Hierarchical fiber bundle model to investigate the complex architectures of biological materials

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The mechanics of fiber bundles has been widely studied in the literature, and fiber bundle models in particular have provided a wealth of useful analytical and numerical results for modeling ordinary materials. These models, however, are inadequate to treat bioinspired nanostructured materials, where hierarchy, multiscale, and complex properties play a decisive role in determining the overall mechanical characteristics. Here, we develop an *ad hoc* hierarchical theory designed to tackle these complex architectures, thus allowing the determination of the strength of macroscopic hierarchical materials from the properties of their constituents at the nanoscale. The roles of finite size, twisting angle, and friction are also included. Size effects on the statistical distribution of fiber strengths naturally emerge without invoking best-fit or unknown parameters. A comparison between the developed theory and various experimental results on synthetic and natural materials yields considerable agreement.

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I. INTRODUCTION

The origin of how naturally occurring biomaterials (e.g., cellular protein filaments, spider silk, bone, tendon, skin) are capable of unifying disparate mechanical properties such as strength (ability to sustain large stresses without fracture) and toughness (ability to undergo deformation and thus dissipate energy without fracture, despite the presence of defects) is of great interest in materials science [1–3]. The performance of synthetic materials such as carbon-nanotube composites in this and other respects (e.g., superadhesive or antiadhesive properties) is constantly improving [4], but remains substantially poor [5]. Thus, to mimic nature is potentially an extremely promising approach in the design of new nanostructured materials, because naturally occurring high-nanotech smart material strategies can often be revealed [6–10]. The "secret" of these materials would seem to lie in "hierarchy" [11–13]. Indeed, several hierarchical levels can often be identified in biomaterials, from nanoscale to microscale: two in nacre, and up to seven in bone and dentin [12,14]. Using theoretical tools to investigate these issues, however, is often inadequate in tackling the large range of size scales involved, ranging from nanometers to meters or even kilometers [15,16].

First developed by Daniels [17], one of the most common theoretical approaches used in the engineering and physics communities to investigate the fracture and breakdown of disordered media is a so-called fiber bundle model (FBM) [18], which allows the derivation of the mechanical property sets for parallel arrangements of fibers with statistically distributed strengths. In general, a fiber bundle consists of a set of N_y parallel fibers with statistically distributed strengths, and a chain of bundles consists of a set of N_x bundles arranged in series [19]. The sample is loaded parallel to the fiber direction and the fibers fail if their stress threshold value is exceeded. Through statistical considerations, a relation between the strength of a bundle and the strength of its constituent fibers is found. This very simple approach has been widely used and further developed to include size and/or length dependency, random slack of fibers [20], localized load-sharing mechanisms during fiber breakage [21], fiber twisting [22], friction effects [23], generalized damage laws, interaction between fibers [24], etc. Also, much attention has been given to the development of models for composite materials, when the fibers are embedded in a matrix [25]. Numerical approaches have been adopted to introduce hierarchy in FBMs [16,26–28], but a systematic analytical theory is currently missing.

Here, we develop a theory, basically the hierarchical extension of Daniels' pioneering model, complementary to a recently introduced numerical hierarchical fiber bundle model (HFBM) [16]. This purely analytical theory, which does not require best-fit or unknown parameters, can be used to analyze structures typically found in biological or bioinspired materials, and could potentially be of great help in the domain of nanomechanics, replacing cumbersome and time-consuming numerical approaches.

The paper is structured as follows: The model is outlined in Sec. II, and numerical calculations are analyzed and compared to a number of experimental results from the literature in Sec. III.

II. MODEL

A. Hierarchical generalization of Daniels' theory

The structure of many fibrous biological materials can be seen as that of a rope, i.e., a hierarchical ensemble of fibers, as schematically shown in Fig. 1 (left). Different hierarchical levels can be identified, starting from single fibers (level 0). A bundle of fibers corresponds to a yarn (level 1), a bundle of yarns corresponds to a strand (level 2), and a bundle of strands corresponds to a rope (level 3). "Twisting" can be introduced at any level, and in the general case, the hierarchical structure can extend over many (n) levels. This arrangement suggests

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