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Characteristic lengths in natural bundle assemblies arising from fiber-matrix energy competition: A floquet-based homogenization theory

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ABSTRACT

The physical heterogeneity and the geometrical periodicity of several bundle architectures found in biological materials play a key role in determining their superior mechanical performances. The underlying mechanism is based on the shear stress transfer between hard fibers and soft matrix. This process yields a size-dependent behavior characterized by specific lengths scales. Here, we elaborate a Floquet-based homogenization valid for arbitrary periodically heterogeneous fiber bundles with fibers subject to mutual interactions. This approach allows us to separately evaluate the energy distribution within the fibers and the matrix, and to define an efficiency function able to optimize the mechanical response of the bundle. We show the existence of a characteristic length scale that maximizes the transfer of the elastic energy from the fibers to the matrix, thus reducing the fibers solicitation and enhancing the overall mechanical response. This theory is able to describe the geometrical features of several biomaterials, such as nacre shell, muscle sarcomere, collagen fibril, and spider silk, in excellent agreement with experimental data. Moreover, it can be used to design bioinspired artificial structures with optimal response.

1. Introduction

The process of evolution over millions of years has generated a wide range of different natural materials and architectures. Among these, fiber bundle assemblies have outstanding mechanical properties, exhibiting a remarkable balance between stiffness, strength and fracture toughness (Smith et al., 1999; Fratzl and Weinkamer, 2007; Meyers et al., 2008; Ashby et al., 1995; Gibson et al., 1995; Ji and Gao, 2004). Such performances are attributed to their peculiar heterogeneous and hierarchical microstructure, with organizations ranging from the molecular to the macroscopic scale (Gao et al., 2003; Yao et al., 2011; Bosia et al., 2012). The smallest units in such materials are simple fibers embedded in a soft matrix. The most important mechanism at the base of the mechanical behavior is the stress transfer between fibers and matrix, which is mediated by shear interactions. There is an overall consensus on the fact that the above general structure, combined with the shear mechanism, is definitively beneficial for the mechanical response of biological bundles (Gao et al., 2003; Yao et al., 2011; Bosia et al., 2012; Cranford, 2013). Nacre shells, muscle sarcomeres, collagen fibrils, and spider silks are remarkable examples of such high-performance materials. The architecture of these structures is shown in Fig. 1. The nacre (mother-of-pearl) is composed of blocks of aragonite $CaCO_3$ and a protein organic phase, assembled in a brick and mortar geometry, see panel (a). The mineral platelets (bricks) are separated by an organic phase matrix (mortar) and a distribution of nanosized mineral bridges can be observed at the platelet-platelet interfaces (Shao et al., 2014; Okumura and de Gennes, 2001; Sun and Bhushan, 2012). Panel (b) shows the muscle and sarcomere structures. The geometry of the sarcomere unit is constituted by interdigitating antiparallel filaments of actin and myosin, the elastic titin filaments and the cross-linker proteins (Kossmann and Huxley, 1961; Tedesco et al., 2010). In this case, the shear among actin and titin-myosin filaments is mediated by the matrix of cross-linker proteins. In this work, we always refer to the passive response of the sarcomere structure, the active behavior being not relevant here. Panel (c) shows the structure of collagen-I, the building block of eye's cornea,

