin enough to permit the penetration by electric tunnel effect. It is important to note that this analysis/equation is used for low-temperature conditions, so as the current induced by the thermal energy of the electrons has been neglected. In addition to this, this equation is valid only fir the case of low voltage applied to the electrodes.

From Eq. (1), it can be noted that the tunneling conductance decays exponentially with distance d having a characteristic decay length in the order of a few nanometers. In Fig. 1, R_{tunnel} is plotted in log scale against d for different values of λ. The use of log scale transforms the relation from exponential to linear.

3. FE modeling

3.1. Basic assumptions – model development

The geometry of the nanocomposite modeled belongs to a square 3D plate with thickness equal to 10 CNT's diameters. The plate was modeled using the 3D 20-node electric solid element SOLID231 [13]. The side of the plate is five times CNT's length, a value that has been proven to be sufficient enough to represent the typical nanocomposite conductive architecture [10]. Through the thickness of the plate ten elements were used, while the number of elements at the two sides of the plate was determined by the number of elements representing each CNT as well as by the CNT's geometrical characteristics.

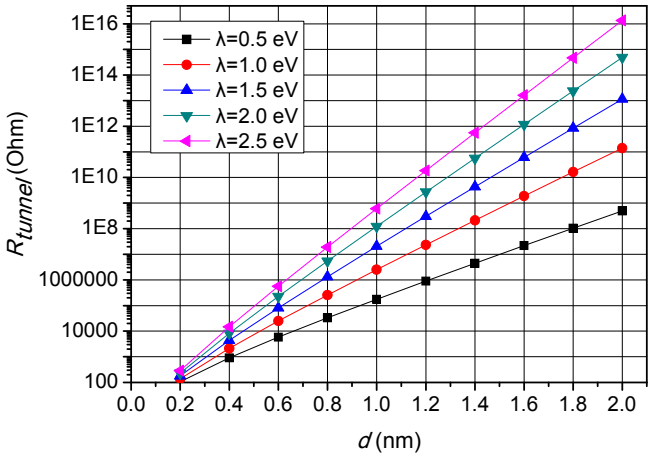

Fig. 1. Variation of tunneling resistance R_{tunnel} (in log scale) with regard to thickness of insulated resin d for different values of height of barrier λ.

The theory of SOLID231 element [13] is based on electromagnetic field theory described by Maxwell equation. By neglecting the magnetic field and applying a series of transformations one obtains the governing equation for quasi-static field

$$-\nabla\cdot([\sigma]\nabla V) - \nabla\cdot\left([\varepsilon]\nabla\frac{\partial V}{\partial t}\right) = 0 \quad (2)$$

where V is the electric scale potential, $[\sigma]$ is the electrical conductivity matrix equals to $\begin{bmatrix} \frac{1}{\rho_{xx}} & 0 & 0 \\ 0 & \frac{1}{\rho_{yy}} & 0 \\ 0 & 0 & \frac{1}{\rho_{zz}} \end{bmatrix}$ and $[\varepsilon]$ is the permittivity matrix equals to $\begin{bmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}$. Eq. (2) is the constitutive relations of SOLID231 element and is used to approximate time-varying electric fields. Neglecting time-variation of electric potential, Eq. (2) reduces to the governing equation steady-state electric conduction

$$-\nabla\cdot([\sigma]\nabla V) = 0 \quad (3)$$

The finite element matrix equations are be derived from variational principles. These equations exist for linear and nonlinear material behavior as well as for static and transient response. The electric scalar potential V is approximated over the element as follows:

$$V = \{N\}^T\{V_e\} \quad (4)$$

where $\{N\}$ is the element shape function and $\{V_e\}$ is the nodal electric scalar potential. The application of variational principle and finite element discretization to the differential Eq. (2) produces the matrix equation of the form

$$\left[C^V\right]\{V_e\} + \left[K^V\right]\{V_e\} = \{I_e\} \quad (5)$$

where $[K^V] = \int_{vol} (\nabla\{N\})^T[\sigma^{eff}](\nabla\{N\}^T)d(vol)$ is the element electrical conductivity coefficient matrix, $[C^V] = \int_{vol} (\nabla\{N\})^T[\varepsilon](\nabla\{N\}^T)d(vol)$ is the element dielectric permittivity

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