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A new Monte Carlo model for predicting the mechanical properties of fiber yarns

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ABSTRACT

Understanding the complicated failure mechanisms of hierarchical composites such as fiber yarns is essential for advanced materials design. In this study, we developed a new Monte Carlo model for predicting the mechanical properties of fiber yarns that includes statistical variation in fiber strength. Furthermore, a statistical shear load transfer law based on the shear lag analysis was derived and implemented to simulate the interactions between adjacent fibers and provide a more accurate tensile stress distribution along the overlap distance. Simulations on two types of yarns, made from different raw materials and based on distinct processing approaches, predict yarn strength values that compare favorably with experimental measurements. Furthermore, the model identified very distinct dominant failure mechanisms for the two materials, providing important insights into design features that can improve yarn strength.

1. Introduction

Since their discovery in 1991, carbon nanotubes (CNTs) have attracted considerable attention in the mechanics community for their superior strength (up to 100 GPa) and elastic modulus (up to 1 TPa) (Iijima, 1991; Zhang et al., 2004). These outstanding mechanical properties make CNTs the ideal building blocks for macroscopic composites that require light weight and high mechanical performance for use in aerospace and automotive applications. One promising approach to scale up the mechanical properties of CNTs is to spin them into macroscopic yarns. Two main techniques have been developed to make macroscopic yarns, for instance: (i) dry spinning of CNT yarns by drawing and twisting from CNT arrays, aerogels, or mats (Denis-Lutard et al., 2010; Koziol et al., 2007; Min et al., 2012; Naraghi et al., 2010; Ryu et al., 2011; Tran et al., 2009; Zhang et al., 2004, 2008); and (ii) wet spinning of CNT yarns by drawing and twisting from CNT sources embedded in chemical solutions (Li et al., 2004; Zhang et al., 2007). Similar to the micromechanics in staggered hierarchical biological composites, such as nacre shell (Barthelat et al., 2007; Meyers et al., 2008), collagen fibril (Fratzl et al., 1998) and spider silk (Keten et al., 2010), the load in CNT yarns is transferred over the overlap distance between fibrils via shear stresses at the interfaces. The nanoscale building blocks have two distinct failure modes – fibril rupture and interface sliding – that can eventually cause the failure of macroscopic yarns. Which of the two modes will dominate the composite failure depends on the critical dimensions and the mechanical properties of the building blocks (Bar-On and Wagner, 2013; Begley et al., 2012; Selle et al., 2015; Yao et al., 2013). For yarns consisting of bare CNTs, the weak van der Waals interactions between carbon atoms cannot offer an interface strong enough to hold the integrity of yarns at a high load. Researchers have

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developed various techniques to improve the load transfer ability of the inter-fibril interfaces via either non-covalent bonds between functional chemistries on the CNTs surfaces or covalent bonds formed between cross-linked tubes (Filleter and Espinosa, 2013; Kis et al., 2004; Lu et al., 2012). Despite these efforts, the strengths of CNT yarns reported to date still fall short of the strength of individual CNTs. Identifying the primary cause of the yarn failure among the two competing failure modes – fibril rupture and interface sliding – is critical to advance this research.

Theoretical models have been explored to attempt to understand the predominant mechanisms of yarn failure. The first yarn model proposed by Daniels (Daniels, 1945) treated the yarn as a bundle of parallel fibers that were evenly clamped at each end and had no interactions between each other. These fibers had the same length and cross-sectional area; however, the fiber strength distribution followed a Weibull probability function, i.e., the failure probability for a fiber under an applied stress $\sigma$is given by.

$$P(\sigma) = 1 - \exp\left[- \frac{L_b}{L_0}\left(\frac{\sigma}{\sigma_0}\right)^m \right] \tag{1}$$

where L_0 is the reference fiber length, L_b is the fiber length, σ_0 is the scale factor, and m is the shape factor. Daniels showed that when the load redistributes equally on intact fibers, the strength of the yarn asymptotically approaches a *Gaussian distribution*. Other models extended this approach to include more geometric factors. The continuum model developed by Hearle investigated the effects of fiber length, twisting angle, and fiber migration on the yarn mechanical properties (Hearle et al., 1969). Hearle's model used a static friction law to simulate the interaction between fibers. Thus, statistics of the fiber strength and evolution of the microstructures, such as load redistribution after fiber breaks, are absent in Hearle's model. Porwal et al. (2006) extended Daniels' model and developed a Monte Carlo model to predict the statistical strength of a twisted fiber yarn using a twist-modified equal load sharing (TM-ELS) rule. Porwal's model takes into account the statistical variation of fiber strength and simulates fiber break initiation and progression for a yarn under tension. Later, with some modifications to the load sharing rule, this model was adopted to predict the mechanical strength of CNT yarns (Beyerlein et al., 2009; Porwal et al., 2007). These existing models simplify interactions at the interfaces as a static friction law that requires a transverse pressure on fibers to cause load transfer. Furthermore, the friction law implies that the interactions between fibers can be enhanced linearly when the overlap distance increases, which is inconsistent with the experimental observation where the load transfer capability tends to saturate at some overlap distance (Wei et al., 2012). Therefore, the friction law is an oversimplification of the interfaces and may not accurately simulate the load distribution on fibers along the overlap distance.

In this study, we developed a new Monte Carlo model for fiber yarns in which the history of stochastic fibril rupture and interface sliding in macroscopic yarns is simulated and their effects on the mechanical properties of the fiber composites investigated. The interface is modeled as a soft thin layer that undergoes only shear deformation. The mechanical properties of the building blocks, fibril statistical strength and interface shear strength, are inputted from nanoscale experiments (Filleter et al., 2011; Filleter and Espinosa, 2013; Naraghi et al., 2013', 2010). Case studies on two types of CNT yarns were performed using this model, and distinct bottlenecks for the mechanical performance of both types of yarns were identified.

2. Model development

2.1. Yarn geometry and model discretization

A twisted fiber yarn consisting of fibers in a hexagonal close-packing structure was assumed in our stochastic Monte Carlo model (Fig. 1). Axial positions of individual fibers were randomly distributed to account for a random distribution of overlap lengths. Each fiber is discretized into a series of 1-D elements along the fiber axis, and thus the normal stress in a

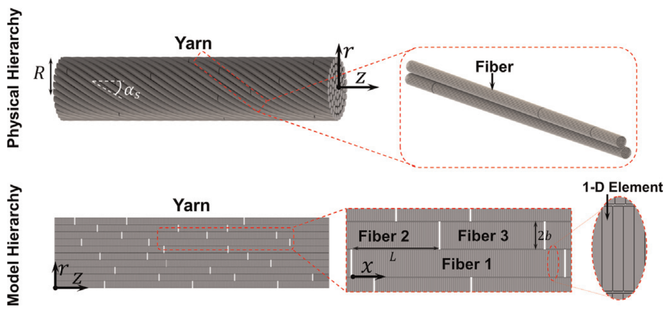

Fig. 1. Schematics of idealized yarns depicting (left to right): the cross-sectional view of the yarn model, randomly distributed fibers (in this study, a fiber refers to a bundle consisting of 60 to 100 double-walled carbon nanotubes), and a fiber discretized by 1-D elements. (Top) hierarchical structure of a 3-D ideally twisted yarn consisting of hexagonal close-packed discontinuous fibers; (bottom) yarn hierarchy in the Monte Carlo model (section view) reported here.