Analysis of composites reinforced by wavy carbon nanotubes

Radosław Górski and Piotr Fedeliński

Department of Strength of Materials and Computational Mechanics, Silesian University of Technology
Konarskiego 18A, 44-100 Gliwice, Poland
e-mail: Radoslaw.Gorski@polsl.pl, Piotr.Fedelinski@polsl.pl

Abstract

The paper presents a micromechanical modelling of carbon nanotube-reinforced composites in order to calculate their effective elastic properties. The polymer matrix of two-dimensional representative volume element (RVE) of the nanocomposite is modelled by the boundary element method (BEM) and the nanotubes by the finite element method (FEM). The effect of a waviness of aligned or randomly oriented nanotubes is investigated. The nanotube waviness is modelled by prescribing a sinusoidal shape as shown by other authors, or by any arbitrary shape using the NURBS curves. The effective properties of composites with wavy or straight nanotubes and their different volume fractions are computed and compared. The influence of the particle/matrix modulus ratio on the effective elastic properties is also investigated. The numerical solutions will be compared with other available numerical and experimental results or obtained by analytical micromechanical methods.

Keywords: boundary element methods, finite element methods, composites, homogenization, material properties, microstructures

1. Introduction

An experimental materials testing is usually expensive and time consuming, thus a computer modelling and simulation play a significant role in predicting and designing material properties of composites. The analysis of these materials is performed by different computational methods covering different scales. The so called continuum methods, ranging from simple closed-form expressions to complex micromechanical models and numerical methods, can be successfully applied in predicting the effective properties of different composites. Among the numerical methods, the finite element method (FEM) and the boundary element method (BEM) are the most frequently used.

New composites of required properties can be fabricated by combining two or more materials. A combination of polymers with carbon nanotubes (CNTs), acting as a matrix and fillers, respectively, results in a new class of materials, called carbon nanotube-reinforced polymers (NRPs). They can have an extraordinary functional and an enhanced mechanical properties, due to a unique physical and mechanical properties of CNTs. The unusual properties of CNTs, including for instance small size, low density, excellent electronic and thermal properties and extremely high stiffness and strength, can be utilized in the composite materials science, if they play the role of reinforcement. However, in order to expose these properties influencing the reinforcing effectiveness in NRPs, several issues should be examined and well understood. They include for instance dispersion and orientation of CNTs within a polymer, bonding and interaction between them, and so on. In the latest studies, the waviness of CNTs as an additional important issue influencing the effective mechanical properties of NRPs is investigated.

Many authors have undertaken a study on analysis of NRPs by continuum methods but most of it deals with straight CNTs. The evaluation of the effective properties of carbon nanotube-based composites with straight CNTs by the FEM and BEM is presented for instance in [3] and [7], respectively. Fisher et al. [6] have developed a hybrid model that allows the effects of CNTs waviness to be incorporated into micromechanical method. The model combines the finite element results and a micromechanical method for predicting the effective reinforcing modulus (ERM) of a wavy nanotube. The ERM is then used in the Mori-Tanaka method [8] to predict the effective modulus of NRPs. The same authors have presented a similar approach, in which the finite element model of a wavy CNT is used to numerically evaluate the dilute strain concentration tensor [2]. It is then utilized in the Mori-Tanaka method to predict the effective modulus of NRPs with aligned or randomly oriented CNTs. A closed form analytical model, incorporating the nanotube curvature, length and both 1D and 3D arrangement, for estimating the effective elastic modulus of carbon NRPs, is developed by Anumandla and Gibson [1]. The above models, although accurate and efficient, assume a perfect bonding between a matrix and nanotubes, which are treated as solid elements not hollow. Pantano et al. [10], [11] have developed the FEM models, in which the curvature of CNTs and their interaction with a matrix are taken into account. The nanotubes are modelled as hollows and perfect or weak bonding between a matrix and CNTs is analyzed. Shao et al. [12] have presented a simple analytical model to investigate the influence of CNTs waviness and debonding. Recently, Omidi et al. [9] have proposed a new form of the rule of mixtures, which includes many important factors influencing the reinforcing efficiency, for instance waviness and orientation of inclusions. The method allows for more accurate prediction of mechanical properties of NRPs. Generally, in the papers discussed above, a significant influence of the CNTs waviness and the interface interaction on the effective elastic modulus of carbon nanotube-reinforced composites, have been observed.

