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A multi-scale modeling approach for simulating crack sensing in polymer fibrous composites using electrically conductive carbon nanotube networks. Part I: Micro-scale analysis

Konstantinos Tserpes*, Christos Kora

Laboratory of Technology & Strength of Materials, Department of Mechanical Engineering & Aeronautics, University of Patras, Patras 26500, Greece

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ABSTRACT

This is the first of a two-paper series describing a multi-scale modeling approach developed to simulate crack sensing in polymer fibrous composites by exploiting the interruption of electrically conductive carbon nanotube (CNT) networks. The approach is based on the finite element (FE) method. FE models at three different scales, namely the micro-scale, the meso-scale and the macro-scale have been developed using the ANSYS PDL environment. In the present paper, the micro-scale analysis is described. In the micro-scale, two representative volume elements (RVEs) have been developed: a RVE of a CNT/polymer for validating the computation of the effective electrical conductivity of the nanocomposite and a RVE of a CNT/composite for evaluating the effect of crack presence on the effective electrical conductivity. In the CNT/composite RVE, carbon fibers and glass fibers have been modeled. The computed effective electrical conductivity of the CNT/polymer shows a very good agreement with experimental results from the literature, something which validates the proposed electrical modeling approach. The model of the CNT/composite shows a large sensitivity on the presence of the crack. The model with the carbon fibers shows a more homogeneous electrical response compared to the model with the glass fibers which is due to the conductive nature of carbon.

1. Introduction

Structural Health Monitoring (SHM) aims to provide at every moment during the life of a structure, a diagnosis of the “integrity” of the constituent materials, of the different parts, and of the full structure. According to [1], an effective SHM system potentially minimizes the time for ground inspections, increases the availability of the aircraft and allows a reduction of the total maintenance cost by more than 30% for an aircraft fleet. These advantages represent a major contribution towards greener aviation. SHM is comprised from the diagnosis and prognosis functions. The diagnosis function is based on a monitoring system, which usually consists of a network of a limited number of sensors distributed over a relatively large area of the structure. However, with such a monitoring system only major damage conditions can be detected. The current trend is the development of dense wireless networks of miniaturized sensors. In addition, multifunctional materials for SHM have gained attention for their versatility to sense, actuate and harvest energy from ambient vibrations.

Combining extraordinary mechanical [2–5], thermal [6] and electrical properties [7] with fiber-like structure, CNTs are used as reinforcements to produce multifunctional polymers (nanocomposites) and fiber composites. Amongst the targeted functionalities is strain and damage sensing. Damage sensing in fiber composites by conductive CNT networks has been initially proposed by Fiedler et al. [8]. Since then, numerous works, mainly experimental (e.g. [9–13]), have been reported. On the contrary, there have been reported only two works on the modeling of damage sensing by CNT networks, one for fiber composites [11] and one for nanocomposites [12]. Li and Chou [11] modeled damage sensing in [0/90]s cross-ply glass fiber composites using embedded CNT network. The contact resistances of CNTs were modeled considering the electrical tunneling effect and the effective electrical resistance of the percolating nanotube network was calculated by considering nanotube matrix resistors and employing the finite element (FE) method for electrical circuits. The loading process of the composite, from initial loading to final failure, has been simulated also by the FE method. The deformation and damage induced resistance change has been identified at each loading step. The results demonstrated that the simulation model captures the essential parameters affecting the electrical resistance of nanotube networks. The authors did not carry out any parametric study. Kuronuma et al. [12] presented

* Corresponding author.
E-mail address: kitserpes@upatras.gr (K. Tserpes).

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an analytical model of strain sensing behavior of CNT-based nanocomposites. The model incorporated the electrical tunneling effect due to the matrix material between CNTs to describe the electrical resistance change as a result of mechanical deformation. The model deals with the inter-nanotube matrix deformation at the micro/nanoscale due to the macroscale deformation of the nanocomposites. A comparison of the analytical predictions with the experimental data showed that the proposed model captures the sensing behavior.

From the above, we conclude that the understanding of the key factors governing the sensing effectiveness of CNT networks has been mainly attempted by experimental means. However, in this process, reliable models and simulation-driven design tools could be very useful as they are cost and time-effective. In this context, in the present work, proposed is a multi-scale FE-based modeling approach for simulating the basic mechanisms of crack sensing by conductive CNT networks in polymers and fibrous composites. The modeling approach is described in two papers. The present paper describes the basic electrical theory applied, the electrical FE modeling, the validation of the computation of the CNT/polymer's electrical conductivity and the electrical response of CNT/composites in the presence of a crack. The second paper describes the meso-scale and macro-scale models. It is important to mention that the proposed model does not consider the actual CNT/polymer interphase and the formation of CNT agglomeration for which many experimental e.g. [13] and theoretical studies e.g. [14–19] have shown that have significant effect on the mechanical properties and fracture behavior of nanocomposites. On the contrary, it considers the interphase-conduction phenomenon through the simulation of the quantum tunneling phenomenon.

