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Research Paper

Multiscale damage and strength of lamellar bone modeled by cohesive finite elements

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ABSTRACT

A computational multiscale model of damage mechanisms and strength of lamellar bone is presented. The analysis incorporates the hierarchical structure of bone spanning the nanoscale (mineralized collagen fibril), the sub-microscale (single lamella) and the microscale (lamellar structure) levels. Due to the presence of several constituents (collagen, hydroxyapatite minerals, and non-collagenous proteins) and the different microstructural features at each scale, various deformation and failure mechanisms occur in bone at its several levels of hierarchy. The model takes into account the dominant damage mechanisms at the above mentioned three scales and predicts the strength of bone by using a cohesive finite element method. Elastic moduli of bone at these three different scales are also obtained as part of these calculations. The obtained modeling results compare well with other theoretical and experimental data available in the literature.

1. Introduction

Bone is a mineralized biological tissue which gives body its support and stability. It is a natural nanocomposite material consisting of an organic phase (collagen and non-collagenous proteins (NCPs), 32–44% of bone volume), an inorganic phase (hydroxyapatite (HA) crystals, 33–43% of bone volume), and water (15–25% of bone volume) (Olszta et al., 2007). Mechanical properties of the main components of bone are very different: collagen is soft and highly deformable (Buehler, 2008), while mineral crystals are stiff and strong but brittle. These constituents are combined to form a hierarchically structured and nature-optimized bone tissue which is stiff, strong, and tough. Yet, the underlying structural, physical, and mechanical foundations for such material behavior are not fully clear. These provide motivation for the current study.

The following structural scales can be distinguished in the hierarchical structure of bone (Fig. 1): macroscale, mesoscale, microscale, sub-microscale, nanoscale, and sub-nanoscale (Hamed et al., 2012, 2010). The macroscale represents the whole bone level. At the mesoscale the bone tissue is composed of the dense cortical bone and the spongy trabecular bone. The mature human cortical bone consists of osteons embedded in an interstitial bone and surrounded by a circumferential bone, whereas the trabecular bone is made of a porous network of trabeculae. At the microscale both cortical and trabecular bones have lamellar structures

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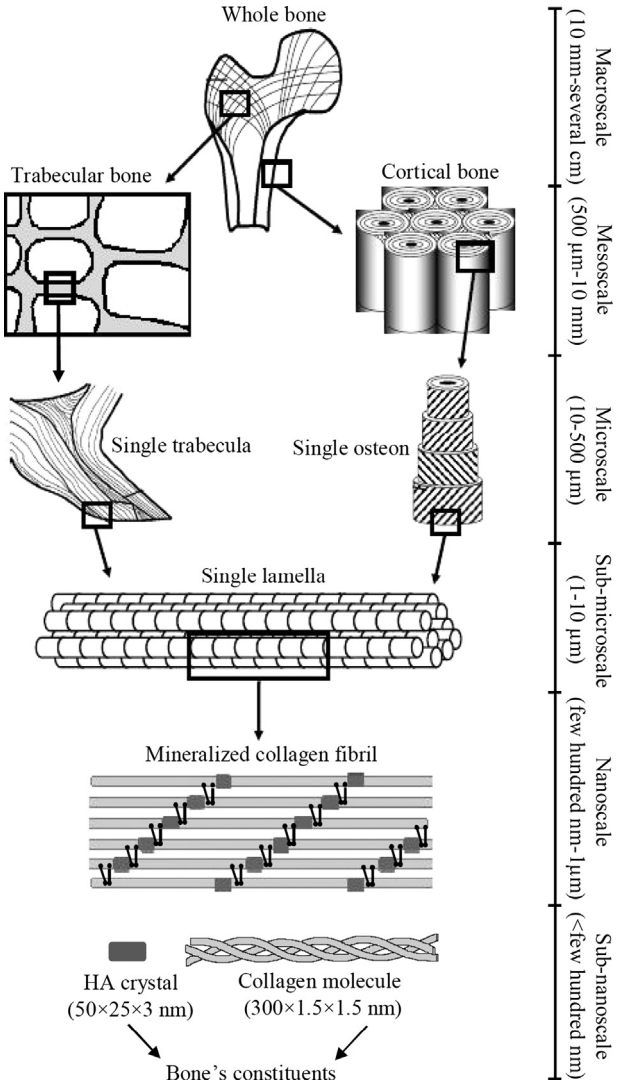

