CARBON NANOTUBE FIBERS: CHALLENGES AND OPPORTUNITIES

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Abstract:
This paper accesses the recent advancements in the science and technology of carbon nanotube (CNT) fibers, in terms of their fabrication methods as well as characterization and modeling of mechanical and physical properties. The challenges and opportunities in CNT fiber research are also evaluated.

Keywords: *carbon nanotubes; fibers; mechanical properties; challenges and opportunities*

1. Introduction

The superb mechanical and physical properties of individual carbon nanotubes (CNTs) provide a great opportunity for researchers in developing high-performance continuous fibers based upon CNTs [1,2]. Due to the good alignment and high volume fraction of constituent CNTs, CNT fibers have shown excellent mechanical and physical properties[3,4], and demonstrated the high potential for their usage as reinforcements in multifunctional composites as well as strain sensors [1,2,5]. In this paper, we assess the recent advances in CNT-based continuous fibers. The review is conducted in terms of their fabrication methods as well as characterization and modeling of mechanical and physical properties. The challenges and opportunities in CNT fiber research are also evaluated.

2. Fabrication of CNT fibers

The highly aligned individual CNT bundles can be assembled to a form a microscope fiber mainly by the inter-tube van der Waals interactions. There are three major techniques for fabricating CNT fibers:

(1) Spinning fibers from a lyotropic liquid crystalline suspension of nanotubes, in a wet-spinning process similar to that used for polymeric fibers such as aramids, as shown in Fig. 1a. Both fibers with and without polymer can be obtained by this method[6-10].

(2) Spinning fibers from multi-walled CNTs previously grown on a substrate as ‘‘semi-aligned” carpets (forests) [3, 11-16], as shown in Fig. 1b, and

(3) Spinning fibers directly from an aerogel of single-walled and multi-walled CNTs as they are formed in a chemical vapor deposition reactor [17-19], as shown in Fig. 1c.

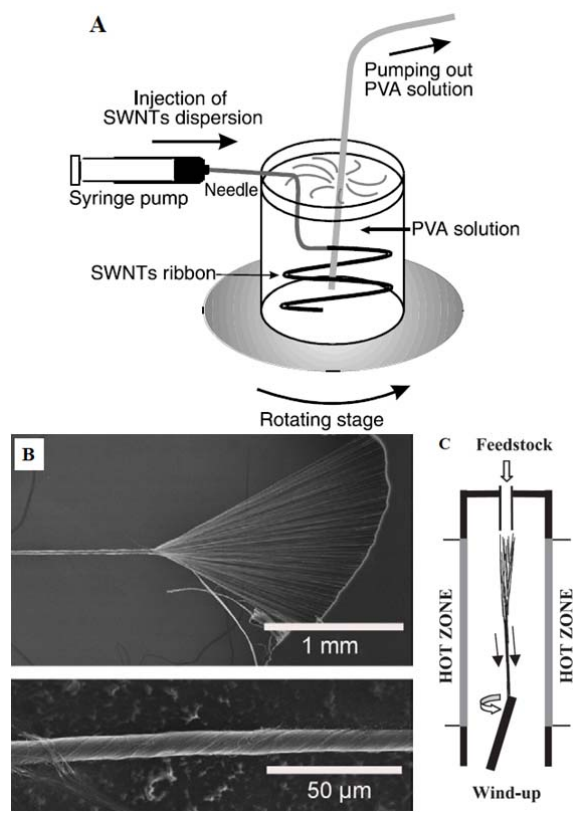

Fig. 1. CNT fiber spun from (a) CNT solution [6], (b) CNT forest[5], and (c) CNT aerogel[17], respectively.

3. Characterization of CNT fiber properties

In the past decade, intensive experimental studies have been conducted by researchers to characterize the performance of CNT fibers. Fig. 2(a) summarizes the tensile strength and modulus of CNT fibers fabricated from the aforementioned methods. It is found that fibers spun from CNT aerogel possess the highest tensile strength so far. CNT length has significant effect on fiber tensile properties. For example, Zhang et al. [15] spun CNT fibers with comparable diameters (about 4 μm) from arrays of 300, 500, and 650 mm in length and compared their strength. As shown in Fig. 2(a), the tensile strength increases with increasing CNT length, from 0.32 to 0.56 and to 0.85 GPa, respectively. It is suggested that longer nanotube could not only lead to a higher friction force at the nanotube interfaces, but also reduce the fraction of CNT ends, which are regarded as defects in the fiber. Koziol et al.[19] pointed out that CNTs of larger diameter with fewer walls would collapse during fiber fabrication, which could increase the contact area between CNTs and enhance the load transfer efficiency.

