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A comparative study of the load transfer mechanisms of the carbon nanotube reinforced polymer composites with interfacial crystallization

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ABSTRACT

With the help of shear-lag theory, load transfer analysis is performed on the carbon nanotube reinforced polymer composites with interfacial crystallization of different morphologies, including transcrystallinity layer (TCL) and nanohybrid shish-kebab (NHSK) structures. By comparison, we find that the TCL structures can ease the burden of the CNT while the NHSK structures can lead to a fluctuating distribution of the axial stress in the CNT. Both structures can improve the effective elastic modulus of the composites, though the effect of the TCL structures is more pronounced. Besides, the enhancement of the load transfer efficiency of the composites is also observed, the study of the interfacial stress on different kinds of interfaces shows that the reinforcing effect of the TCL structures is sensitive to both the CNT/crystalline polymer interface and crystalline polymer/amorphous polymer interface, while the major decisive factor for the NHSK structures is confined to be the CNT/crystalline polymer interface because of the interlocking effect. Based on these features, some suggestions are given for tailoring the high-performance carbon nanotube reinforced polymer composites.

1. Introduction

Polymer nanocomposites have drawn intensive attention in the past two decades owing to their wide scope of potential application [1–3]. The nanocomposites incorporating high aspect ratio fillers, such as carbon nanotube (CNT) and carbon nanofiber (CNF), are expected to exhibit extraordinary mechanical properties [4–7]. However, the achievement of high-performance CNT reinforced nanocomposites is hindered by the aggregation of CNTs and the poor load transfer efficiency between the pristine CNT and polymer matrix [8,9]. Being one of the strategies dealing with the problems aforementioned, the CNT induced interfacial crystallization has attracted tremendous interests in the past several decades [10,11]. The interfacial crystallization improves the mechanical performance of the composites by three mechanisms [12]. First, the interaction between the CNT and the matrix is enhanced as the CNT/crystalline polymer interface is stronger than the CNT/amorphous polymer interface. Second, the crystalline polymer, which is stiffer and stronger than the amorphous polymer, is added to the composite system as the third constituent. Third, the aggregation of the CNTs can be alleviated after the introduction of crystalline polymer.

Two typical structures can be acquired by the interfacial crystallization. One is the transcrystallinity layer (TCL) shown in Fig. 1(a). The formation of a TCL is attributed to a high density of active nucleation at the interface, which confines the crystal growth to the direction of the CNT axis [13,14]. Considering the strong CNT/TCL interface as well as the high modulus and strength of the TCL, a better reinforcing effect can be expected. However, a new kind of interface is introduced into the composite system, namely the crystalline polymer/amorphous polymer interface. Owing to the difference of molecular alignment, strong interactions between these two kinds of polymers could not be guaranteed [15].

The other is the nanohybrid shish-kebab (NHSK) structure, in which the CNT serves as the shish and the crystalline polymer lamellae forms the kebabs [17–19]. As shown in Fig. 1(b), the CNT is decorated with crystalline polymer lamellae which are uniform in size and periodically located along the CNT. Compared to the TCL, the morphology of NHSK is more complicated, resulting in more sophisticated reinforcing mechanisms. Besides, three different types of interfaces exist in the NHSK reinforced composites, namely

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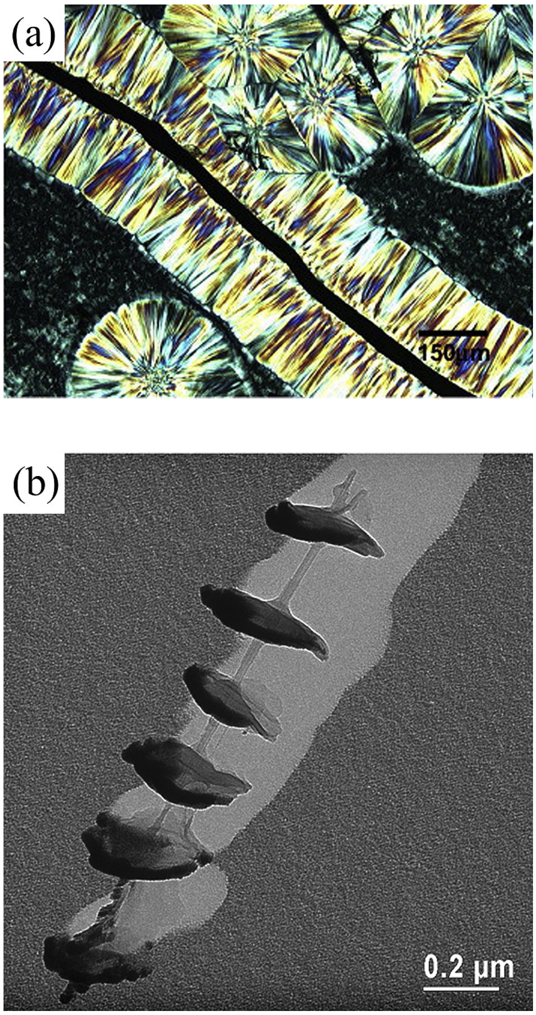

Fig. 1. TEM micrograph of CNT induced interfacial crystallization. (a) The transcrystallinity layer (TCL) [16]; (b) The nanohybrid shish-kebab (NHSK) structure [17].

the CNT/amorphous polymer interface, CNT/crystalline polymer interface and the crystalline/amorphous polymer interface, which may have pronounced effects on the performance of the composites.