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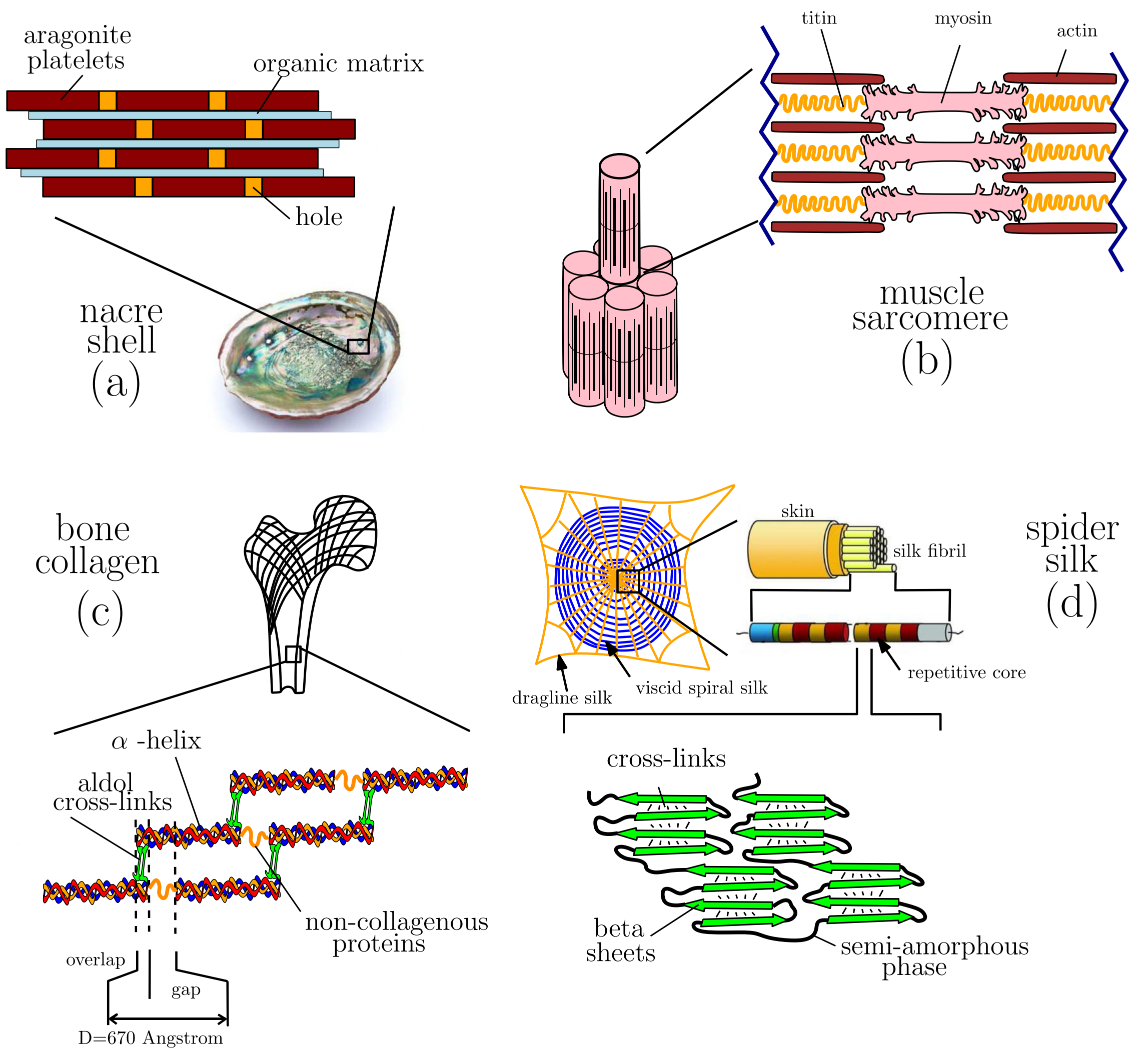

Fig. 1. Architectures of biological materials. Panel (a): bricks-and-mortar structure of nacre (or mother-of-pearl). Panel (b): structure of the muscle fibers based on the sarcomere unit; it is composed of actin, myosin and titin filaments and the cross-linker proteins. Panel (c): collagen structure and schematic representation of the axial arrangement of molecules showing a periodic nanomorphological heterogeneity. Panel (d): schematic orb-web built by a spider composed of fibers with a skin-core structure. We can observe the composition of a silk core fibril: proteins contain highly oriented alanine-rich nanocrystals of antiparallel beta-sheets along the fiber axis embedded in a glycine-rich matrix of random polypeptide chains and moderately oriented helical structures (adapted from Huang et al., 2012, with permission).

skin, tendon and bone. Tropocollagen molecules (length ~300 nm) are assembled in fibrils (length ~1μm), which arrange to form the collagen fiber (length ~10μm) (Holmes et al., 2001; Jäger and Fratzl, 2000; Hulmes et al., 1995). Here, the shear transfer between fibers is supported by the aldol cross-links. Finally, panel (d) shows the scheme of the spider silk structure. One can find an orb-web built by a spider and its architecture going from the skin-core structure to the organization of the repetitive core (Huang et al., 2012; Cranford et al., 2012). This core exhibits the typical brick and mortar geometry composed of beta-sheets and a semi-amorphous phase. These examples share three important features: (a) the physical heterogeneity, (b) the geometrical periodicity, and (c) the stress-transfer mechanism between fibers and matrix of the bundle. These features represent the starting point of the theory here developed.

From the theoretical point of view, several investigations have been conducted in bundle systems. One of the most important paradigm is the classical "shear-lag" interaction scheme among fibers. Originally introduced to study the elasticity and the strength of paper and other fibrous structures (Cox, 1952), the shear-lag model was after exploited to understand the behavior of composite materials (Hutchinson and Jensen, 1990; Nairn, 1997), and to analyse failure phenomena through the well-known fiber bundle model (FBM) (Pradhan et al., 2010; Kawamura et al., 2012). Initially introduced for studying the failure of spun cotton yarns (Peirce, 1926), the FBM was further elaborated for considering a parallel arrangement of fibers with statistically distributed strength (Daniels, 1945). In the FBM context, the shear-lag model has been largely adopted to study the matrix power-law creep compliance (Lagoudas et al., 1989; Beyerlein et al., 1998; Mahesh and Phoenix, 2004), the nonlinear matrix (Mason et al., 1992) and the matrix plasticity (Beyerlein and Phoenix, 1996). Further, the shear-lag model has been recently used to investigate the effects of a population of cracks on the overall mechanical bundle behavior (Manca et al., 2014a, 2015). The matrix-fibers interaction, based on the shear-lag paradigm, has been shown to yield a spatially non-local elasticity with a size-dependent behavior (Wada and Tanaka, 2011). This behavior is at the origin of optimal length scales controlling both the fiber length and their overlapping in the bundle macrostructure (Buehler, 2006, 2008; Chen et al., 2009; Wei et al.,