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Numerical analysis of the elastic–plastic properties of the composites incorporating nanohybrid shish-kebab structures

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ABSTRACT

The nanohybrid shish-kebab (NHSK) structure, in which randomly dispersed and wavy carbon nanotubes (CNTs) serve as shish and crystal lamellas periodically decorated onto the CNTs serve as kebabs, has attracted extensive attentions due to its more excellent enhancement in comparison with pristine CNT for polymer matrix composites. In this paper, a new method, based on a modified random sequential adsorption (RSA) algorithm, is proposed to construct the 3D finite element model of the NHSK reinforced composites. The Young's modulus calculated by this model agrees with the experimental result. Moreover, we present a comparison between the pristine CNT reinforced composite and the NHSK reinforced composite in terms of elastic–plastic behavior. Different load transfer mechanisms are analyzed for the two kinds of composites. Furthermore, we explore the effects of the crystal kebab's material property, diameter and the periodicity of the kebabs on the elastic–plastic properties of the composite. The results show that the effective mechanical properties of the composites have a large improvement with the existence of crystal kebabs in comparison to the pristine CNT reinforced composite, which indicates that the NHSK structure can improve the load transfer efficiency between the CNT and the matrix and act as another enhanced phase in the composite. The proposed model can be used for the virtual design and optimization of CNT/semicrystalline polymer composites since it has proven capable of assessing the effects of different material and geometrical parameters on the elastic–plastic properties of the composites.

1. Introduction

Since discovered in 1991 [1], the carbon nanotube (CNT) has attracted considerable attention for its extraordinary mechanical, thermal and electrical properties. These properties, especially the impressive mechanical behaviors with Young's modulus as high as 1 TPa and strength higher than 1 GPa, tend to make CNTs promising fillers to enhance the polymeric matrix composites [2,3]. However, some studies have shown that the absolute increases of mechanical properties for the composites incorporating CNTs are somewhat disappointing, which is attributed to the poor load transfer efficiency between the CNT and polymer matrix and the aggregation of the CNT due to high specific surface area and strong van der Waals forces [4]. For these problems, quantities of strategies aiming at strengthening the CNT/polymer interface have been proposed in the past few years [5], one of which is the nano-scale interfacial crystalline for the composites systems composed with CNT and semicrystalline polymer [6]. Interfacial crystalline, unlike chemical functionalization, not only can improve the interface bonding between the CNT and polymer, but also ensure the perfect atomic structure and excellent properties of the CNT. By controlling the crystallization conditions, Li et al. [7,8] firstly decorated the CNTs periodically with polymer single crystals and obtained a novel nano-structure, which is named as "nanohybrid shish-kebabs (NHSKs) structure". Henceforth, plenty of researches have been carried on related issues, such as preparation methods [9–13] and mechanical properties [14–16].

The NHSK structure, in which the CNT serves as a shish and the crystal lamellae serve as the kebabs periodically decorating on the CNT, has a rougher surface to enhance the interfacial interaction between the CNTs and the polymer matrix without sacrificing the mechanical properties of the CNT. The size and periodicity of the kebabs can be readily controlled by varying crystallization conditions [9]. As known to be stiffer and stronger than the amorphous polymer, the crystalline polymer can also be considered as another phase of enhancement for the CNT/semicrystalline polymer composites [17]. According to experiments [14,15], a considerable enhancement of the mechanical properties of the composites is achieved after the interfacial crystallization. For instance, Ref.

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[15] has reported an enhancement in Young's modulus of 11.9% and ultimate tensile strength of 11.8% of the NHSK/PMMA composite compared to the pristine CNT (P-CNT)/PMMA composite under the condition of same volume fraction of CNTs. In conclusion, the NHSK structure can not only improve the load transfer efficiency between the CNT and the matrix, but also bring in a new phase of reinforcement for the CNT/polymer composites. However, few analyses have been reported in the open literatures for the NHSK reinforced composites. Therefore, it is necessary to explore the reinforcing mechanism of the NHSK structure for the polymeric composites.