The research and application of the interfacial crystallization call for a comprehensive understanding of its effect on the mechanical properties of the composites. Up to now, considerable experimental studies have been conducted to address this issue. The improvement of the elastic modulus and the strength of the composites with interfacial crystallization, no matter TCL or NHSK structure, have been observed in most macroscopic experiments reported [16,20–23]. To specify the microstructure of the composites and to analyze the load transfer from the matrix to the CNT, in situ spectroscopic analysis, including Fluorescence, Raman and X-ray spectroscopy, is also employed in this area [12]. For instance, by detecting the strain of the CNT using Raman spectroscopy, a considerable reinforcing effect of the CNT with TCL structures was confirmed, indicating a high load transfer efficiency of the composites [24]. Similarly, the enhanced load transfer was also observed by the Raman spectroscopy characterization for the composites incorporating NHSK structures [25]. In addition to the experimental studies, some researchers have attempted to illustrate the mechanisms of the CNT-induced crystallization by Molecular Dynamic (MD) simulation [26–28]. All the studies aforementioned have enhanced the comprehension of the crystalline mechanisms of the CNT-polymer system and provided some evidence that efficient load transfer does exist in the composites incorporating TCL or NHSK structures. However, to the best of our knowledge, the detailed load transfer characteristics of the composites have not been specified. Besides, the comparison between the reinforcing effects of the TCL and NHSK structures remains to be an interesting issue that has not been addressed yet.

The shear-lag model based load transfer analysis is proved to be an efficient method to evaluate the efficiency of reinforcement in the composite systems [29,30]. With the rapid development of the nanocomposites, the shear-lag model is being more and more frequently utilized to analyze the load transfer characteristics in the composites incorporating the nano-fillers, including nanotube and nanofiber [31–35]. For instance, Gao and Li [32] applied the shear-lag theory to the CNT-reinforced composites and analyzed the effect of the nanotube aspect ratio on the load transfer characteristics of the composites. Considering the CNT-induced polymer interface of the composites, Zhang and He [33] analyzed the viscoelastic behavior of the CNT-reinforced composites using a three-phase shear-lag model. Besides, the effects of other factors like the CNT curvature and the interfacial defects have also been studied by some researchers [35,36]. To sum up, the load transfer characteristics of the composites incorporating pristine CNT and TCL structures could be addressed by the current two-phase shear-lag model and three-phase shear-lag model, respectively. However, as far as we know, the load transfer characteristics of the NHSK reinforced composites have not been addressed theoretically because of the discontinuity of the matrix and interface in the longitudinal direction.

It can be expected that different load transfer characteristics reflecting distinct reinforcing mechanisms may be possessed by the composites after interfacial crystallization. Thus, it is critical to clarify the different load transfer characteristics of three kinds of composites, namely the composites incorporating the pristine CNTs, the TCLs and the NHSK structures. In this paper, a shear-lag model targeted at the composites incorporating NHSK structures is proposed by including the discontinuity of the matrix and interface. Then the load transfer characteristics of the three kinds of composites are clarified with the help of newly developed model. By comparisons, we try to characterize the distinct features of each composite and give some advices on tailoring the interfacial crystallization for high-performance composites.

2. Load transfer analysis on the CNT-reinforced composites with interfacial crystallization

The prerequisite of the shear-lag analysis is taking a cylindrical representative volume element (RVE) out of the composites as an object of study. Three different RVEs for composites incorporating the pristine CNTs, TCLs, and NHSKs are depicted in Fig. 2. Comparisons show that the former two RVEs can be regarded as special cases of the third one, in which the thickness of the crystalline polymer kebab and the gap between the neighboring kebabs are set to zero respectively. Thus, rather than deriving the formula for each case individually, we primarily focus on developing the shear-lag model for the NHSK reinforced composites, which can be degenerated to the cases of the pristine CNT and TCL afterwards.

As shown in Fig. 2(c), the radius and the length of the RVE are denoted as R and L, respectively. A uniform tensile stress σ is applied on the sections of the matrix at two ends of the RVE. Embedded in the RVE is a CNT of radius a, decorated by N crystalline polymer kebabs of radius b. The RVE can be divided into two types of segments, namely the two-phase segments and the three-phase