STRENGTH PREDICTION OF CARBON NANOTUBE YARNS USING A STRUCTURAL MECHANICS APPROACH

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1 Introduction

Recently, carbon nanotubes (CNTs) have been processed to yarns, woven and braided textiles via textile technologies, aiming to utilize their remarkable mechanical and electrical properties in micro/macro scales [1]. Since yarns are the fundamental unit of all these structures, their mechanical properties, such as tensile modulus and strength, are important factors to determine the mechanical performance of such textiles. As such the mechanical modeling of yarns in the macro and micro scale has been researched in the textile community since 1940. It is, however, uncertain that such modeling can be used to predict the mechanical properties of CNT yarns due to their nanoscale constituents (CNTs). This study is to investigate and modify a mechanical model, which was developed for textile yarns consisting of microfibers, and finally to develop a suitable model for predicting the tensile strength of CNT yarns based on their manufacturing conditions.

2 Theoretical models for yarn strength

2.1 Classical methods

Many mechanics models have been developed to predict the strength of staple yarns (consisting of short microfibers). We noted that a mechanical model developed by Pan [2] can be highly applicable to CNT yarns. Considering the fiber fragmentation mechanism, he derived the following equation for predicting the strength (σ_y) of staple yarns.

$$<\sigma_y> = \eta_q V_f \gamma (l_e \alpha \beta)^{-1/\beta} \exp(-1/\beta) \qquad (1)$$

Here η_q is the orientation efficiency factor determined by both the helix angle and Poisson's ratio. V_f is the fiber volume fraction within yarn. Note that we introduced a new parameter (γ) to consider the tubular structure of the constituents (CNTs). γ was defined as a geometric factor considering the cross section of a tube as follows.

$$\gamma = \frac{r^2 - (r-t)^2}{r^2} \qquad (2)$$

where r and t are the outer radius and the wall thickness of the nanotube, respectively. Assuming that stresses are transmitted to each staple fiber (CNT) by the frictional mechanism, l_e was defined as the effective length for the load transfer as follows.

$$l_e = \frac{r_f \sigma_f}{\mu g} \qquad (3)$$

where r_f is the fiber radius, σ_f is the fiber tensile stress, and μ and g is the frictional coefficient and lateral pressure in a twisted yarn, respectively. α and β in Eqn (1) are the scale and shape parameters in Weibull distribution of the strength of CNT fibers. Though Eqn (1) was developed for staple yarns with short microfibers, it can be used to predict the strength of CNT yarns assuming that the load transfer mechanism between CNTs inside the yarn is the same as that of short microfibers, i.e., accepting the scaling law. Then, several parameters in Eqn (1) can be determined for CNT yarns. A Weibull distribution (α and β), which were determined from multiwall CNTs [3], was used in this study. Since the orientation efficiency factor and fiber volume fractions are design parameters for a specific CNT yarn, they can be assumed or parameterized for the calculation. Lastly, the effective length should be provided, requiring μ and g, which can be determined experimentally or theoretically. Note

that experimental approaches for determining the two parameters (μ and g) are not routine due to the nanoscale CNTs. Therefore, in this study they were determined theoretically using finite element analysis. For this calculation, the properties of each CNTs were determined using a structural mechanics approach, which may be considered as an alternative to molecular dynamics (MD).

2.2 Structural mechanics approach

MD is a powerful method to calculate the frictional coefficient and lateral pressure between CNTs inside CNT yarn; however a long computational time is a definite disadvantage. To overcome this, a structural mechanics approach was developed and used to calculate the mechanical behavior of CNTs [4]. Structural mechanics considering the potential function in MD can be an alternative option because it can readily incorporate the properties of CNTs into continuum scale structure and their mechanical behavior can be calculated using well established methods such as finite element method. Here, the mechanical properties of CNTs are important in this approach and can be determined using MD simulation. In this research the following mechanical properties were used for each CNT [4].

Table 1. Mechanical properties of CNTs for structural mechanics approach.

Modulus(Young's) [GPa]	Poisson ratio
E_1: 113 E_2: 113 E_3: 1130 G_{12}: 44.6 G_{13}: 470 G_{23}: 470	ν_{12}:0.267 ν_{13}:0.048 ν_{23}:0.048

Then, a finite element model was constructed by modeling each CNT inside CNT yarns using a 3D element and used to determine the parameters in Eqn (3) as follows.

2.3 CNT yarn model

A geometric model for CNT yarn was constructed as shown in Fig. 1. A twisting operation was then simulated by imposing the fixed boundary condition on the bottom side of each CNT, while its top side was tensioned parallel to the yarn axis. Seven CNTs were used in the modeling assuming the hexagonal close-packed structure of CNTs inside yarn. The finite element analysis was carried out to calculate the lateral pressure between CNTs inside the yarn according to tension applied to each CNT. Van der Waals interaction, which was calculated by Lennard-Jones potential between CNTs (see Fig 2), was included in addition to the frictional force during the lateral pressure calculation.

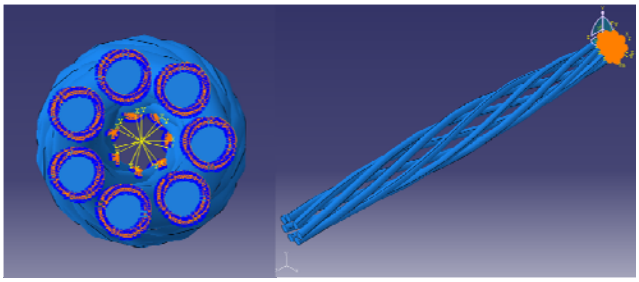

Fig.1. CNT yarn model with close-packed structure (left) and the boundary conditions for twisting operation (right).