Fig. 1 – Hierarchical structure of bone.

formed through stacking of lamellae in different orientations. At the sub-microscale a single lamella is made of preferentially oriented mineralized collagen fibrils perforated by ellipsoidal cavities called lacunae. At the nanoscale the mineralized collagen fibril is a composite structural unit consisting of the collagen type I, nano-sized hydroxyapatite crystals, water, and a small amount of non-collagenous proteins. The sub-nanoscale represents the atomic scale of bone's constituents: tropocollagen molecules and crystals (Olszta et al., 2007; Weiner and Traub, 1992).

Understanding the failure and fracture behavior of bone is of significant clinical importance. Osteoporosis is a bone disease characterized by bone fragility and increased risk of fractures (Cummings et al., 1985; Kanis, 1994; Klotzbuecher et al., 2000). Many factors, such as bone disuse, aging, and post-menopause among others, affect the onset and progression of osteoporosis. Bone fractures can lead to further disabilities and morbidity. Given these severe consequences of fractures, the primary goal of any treatment should be the prevention of fractures in osteoporotic patients. This demands an accurate diagnosis of bone quality, strength and fracture toughness. Traditionally, bone fracture risk is determined by the bone mass or bone mineral density (BMD). However, BMD is not the only factor responsible for bone fracture and not an accurate predictor of bone strength (Ritchie et al., 2009; Licata, 2009). For example, Hui et al. (1988) showed that the fracture risk increases ten times with aging, independent of BMD. These findings emphasize the need to better understand the factors affecting the bone quality and bone fracture and strength.

Fracture is a mutual competition between damage mechanisms and toughening crack-shielding mechanisms (Ritchie, 1999). Both mechanisms exist at all hierarchical length scales in bone. However, the connections between the structural features, damage and toughening mechanisms, and fracture and strength are not yet well understood in bone, especially at smaller scales. If more insights can be obtained on the structure–strength relationships in bone, newer and more effective techniques could be developed to assess bone strength and fracture risk and to treat bone diseases.

Compared to a large number of models available in literature for the prediction of bone's stiffness, there are only few models to predict bone's strength. At the nanoscale, Mammone and Hudson (1993) used a micromechanics approach to obtain tensile strength of bone by representing bone as a polymeric composite containing a collagenous matrix and HA fillers. Jager and Fratzl (2000) proposed a geometric model of collagen fibrils with a staggered arrangement of HA platelets and used a shear lag model to predict the effective elastic modulus and strength of such a system. Wang and Qian (2006) proposed a two-dimensional (2D) shear lag model to predict stress concentration fields around a crack in a mineral–collagen composite. Siegmund et al. (2008) used a cohesive finite element method (FEM) analysis to assess the effect of collagen cross-linking on the stiffness and strength of a mineralized collagen fibril, while Luo et al. (2011) employed a cohesive FEM model to study the effect of mineral–collagen interfacial behavior on the microdamage progression in bone. Atomistic simulations were also employed to study the deformation mechanisms and fracture behavior of collagen–HA systems at nanoscale (Buehler, 2007; Nair et al., 2013; Dubey and Tomar 2008). Fritsch and Dormieux (2009) used a multiscale micromechanics model to obtain the strength of bone at the nano and sub-microscales. At the microscale, there are no models available in literature for predicting the strength of bone. However, rich literature on modeling the failure and fracture mechanisms of composite materials, especially of laminated composites which behave similarly to the lamellar structures of bone, could be generalized and applied to model bone at this scale. At the mesoscale, the nucleation and propagation of microcracks and cracks in bone were studied using different analytical and computational methods, such as a linear elastic fracture mechanics (Raeisi Najafi et al., 2007), a classical FEM analysis (Raeisi Najafi et al., 2011; Ota et al., 1999), a cohesive zone FEM method (Ural, 2009; Ural et al., 2011; Ural and Vashishth, 2006; Mischinski and Ural, 2011), and an extended FEM (X-FEM) modeling (Budyn and Hoc, 2006; Abdel-Wahab et al., 2012; Budyn et al., 2008). However, most of such models focused mainly on obtaining the fracture toughness of bone rather than its strength and focused on one structural scale.

The current study involves the multiscale finite element modeling of strength of lamellar bone. The modeling starts