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Elastic properties of coiled carbon nanotube reinforced nanocomposite: A finite element study

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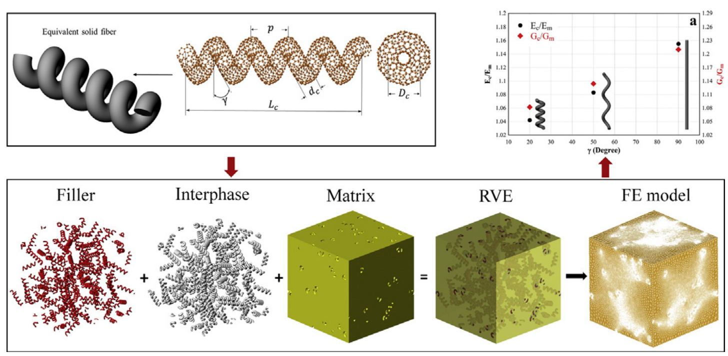
HIGHLIGHTS

- Modeling and analysis of coiled carbon nanotube (CCNT) reinforced polymer nanocomposites are presented.
- Elastic and shear moduli of CCNT-composites are predicted based on the interphase and geometrical parameters of fillers.
- Comparison of the reinforcing effects of CCNT and SWCNT fillers is presented.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper presents modeling and analysis of coiled carbon nanotube (CCNT) reinforced polymer nanocomposites. A new algorithmic representative volume element (RVE) generation method and an RVE based finite element analysis are proposed to predict the elastic properties of CCNT nanocomposites. The elastic properties of CCNT polymer nanocomposites are studied with respect to their interphase, volume fraction, orientation, number of coils and geometrical variations such as tube diameter, coil diameter and helix angle using the proposed finite element analysis. The results show that the elastic moduli of randomly and unidirectionally dispersed CCNT nanocomposites decrease when the coil tube or the coil diameter increases. In addition, reinforcement ratio increases by increasing the number of coils. It was also observed that single walled carbon nanotube (SWCNT) fillers have better reinforcement compared to CCNT inclusions with the same volume to surface area ratio.

1. Introduction

In recent years the development of new composite materials is of a great importance in various engineering applications. Numerous research studies have been carried out for improving various aspects of these materials, in particular, their quality and functionality. Different types of nanomaterials as filler have been used to promote the mechanical, thermal and electrical characteristics of nanocomposite materials. Especially, carbon-based nanomaterials including graphene sheets [1–3], carbon nanotubes (CNTs) [4,5], carbon nanocones [6,7], CNT based network [8,9] and coiled CNTs (CCNTs) [10–13] are receiving tremendous attention in the field of nanotechnology.

Among carbon nanostructures, a great deal of interest has been recently focused on CCNTs due to their specific mechanical and electrical properties which stem from the specific helical structures in

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combination with CNTs unique properties [13]. The mechanical properties of CCNTs are studied by a number of researchers. Chen et al. experimentally characterized the mechanics of coiled carbon nanotubes by clamping a CCNT between two AFM cantilevers while a tensile force was applied up to a maximum value. They showed that the spring constant of CCNTs achieved from experimental data are in a good agreement with their analytical model [14]. The optimum conditions for various possible structural configurations of CCNTs were also studied by Chuang et al. [15]. The effective elastic properties of composites of helical fillers in an elastic matrix were studied in [16], by implementing the superposition of fundamental solutions for the matrix and the constitutive equations for the fillers. The geometry of fillers considered in this study was limited to the regular shapes.

Molecular mechanics and molecular dynamics are used to study the elastic, plastic, vibration, spring constants, shear modulus and fracture of CCNTs [17–23]. It is well known that geometry, additive concentrations and properties are the main factors affecting the reinforcement of nanocomposite materials. Wang et al. employed molecular dynamics to differentiate the mechanical properties of the CNTs with the CCNTs where compression, tension, re-compression, re-tension and pullout from a polyethylene matrix were evaluated in [24]. They concluded that CCNTs can be regarded as a suitable filler for tough and lightweight nanocomposites.

The synthesis methods and the applications of CCNTs as fillers in composites were investigated by [25,26]. They reviewed the synthesis procedures of CCNTs and the advantage of a tighter bond with the composite matrix which can result in a variety of engineering applications. Owing to specific geometry of CCNTs, the authors believed that mechanical strength and fracture toughness of the nanocomposite can be substantially enhanced. This unique property can exist even in the absence of any chemical bonding between the CCNT fillers and the matrix.

