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Multi-scale study of the strength and toughness of carbon nanotube fiber materials

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ABSTRACT

The control mechanisms of the strength and toughness of carbon nanotube (CNT) fibers are revealed by analyzing the load-bearing and deformation characteristics of multi-scale structures in the fiber under tensile loading. A theoretical model is established to investigate the effect of the multi-scale structures on the strength and toughness of CNT fibers. Based on our previous experimental results on tension with in situ micro-Raman monitoring [Li et al., Nanotechnology 22, 2011], the macro- and micro-mechanical behaviors of the fiber are analyzed. The tensile behaviors of the fiber are correlated with the load-bearing and deformation processes involved in the multi-scale structures in the fiber, such as the nanotube bundle and the thread in microscopic scale, and the CNT in nanoscale. The CNT fiber exhibits high strength and toughness simultaneously depending on the multi-scale structure of the material, the differences in the properties between bundles and threads, and the unique interfaces formed by the tabular geometric configuration of double-walled CNTs. A constitutive relationship for CNT fiber materials is developed to provide information on the role of multi-scale structures on the strength and toughness of fibers. Both strength and toughness of CNT fibers can be enhanced by increasing the volume ratio of bundles to threads, the interfacial shear strength, and the interface slippage friction resistive force among the CNTs.

1. Introduction

Due to their excellent mechanical properties, carbon nanotubes (CNTs) have been investigated for building high-performance engineering materials since their discovery in 1991. A variety of macroscopic materials assembled using CNTs, including films [1], fibers [2], and blocks [3], have been developed progressively. Among them, CNT fibers generally exhibit high strength and high toughness, which makes them attractive for a wide range of applications in practical engineering. Thus, understanding the underlying mechanisms involved in the development of high strength and toughness in CNT fiber materials is important.

Over the past two decades, much effort has been devoted to investigating the mechanical properties of CNT-based materials in experimental and model characterization. For example, Cheng et al. demonstrated that the winding of single-walled CNT fibers could enhance their material strength to a certain degree through tensile testing [4]. Beyerlein et al. investigated the effects of fiber diameter and gauge length on the statistical strength of CNT fibers [5]. Liu et al. presented a hybrid atom/continuum model to study the nonlinear elastic properties of single-walled CNT bundles as bulk materials [6]; Vilatela et al. developed an analytical model to calculate the theoretical axial strength of CNT fibers [7]. However, the control mechanism for the strength and toughness of CNT fiber materials is still not clear. Generally, the mechanical properties of CNT fibers are strongly affected by fabrication methods and processing techniques because the arrangement of CNTs and their interactions depend significantly on the fabrication process. For example, the strength of CNT fibers spun from CNT suspensions is about 0.15 GPa and their elongation is about 2% [8]; the strength of fibers drawn out from multi-walled CNT arrays is approximately 0.46 GPa with 10% elongation [9]; and fibers spun from CNT aerogel formed with chemical vapor deposition (CVD) can reach a tensile strength of up to 1.46–9 GPa. The corresponding elongation ranges from 5% to 10% [2,10,11]. The studies cited above indicate that multi-scale microstructure and deformation performance are two major control mechanisms of the mechanical properties of CNT fibers. Meanwhile, little attention has been paid in the literature to the toughness of CNT fibers, although strength and toughness are the two most important mechanical properties. Improving the strength and toughness of most CNT-based materials is not possible because of lack of critical knowledge on the underlying

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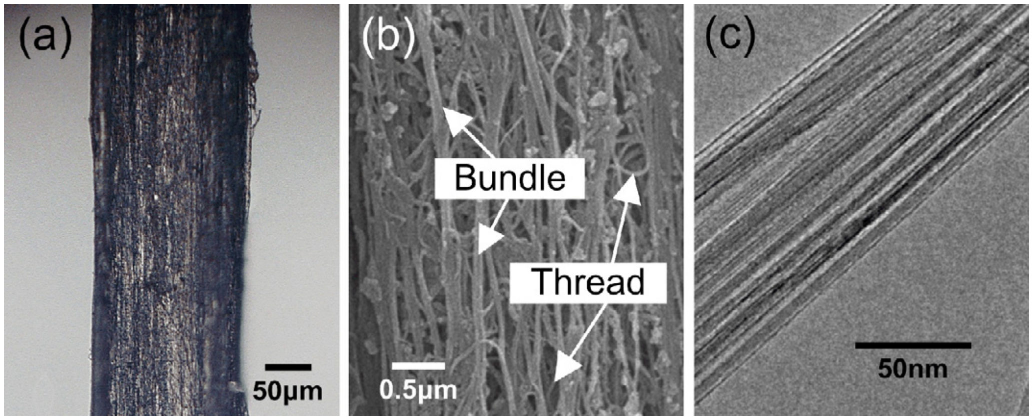

Fig. 1. Macro- and microscopic morphologies of the CNT fiber. (a) An optical photo of the CNT fiber. (b) SEM image of the fiber surface. (c) TEM image of a bundle (or thread) in the fiber.

mechanisms. Therefore, the following questions should be addressed: Why do some CNT fiber materials possess high strength and high toughness simultaneously? How are the strength and toughness of the materials affected by their microstructures? How can we effectively characterize the strength and toughness of these CNT fibers?