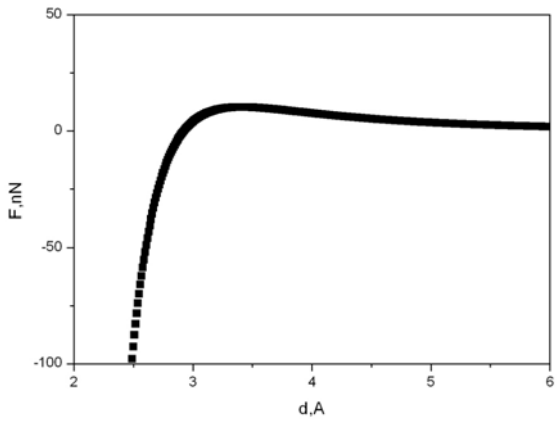

Fig. 2. Van der Waals forces between two identical CNTs (diameter 10nm).

3 Results and discussion

The lateral pressure was calculated using finite element analysis (see Fig. 3). The maximum lateral pressure (3.50GPa) was calculated when the stress (18.60GPa) was applied to each CNT. The frictional coefficient of CNTs is generally determined by their

arrangements [5]. When CNTs were vertically aligned, the frictional coefficient was found to be about 0.9. This value was adopted in this study. Due to the high friction and the CNT migration in the yarn, the yarn interior is not hexagonal close packed structure. Geometric irregularities within CNT yarn exist and may reduce lateral pressure than hexagonal close packed case, which can again lower the mechanical properties of CNT yarns.

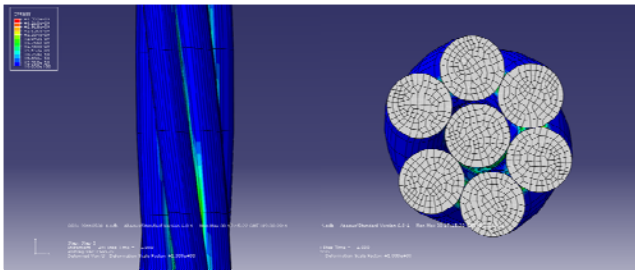

Fig.3. Twisted and deformed shape of CNT yarn (left) and its cross section (right).

Then, the volume fraction of the CNT yarns was estimated using the cross section of geometric model (see Fig. 4.). The yarn diameters were measured in several locations along the yarn axis and the volume fraction was calculated considering the proportion of the yarn area to the CNT area. The average volume fraction was obtained to be about 0.7.

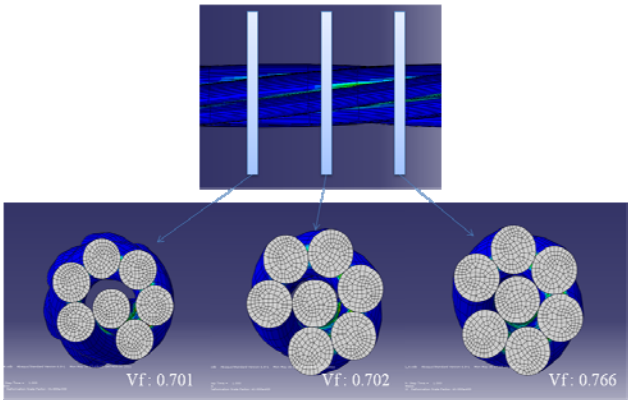

Fig.4. The estimation of CNT volume fraction considering its migration within the yarn.

The parameter α and β determined from multiwall CNTs Weibull distribution were used: $6.343 \times 10^{-4} m^{-1} GPa^{-1}$ and 7.7 [3]. The helix angle was assumed to be 30°, and γ was calculated to be 0.1314 for CNTs with a diameter of 10nm. Using calculated parameters and the lateral pressure (frictional coefficient), the strength of CNT yarn was determined to be 1.27GPa. The calculated value is much higher than experimental values which have been reported, e.g., 150~750MPa[1][6-8], for similar yarn manufacturing condition. The discrepancy can be explained by the modeling approach (the current geometry is closed to filament yarn). Generally, for the same material, staple fiber yarns have the tensile strength two thirds lower than its corresponding filament yarns due to irregular inner structure inside staple yarns. Furthermore, the experimental values we compared were obtained from CNT yarns produced by a dry method (a spinning process from aligned CNT arrays). The inner structure of CNT yarns created by this process is not densely packed and constituent CNTs are not straight. It will reduce the volume fraction and decrease the stresses in CNTs within the yarn due to the obliquity effect. As a result, the actual strength of CNT yarns was lower than their theoretical value. Nevertheless, the current model can provide a pathway to realize the theoretical strength of CNT yarns, the detail of which will be presented at the Conference.

4 Conclusions

A methodology was presented that can calculate the tensile strength of CNT yarns. It combined a mechanical model, which was originally developed for staple yarns with microfibers, with nanoscale calculations, which were performed a finite element analysis. For the nanoscale calculation, the mechanical properties of CNTs were provided from a literature, based on which some parameters necessary for strength calculation were calculated from a structural mechanics approach. The lateral pressure considering Van der Waals interaction which was calculated by Lennard-Jones potential was calculated and used to determine the effective length for load transfer in the CNT yarn. The validation of the current method was discussed by comparing its results with existing experimental values, demonstrating that the present methodology is simple enough to design CNT yarns considering yarn manufacturing conditions.

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