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Micromechanical design of hierarchical composites using global load sharing theory



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ABSTRACT

Hierarchical composites, embodied by natural materials ranging from bone to bamboo, may offer combinations of material properties inaccessible to conventional composites. Using global load sharing (GLS) theory, a well-established micromechanics model for composites, we develop accurate numerical and analytical predictions for the strength and toughness of hierarchical composites with arbitrary fiber geometries, fiber strengths, interface properties, and number of hierarchical levels, N. The model demonstrates that two key material properties at each hierarchical level-a characteristic strength and a characteristic fiber length-control the scalings of composite properties. One crucial finding is that short- and long-fiber composites behave radically differently. Long-fiber composites are significantly stronger than short-fiber composites, by a factor of 2^N or more; they are also significantly tougher because their fiber breaks are bridged by smaller-scale fibers that dissipate additional energy. Indeed, an "infinite" fiber length appears to be optimal in hierarchical composites. However, at the highest level of the composite, long fibers localize on planes of pre-existing damage, and thus short fibers must be employed instead to achieve notch sensitivity and damage tolerance. We conclude by providing simple guidelines for microstructural design of hierarchical composites, including the selection of N, the fiber lengths, the ratio of length scales at successive hierarchical levels, the fiber volume fractions, and the desired properties of the smallest-scale reinforcement. Our model enables superior hierarchical composites to be designed in a rational way, without resorting either to numerical simulation or trial-and-error-based experimentation.

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1. Introduction

Many natural composites employ a multi-scale or *hierarchical* microstructure (Fratzl and Weinkamer, 2007; Rho et al., 1998). Motivated by the conjecture that such microstructures have been "optimized" for mechanical performance (Gao, 2006; Zhang et al., 2011), researchers have become increasingly interested in incorporating hierarchical design principles into *synthetic* composites (Brandt et al., 2013). However, given the vast space available for materials design—the selection of individual constituents, their geometry, the number of scales, etc.—a mechanics model is needed to guide materials development. Such a model should be capable of relating composite performance to constituent properties, thereby enabling identification of optimal microstructures and material combinations. To this end, the "tension-shear chain" (TSC) model was developed by Gao and coworkers for single-level biocomposites (Gao et al., 2003; Ji and Gao, 2004; Zhang et al., 2010) and

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extended to hierarchical biocomposites (Gao, 2006; Zhang et al., 2011; Ji and Gao, 2010). The TSC model illustrates the role of hierarchy in controlling tradeoffs between properties such as strength and toughness (Gao, 2006; Bechtle et al., 2010). However, some of its mechanistic underpinnings are approximate, and some of its predictions, including the strength of long-fiber composites and the scaling of composite toughness with matrix volume fraction, conflict with well-established composite mechanics models. Other workers have also concluded that TSC is inadequate for analyzing long-fiber composites (Chen et al., 2009; Liu et al., 2011), and some have attempted to derive more mechanistically sound models for natural composites (Bar-On and Wagner, 2011; Liu et al., 2011). However, these models are limited to elasticity and do not address the fiber *damage* evolution that governs composite strength and toughness.

Here, we approach the problem as a composite mechanics problem. The hierarchical material consists of fibers and matrix at each scale, with the properties of the fibers given by the properties of the composite at the next-lower scale. At each scale, we use Global Load Sharing (GLS) theory, a well-established micromechanical model that relates the tensile strength, toughness, and overall stress–strain curve of a composite to the properties of its constituents, and includes effects arising from statistical distributions in fiber strength and (finite) fiber length (Curtin, 1991; Curtin and Zhou, 1995; Hui et al., 1995; Curtin, 1999). The GLS model has achieved success in predicting the mechanical properties of many composite systems (Curtin, 1993b, 1999), including composites with polymer matrices and short fibers (Okabe and Nishikawa, 2009; Hashimoto et al., 2012). As will be shown, it also avoids some of the deficiencies of the TSC model. Therefore, it provides a rigorous framework for investigating the mechanics of composites, whether natural or synthetic, or single-level or hierarchical.

This work is organized as follows. We first recapitulate GLS theory for a single-level fiber composite, and subsequently extend it to hierarchical (multi-level) composites. Hierarchy is found to introduce additional material lengths and strengths at each level, but the basic scalings of the quantities of interest—strength, toughness, etc.—are unchanged. We develop highly accurate analytical approximations to the exact numerical results; these approximations enable "spreadsheet-level" design of hierarchical composites. The predictions of the model are then illustrated using a numerical case study, which demonstrates that short fibers are always inferior to continuous fibers with respect to strength and work of pullout. Most importantly, the work of pullout *accumulates* with each successive hierarchical level in the continuous-fiber case, but not in the discontinuous-fiber case. However, short fibers are desirable at the highest level of the composite to impart tolerance to large-scale damage. We conclude by discussing the implications of our model for design of superior composites.

2. GLS model for hierarchical composites: fiber fragmentation

The hierarchical composite studied here is depicted in Fig. 1(a). In this composite, also analyzed by Gao (2006), each fiber is itself a composite, comprising smaller-scale fibers, matrix, and interface. Thus, the properties of a fiber at level n are given by those of the composite at level n - 1. At each level, the fibers have a radius R_n , average length L_n , and volume fraction $V_{f,n}$, and the interfacial shear stress between fibers and matrix is τ_n . The latter stress may arise from plastic flow in the matrix (for ductile matrices), or from debonding and frictional sliding along the fiber–matrix interface (for brittle matrices) (Curtin, 1999). (For prismatic fibers that are not cylindrical, R_n can be replaced by an effective radius, $R_n = 2A_n/P_n$, where P_n is the perimeter of the cross-section and A_n is the area.) The mechanical properties of the composite, such as strength, are

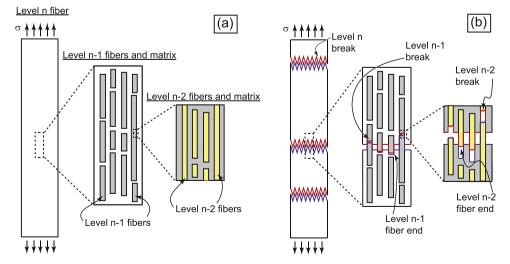


Fig. 1. (a) Schematic of the hierarchical composite of interest. The fiber at level *n* comprises many fibers at level n - 1 and the surrounding matrix; in turn, the level n - 1 fiber comprises many level n - 2 fibers and the surrounding matrix. (b) The same hierarchical composite with damage in the form of (bridged) fiber breaks, indicated with mating red and blue surfaces. Each break is bridged by lower-level fibers. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

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