The effects of the post-processes, such as liquid shrinking and spinning, on the mechanical properties of CNT fibers have also been studied [14-16]. These post-processes could densify the as-spun fibers and enhance the load transfer efficiency between CNTs. Fig. 2c and d are two examples showing the effects of liquid shrinking[14] and spinning[15].

Recently, Deng *et al.* [20] reported several fundament studies relevant to the mechanical behavior of CNT fibers spun from CNT forest. In-situ SEM observations have shown that under tensile loading, several distinct deformation stages can be identified, namely initial tightening of the CNT bundle, followed by loosening, tightening again and final fracture at ultimate load. Figure 3a shows a typical fiber tensile stress-strain curve. The elastic moduli identified on the curve correspond approximately to the first and second tightening stages. Figure 3b shows the data of measured tensile strength at various fiber diameters. The fiber strength decreases with increasing fiber diameter. In order to analyze the statistic characteristic of CNT fiber strength, a modified Weibull strength theory was applied to the test data. It is concluded that the

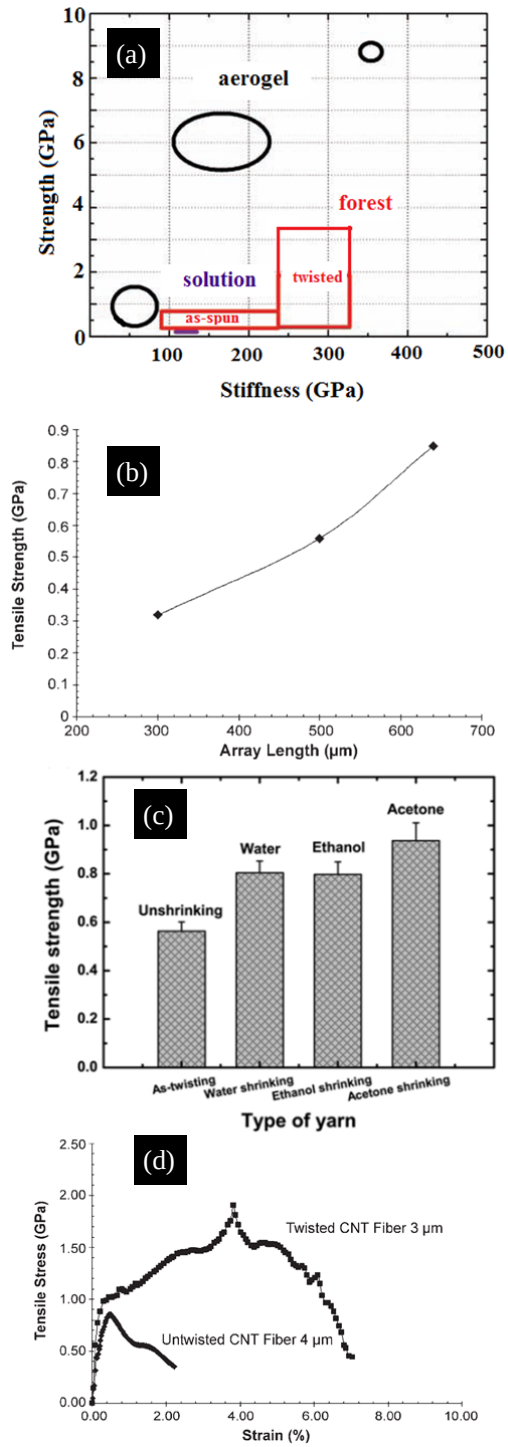

Fig. 2 (a) Comparison of tensile stiffness and strength of CNT fibers fabricated by different methods[3,8,15,19]; and the effects of (b) CNT length[15], (c) liquid shrinking [14] as well as (d) spinning[15].

strength of CNT fibers shows smaller scattering than those of multi-walled CNTs but larger scattering than those of commercial carbon and glass fibers. The interfacial behaviors of CNT fiber in an epoxy matrix have also been investigated through single fiber fragmentation test[20] and microdroplet test[21].