2. The multi-scale modeling approach

The multi-scale model extends at three analysis scales, namely the micro-, the meso- and the macro-scale. The models, the input and the main results for each scale are briefly described in Fig. 1. The three analysis scales have been separated based on the size and the expected outcome. Micro-scale models are the basis of the overall computational approach. Micro-scale models have a maximum size of 100 μm and have been developed so as to derive the effective electrical conductivity of the CNT/polymer and to perform a first assessment on the effect of crack presence on the CNT/composite. In the meso-scale, a parametric crack sensing methodology aiming to link the crack characteristics with the decrease of the effective electrical conductivity of the CNT/composite has been developed. The maximum size of the meso-scale model is 0.2 mm. The need for the meso-scale analysis is due to the large gap between the micro-scale and the macro-scale, i.e. from 100 μm to 10 mm. Finally, in the macro-scale, the crack sensing approach is applied to a square composite section of size of 10 mm. It is noted that small changes in the dimensions of the models are not expected to affect the computed results for each analysis scale.

3. Basic theory

The macroscopic electrical conductivity of a composite material depends on the CNT volume fraction V_{fCNT}. With increasing the V_{fCNT}, the possibility for the formation of contact points of the conductive phase within the insulating phase increases. The V_{fCNT}, for which a continuum conductive network is created, is called the *percolation threshold*.

Given that the insulating resin is not able to conduct (ground) electricity, its charging creates a stable gradient potential through the volume of the insulator, described by the charge density $\rho(\vec{r})$, due to the electrostatic forces among the negative charges (electrons) [20,21]. Subsequently, an electric field can be described by [20,21]

$$\vec{E}(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\iiint \frac{\vec{r}-\vec{r}'}{\|\vec{r}-\vec{r}'\|^3}\rho(\vec{r})d^3r'(V/m) \tag{1}$$

where ε_0 is the vacuum permittivity of free space equals to $8.854 \times 10^{-12}\,C^2\,N^{-1}\,m^{-2}$ and $\vec{r}-\vec{r}'$ is the spatial displacement vector. This electric field can be expressed as the gradient of the electrostatic potential Φ created due to charge distribution; it stands $\vec{E} = -\vec{\nabla}\Phi$.

In the atomic level, given the lack of free electrons, in the presence of electric potential, there are no electrodynamic effects. Therefore, the electrons maintain their superposition and the energy is stored in the form of electrostatic potential energy. With the introduction of CNT fillers, a conduction mechanism is created. The CNTs offer a discharge path between regions with a different charge density since it contains free electrons into their structure. The superpositions of the electrons are not maintained due to the appearance of electrostatic potential and electrodynamic effects. If the effect is continuous from the source of charge to the ground, a steady state current flow is created. A schematic representation of the conduction mechanism caused by the presence of CNTs is given in Fig. 2.

For small CNT contents, for which the formation of a continuous network is not possible, the combination of continuous discharging with the small junction contacts until the grounding might lead to a conducting behavior with, however, very large resistance due to the interphase-dominated conduction. The interphase-dominated conduction takes place through the *quantum tunneling phenomenon* according to which the electrons pass through the barrier of the interphase to the closest quantum tunnel. The specific quantum tunneling resistance is given by

$$\rho_{tunnel} = \frac{1}{\sigma_{tunnel}^{el}} = \frac{h^2}{e^2\sqrt{2m\lambda}}\exp\left(\frac{4\pi d_i}{h}\sqrt{2m\lambda}\right) \tag{2}$$

where h is Planck's constant, d_i is the resistance between the CNTs, e is the electric charge, m is the electron mass and λ is the height of barrier which the electron must overcome in Volts (V).

This phenomenon occurs just before the percolation threshold. For CNT contents larger than the percolation threshold, there is a physical

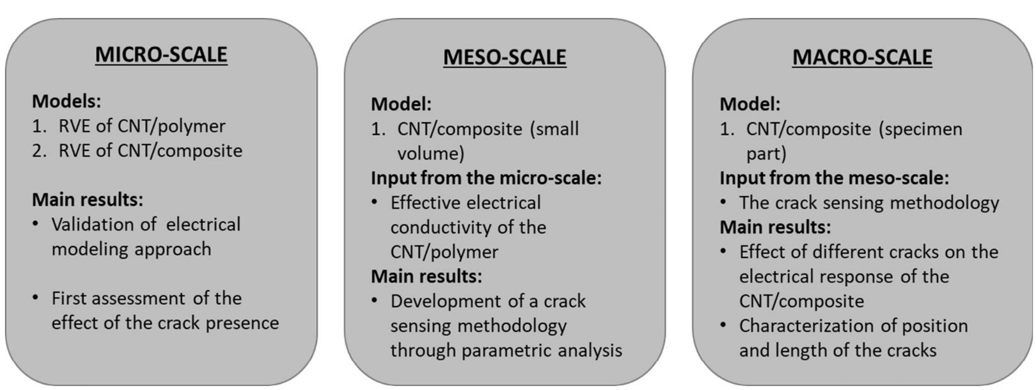

Fig. 1. Models, input and main results on each analysis scale.