Several approaches have been used to study the mechanical properties of nanocomposite materials. Since most of the analytical methods for describing the randomly dispersed nanocomposites are not sufficiently precise and they require long times and costly equipment, computational methods are commonly used to analyze the behavior of nanocomposite materials. Multi-scale modeling, molecular dynamics (MD), molecular mechanics (MM) and continuum mechanics are some of the commonly used methods for modeling of nanocomposite materials. However, MD simulation methods are not applicable to every model due to the complexity of model dimension and the extensive time consuming nature of this method. Because of that, most of the MD simulations of nanocomposite materials are restricted to those models which include only a single reinforcement in the matrix of the composite while in reality, nanocomposites can encompass nanofillers with many different shapes, sizes and a wide variety of orientations and arbitrary distributions. Therefore, MD methods are not always suitable for identification and prediction of mechanical properties of nanocomposites. Continuum mechanics; however, is more efficient in characterization of the material properties when the model is more complex. In addition, the knowledge of stress-strain behavior at the boundaries of a representative volume element (RVE) is adequate to accurately characterize the nanocomposites [27]. Finite element analyses (FEA) have been used to determine the mechanical properties of carbon based polymer nanocomposites [28], in particular, the effect of interphase [29–31] and the dispersion of SWCNTs on the properties of nanocomposites [32–37].

A CCNT is a helical form of a CNT (Fig. 1) with several geometrical parameters such as tube diameter d_c, coil diameter D_c, length of coil tube l_c, coiled length L_c, helix angle γ and number of pitch N_c in comparison to a CNT that only has two effective parameters l_s and d_s. When used as a filler, all of these geometrical parameters could affect the overall mechanical properties of a nanocomposite. A recently published study [24–26] showed that composites reinforced by CCNTs would be good potential candidates for lightweight and tough nanocomposites. To the best of our knowledge, there is no numerical study to evaluate effective mechanical properties based on different morphology and random distribution of CCNT inside polymer nanocomposite. Thus, we are presenting a numerical study based on FE analysis to investigate the effect of different geometrical and intrinsic parameters of CCNTs incorporated in a polymer matrix. To determine whether CCNTs could be considered as an alternative to CNTs in polymer nanocomposites for their mechanical properties, we developed an algorithm to compare the effect of changing filler geometry from the case of SWCNTs to CCNTs. Our proposed model is capable of including interphase effect of polymer/CCNTs in determination of the mechanical response of the system.

In Section 2, an RVE generation algorithm is presented to construct the FE model of randomly dispersed SWCNTs and CCNTs in a polymeric composite. The effective mechanical properties of the designed nanocomposites are evaluated using the developed FEA by changing their filler geometry. Section 3 presents the results obtained from analysis of the models. Our conclusive remarks of the developed study are presented in Section 4.

2. Nanocomposite modeling

2.1. RVE construction

This research work is aimed to evaluate the elastic properties of CCNT nanocomposites by considering their volume fraction, geometry and orientation of CCNTs. A finite element analysis is developed as a computational framework for this study with the following steps: (i)

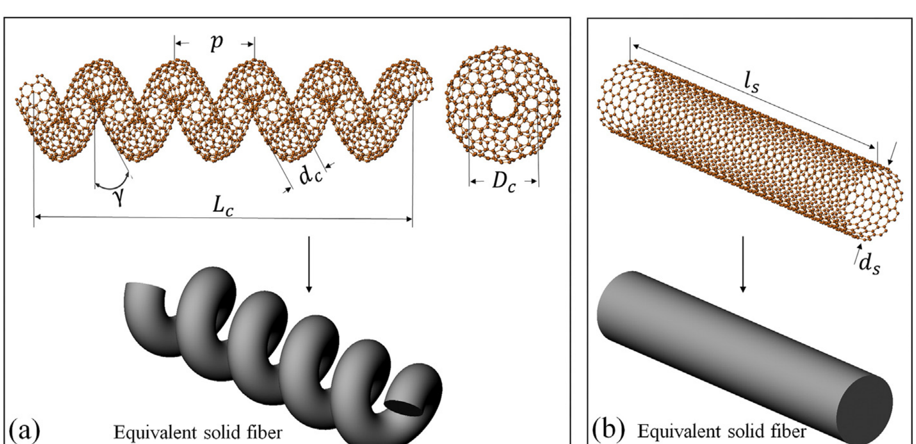

Fig. 1. (a) geometrical parameters and equivalent solid fiber model of a CCNT (b) geometrical parameters and equivalent solid fiber model of a CCNT.