In this paper, the continuum methods are used to analyze carbon nanotube-reinforced composites and evaluate effective elastic properties. The BEM and beam finite elements are used to model and analyze a matrix and carbon nanotubes of two-dimensional RVEs, respectively. The presented approach allows exploiting the advantages of both numerical methods, which have been usually used separately or in a combination with micromechanical methods to analyze NRPs. The nanotubes can be easily modelled as hollows or solids by changing cross-section parameters of beams. Moreover, the method allows easy modelling of NRPs with arbitrary shapes of CNTs embedded in the RVE. The waviness of nanotubes on the effective properties will be investigated and the results for nanocomposites with both straight and wavy nanotubes will be compared.

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2. Coupled boundary and finite element method

In order to compute effective properties, a two-dimensional model of the RVE of the carbon nanotube-reinforced composite is considered. The polymer matrix in plane stress or strain is modelled by the BEM as a plate and the nanotubes by the FEM using beam finite elements. In order to model the reinforcement, additional lines inside the plate and along the reinforcement are introduced. The lines are discretized into boundary and finite elements. This increases a total number of degrees of freedom but it is much smaller than in methods requiring discretization of the whole interior of the plate, e.g. the FEM. Generation of mesh for new RVEs is easier in the present method than in other domain-based methods. The BEM/FEM equations are coupled by assuming conditions of compatibility of displacements and equilibrium of forces between the matrix and reinforcement [4]. A perfect bonding between the plate and reinforcement at the connected nodes is assumed. The method allows modelling of composites with different reinforcement, e.g. nanotubes or nanoclay plateles, by changing cross-section parameters of beams. The shape of the reinforcement, i.e. straight or wavy, can be easily modelled by changing the shape of a one-dimensional line along the attachment. The presented method was successfully applied to the evaluation of the effective Young modulus of polymer/clay nanocomposites with intercalated and aligned nanoclay sheets [5].

3. Numerical model

The carbon nanotube-reinforced composite with aligned or randomly oriented wavy or straight nanotubes is considered and the effective properties are analyzed. The nanotube waviness will be modelled by prescribing a sinusoidal shape as shown by other authors, or the nanotube will have an arbitrary shape modelled by using the NURBS curves. The nanotubes can not intersect themselves and the outer boundary of the RVE. The minimal distance between the nanotubes and also between them and the outer boundary will be assumed. A typical RVE with straight and wavy nanotubes randomly oriented and embedded in the matrix is shown in Fig. 1.

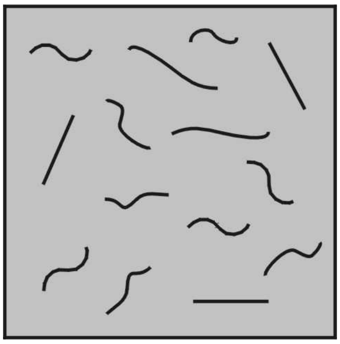

Figure 1: RVE of the carbon nanotube-reinforced composite

The material of the matrix and nanotubes is linear elastic and isotropic. The assumed material properties will be typical values for the polymer and nanotubes.

In order to determine effective elastic constants, the RVEs will be subjected to uniform stresses applied at their edges and displacements of all boundary nodes will be obtained. The effective properties will be determined by taking into account the applied stresses and calculated displacements and strains of the RVEs. Several RVEs for the particular volume fraction of nanotubes will be analysed in order to average the results.

4. Conclusions

In the paper, the nanotube waviness as one of several key mechanisms influencing the reinforcing effectiveness and the effective properties of carbon nanotube-reinforced composites is investigated. The coupled BEM/FEM is used which results in significantly decrease in the number of degrees of freedom in comparison with the FEM, because the outer boundary of the RVE and the lines along the nanotubes are only discretized. The presented method allows easy modelling of composites with different types and shapes of reinforcement.

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