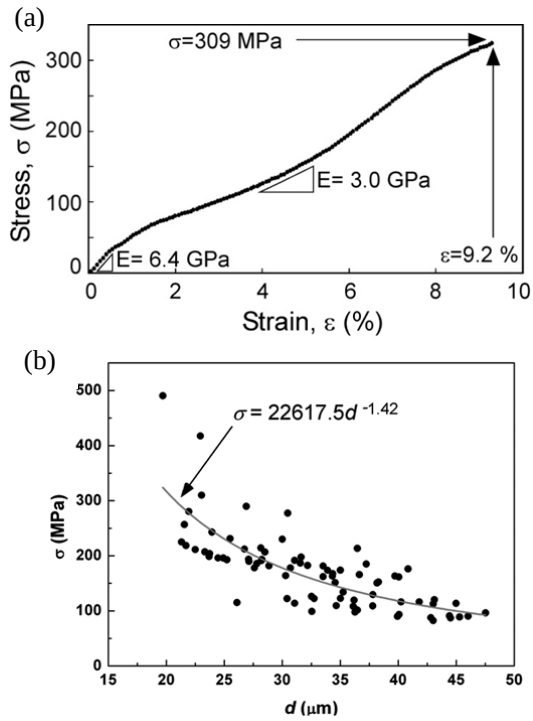

Fig. 3. (a) A typical tensile stress-strain curve of CNT fibers; (b) CNT fiber strength at various fiber diameters[20]

4. Analysis and Modeling

The characterization of CNT fibers as well as their constituent CNTs has motivated some analytical work for modeling their properties. Existing research work has focused on, for example, the statistical fiber strength [22], as well as the entanglement[23] and radial deformation[24] of CNTs in the fiber.

Beyerlein et al. [22] investigated the effects of yarn diameter and gauge length on the statistical strength of CNT fibers spun from CNT forest. A Monte Carlo simulation model has been developed to predict the relationship between fiber nanostructure and tensile strength. Predictions indicate that the mean and statistical variation in strength decrease as the surface twist angle, number of CNTs in the cross section and gauge length of the yarn increase.

CNT entanglements have been observed in CNT fibers and films. Lu and Chou [23] studied the mechanical behaviors of the entanglements using both theoretical analysis and atomistic simulation methods. The CNT entanglement is modeled as two connecting self-folded CNTs (SFCNTs), as shown in Figure 4. The critical length for the formation of the SFCNT is around $12.00\sqrt{EI/\gamma}$, where EI and γ are the CNT bending stiffness and interfacial binding energy, respectively. The mechanical responses of the CNT entanglement under tensile force, as well as the effects of CNT radius and length, have also been studied.

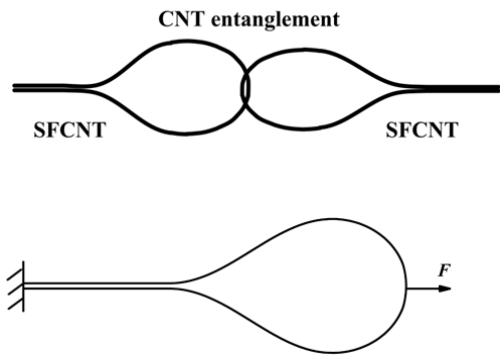

Fig. 4 Theoretical model for analyzing the mechanical response of CNT entanglement in fibers[23]

Contrary to the high stiffness along the axial direction, CNTs are relatively compliant in the radial direction. CNTs are susceptible to deformation or even collapse under the inward force induced by fiber twisting [19, 25, 26]. Lu *et al.* [24] studied the cross-sectional transformation of SWCNTs during radial deformation using both atomistic simulation and continuum theoretical analysis. There exist two critical radii R_1 and R_2, which are 1.05nm and 1.90nm, respectively. For SWCNTs with radius less than R_1, the initial circular states are found to be most stable; for SWCNTs with the radius between R_1 and R_2, the collapsed states are metastable, but the circular states are energetically favorable; and for SWCNTs with radius large than R_2, the fully collapsed state becomes energetically favorable. The energy variation during the radial deformation has also been investigated. Both energy barrier and energy difference for the collapse of SWCNTs decrease with increasing SWCNT radius.

5. Challenges and Opportunities

Laboratory scale CNT fibers, which often possess small fiber size and exhibit high modulus and strength as well as superb thermal and electrical conductivities, have high potential as reinforcements in multifunctional composites.

In spite of the significant improvements in recent years toward developing high performance CNT fibers, there still exist some major challenges. For example, their mechanical and physical performance are at the level far below those of individual CNTs. Also, the scaling-up of current processes to produce continuous fibers suitable for textile processing is imperative.

Lastly, the integration of the knowledge-base developed in fabrication and characterization of CNT fibers will greatly facilitate the development of modeling and simulation methodologies, which are indispensible for the application of CNT fibers in advanced composites.

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