In our previous work [12], tensile tests coupled with in situ Raman detection have been carried out for CNT fibers spun from CNT aerogel formed with CVD. The individual CNTs deform elastically without obvious damage or bond breakage. The yield and fracture of fibers can be due to the slippage among the CNTs. In this work, the strength and toughness of CNT fibers are studied at multi-scale levels. Based on the macroscopic tension tests and in situ micro-Raman detection results and the microstructure characteristics of the fibers observed, the load-bearing and deformation processes of multi-scale structures in the fibers under tension are analyzed to provide an insight into the control mechanisms of the strength and toughness of CNT fibers. More importantly, a constitutive relationship for CNT fiber materials is developed using the analysis described. The constitutive relationship is then used to investigate the influence of the multi-scale structures on the macroscopic strength and toughness of the fibers.

2. Mechanisms of the strength and toughness of CNT fibers

The CNT fiber materials are spun from CNT aerogel formed by CVD [13]. Macro and micro morphologies of the fiber are shown in Fig. 1. The fiber has a multi-scale structure: the fiber itself is in macroscopic scale, the nanotube bundle and thread in microscopic scale, and the CNT in nanoscale. The macroscopic fiber (Fig. 1(a)) contains relatively thick and straight bundles, as well as fine, flexible threads (Fig. 1(b)). The bundles preferentially align along the fiber axis. The threads are distributed among the bundles and combined. Both the bundles and threads are formed by piling double-walled CNTs with a collapsed section (Fig. 1(c)). Further information on this process can be found elsewhere [13].

2.1. Tension experiment of CNT fibers coupled with Raman detection

The uniaxial tension of the CNT fiber is measured by a precise micro-loading device. The fibers are stuck onto the center-hollow paper cards and then mounted in the micro-loading device with cards. The fiber gauge lengths are fixed to 5 mm, and the average strain rate is 0.7% min^{-1}. During the application of uniaxial tension to the fibers, the spectrum data are collected by a Renishaw InVia Raman spectroscope. Detailed information can be found in our previous work [12]. The macroscopic stress–strain curve and the G' Raman band information of the fibers are given in Figs. 2 and 3, respectively.

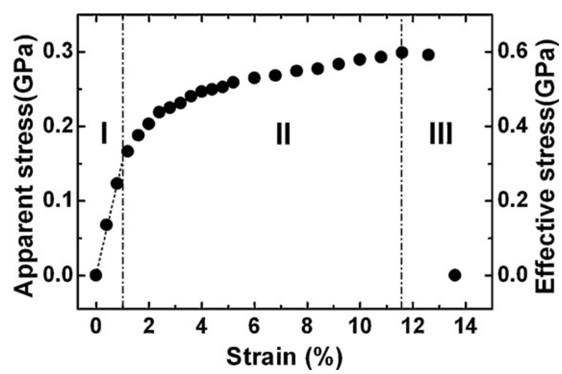

Fig. 2. Change in tensile stress of CNT fiber with strain.

2.2. Mechanisms of the strength and toughness of CNT fibers

The deformation process of the fibers includes three stages, namely, the elastic stage I (strain < 1%), the hardening stage II (1% ≤ strain ≤ 11.5%), and the damage-fracture stage III (strain > 11.5%), as shown in Fig. 2, where the fiber strain is obtained from the ratio of its deformation quantity to gauge length. The fiber deformation quantity is read out from the micro-loading device. The apparent wall thicknesses and circumferences of the fibers are obtained from the scanning electron microscope (SEM) images of the cross-sections of the fibers. The apparent Young's modulus, yield limit ($\sigma_{0.2}$), and strength limit of the CNT fiber are estimated as 15.6, 0.14, and 0.3 GPa, respectively. These data are based on the SEM images where a large space inside the fiber walls exists. Thus, the volume (or area) occupied by the space should be excluded from the total volume (or area) when calculating the effective mechanical properties based on the actual cross-sectional loaded area. According to the SEM observations, the estimated volume fraction of CNTs inside the fiber walls is ≤50%. Thus, the effective calculated Young's modulus, yield limit and strength limit of the fibers should be at least twice of the values mentioned above, namely, 31.2, 0.28, and 0.6 GPa, respectively. The elongation of the fibers given in the experiment is approximately 11%. All these data indicate that the CNT fibers exhibit both outstanding strength and relatively high toughness simultaneously.