For the NHSK reinforced composites, it is worth mentioning that compared with other types of fillers, the characteristics of NHSKs are quite special. On the one hand, the CNTs are always presented as wavy and spatially random due to their extremely high aspect ratio [18]. On the other hand, the size and periodicity of the crystal kebabs are varying under different crystallization conditions [7,9], which is expected to have a significant influence on the effective mechanical properties of the resulting composites. Therefore, it is necessary to investigate the effect of these geometrical parameters on the mechanical properties of the composites. Nevertheless, it is extremely difficult to determine the distribution of these parameters within the polymer and their relative effect on the effective properties of the composites in experiments [19,20]. Furthermore, because of the complex structure, theoretical analysis can hardly give enough predictive results for the NHSK reinforced composites, either. For instance, Chen and Lu [16] analyzed the load transfer mechanism of composites incorporating the NHSK structures by an improved shear-lag model, but could not give the effective properties of the whole composites. However, computational approaches, especially FEA method, can provide more reasonable descriptions of the complex microstructures of the composites and give relative accurate predictions for their properties. For the composites reinforced by random and wavy CNTs, several simulations have been carried on the mechanical properties. Han et al. [21,22] presented two modeling approaches for predicting the elastic properties of the CNT reinforced composites by considering the agglomerations of the CNT networks and the thick polymer interphase regions between the CNT and the surrounding matrix. These two different modeling methods, based on local continuum mechanics and hybrid local/non-local continuum mechanics respectively, provide similar results in terms with homogenized quantities but locally can lead to very different microscopic fields. Vu-Bac and Ghasemi et al. [23–25] proposed a stochastic analysis method to quantify the influence of the correlated key parameters including CNT length, waviness, agglomeration and volume fraction on the elastic properties of polymer composites and predict the interfacial characteristic between the CNT and polymer matrix, and used a reliability and Non-Uniform Rational B-Spline (NURBS) based sequential optimization approach for finding the optimal fiber content and distribution in fiber reinforced composites. Herasati et al. [26] introduced a new method for characterizing and modeling the waviness and alignment of the CNTs in composites and discussed the effect of the CNT's morphology on the effective elastic property of the composites. Yuan and Lu [27] proposed an algorithm to produce the FE model of polymeric composites with randomly dispersed and wavy CNTs. They also explored the effects of the CNT length, orientation and waviness on the elastic–plastic behavior of the composites. In conclusion, FEA can be an effective method to explore the mechanical properties of the composite incorporating the complex NHSK structure.

To the best of our knowledge, numerical simulation on the effective mechanical properties of such NHSK reinforced polymer composites has not been reported in the open literature. In this paper, an algorithm is firstly proposed to construct the FE model of polymeric composites with a plenty of randomly dispersed and wavy NHSKs. The elastic–plastic properties of polymeric composites reinforced by NHSKs are analyzed by considering the complex micro-structure of NHSKs. In Section 2, the details of the FE generation are introduced. Numerical results are presented in Section 3, where we discuss the effect of material properties and structural characteristics of the NHSK on the mechanical properties of composites. Some conclusions are drawn in Section 4.

2. Modeling

It is well known that CNTs embedded in polymer matrix have a certain degree of waviness along their length and a random distribution of position and orientation. The characteristic of the CNT architecture is mainly due to their low bending stiffness and extremely high aspect ratio (length to diameter). In our previous work [27], we have proposed a modified random sequential adsorption (RSA) algorithm to construct the finite element (FE) model of CNT reinforced composite in a cubic representative volume element (RVE) by considering the waviness and randomness of the CNT. Based on the CNT architecture, a method is presented to generate NHSK architecture in this paper. The detailed process is described as follows.

2.1. A 3D random CNT architecture

Each wavy CNT is approximated by numerous interconnected segments of straight cylinders. The total number of CNT (N_c) is a function of the CNT volume fraction V_{f_CNT} and its external diameter. As shown in Fig. 1, each segment has the same length of l and the same radius of r. P_{i-1} and P_i are the two endpoints of the ith segment. The two Euler angles (φ_0, θ_0) determine the spatial orientation of the CNT, while the other Euler angles (φ_i, θ_i) determine the waviness of the CNT. For every CNT, the spatial position of the initial point P_0 is selected randomly in the RVE. The first segment is generated according to the initial point P_0 and the Euler angles (φ_0, θ_0) under the global coordinate system. In the current study, the Euler angles (φ_0, θ_0) are assigned randomly or satisfy a uniform distribution in other words. In the similar way, the ith segment is added into the RVE by randomly generating two Euler angles (φ_i, θ_i) under the local coordinate system which is depended on the previous segment. The number of the segments n_s is determined by the segment's length l and the CNT's length L. Physically, the intersection of any two segments of one or two CNT is not acceptable, requiring that the newly generated candidate segment do not overlap any segments previously accepted in the configuration. It must be mentioned that the time required to generate a new segment satisfying the non-intersection requirements becomes gradually longer as the current volume fraction increases. In order to improve the efficiency, we define two certain iterations (I_{max}, J_{max}) acting as restricted conditions. If the iteration trying to generate a new segment is more than I_{max}, the previous segment is discarded and a new one will be established. Furthermore, if the iteration trying to generate a new segment is more than J_{max}, the current CNT is discarded and a new one will be established. In order to maintain the periodicity of the RVE, parts of the segments that exceed the boundary of the RVE are cut and shifted to the opposite boundary.

By changing the distribution of the initial Euler angles (φ_0, θ_0), CNT architecture with different spatial configurations are generated, such as aligned CNT and random CNT [27]. In the present study, due to the complete randomness of CNT, the initial Euler angle θ_0 follows a uniform distribution in the range of $(0, \pi/2)$. Because the Euler angle φ_0 is random in the range of $(0, 2\pi)$, the sign of the angle θ_0 is not important. It has demonstrated that