EXPERIMENTALLY-BASED MODELING OF TRABECULAR BONE AS A COMPLEX CELLULAR MATERIAL

Iwona Jasiuk[*a)], Elham Hamed[*], Timothy Patterson[*], Jun Li[*] & Alexander Setters[*]
[*]*Department of Mechanical Science and Engineering, College of Engineering, University of Illinois at Urbana-Champaign,1206 W. Green Street, Urbana, IL,61801, USA*

Summary Trabecular bone is a cellular material with a complex hierarchical structure. At mineralized fibril level, bone is modeled as a three-phase composite of collagen molecules, nanocrystals and water. At single lamella level, micromechanics approach is used to model preferentially oriented fibrils. At single trabecula level, composite materials laminate theory is used to model lamellae stacked in different orientations. At trabecular bone level, cellular architecture, imaged via micro-computed tomography, is modeled by finite elements. Inputs for modeling are obtained by multiscale experimental characterization. Theoretical predictions for elastic moduli and strength are in good agreement with experimental data. Computational challenges include modeling of complex, random structure at each structural level and accounting for spatial heterogeneity of bone's properties. Theoretical issues include lack of separation of scales and dependence of properties on specimen size and boundary conditions.

INTRODUCTION

Bone is a biological tissue, which among its other functions serves as a structural support for other tissues in the body. As a structural material, it has excellent properties when healthy: high stiffness, strength, fracture toughness, and light weight. Bone consists of *cortical* bone forming an outer shell and *trabecular* spongy bone filling space within or at long bone's ends. Such structure is optimized to resist loads while being lightweight. Bone is a multi-phase composite material made of soft and deformable proteins (mainly collagen), stiff but brittle apatite minerals, and fluids. These components self-assemble to form a complex structure spanning from nano to macroscale. The superior properties of bone are due to this composite, spatially heterogeneous, and hierarchical structure. The apatite crystals are in the shape of irregular platelets, 20-50 nm in length and width and 1-3 nm in thickness. Cross-linked collagen molecules, which are triple helical protein chains about 1.5 nm in diameter and 300 nm in length with 40 nm gaps between ends, are staggered to form collagen fibrils about 50-100 nm in diameter. These crystals are located both within and around collagen fibrils. The fibrils reinforced with crystals form a mineralized collagen fibril which serves as a building block of bone. These mineralized collagen fibrils are preferentially aligned and arranged into lamellar sheets (3-7 μm in thickness). These are stacked at different orientations and wind around to form cylindrical (or platelike) struts called trabeculae, which are about 0.1 mm in diameter and 1 mm long. This gives trabecular bone a porous cellular-like appearance. Thus, the trabecular bone has a complex hierarchical structure in which different geometrical features occur on several length scales. These scales are classified as follows: a) nanoscale (single fibril and crystals), b) sub-microscale (single lamella), c) microscale (single trabecula), and d) mesoscale (random network of struts or plates). The next structural level, macroscale, represents the whole bone, which includes both trabecular (porous) and cortical (solid) bone types. These structural levels are illustrated in Fig. 1.

EXPERIMENTAL CHARACTERIZATION OF TRABECULAR BONE

Trabecular bone is studied using bone samples from porcine femoral heads, harvested from 6 month old animals. Bone tissue was obtained from the Animal Science Department at the University of Illinois Urbana Champaign. The characterization includes the analysis of bone's structure, chemical composition and mechanical properties at different structural scales. The trabecular bone structure is imaged at different structural levels using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Photographs, representing a wide range of magnifications (10-50,000), are analyzed by Image J software. The data collected includes the area fraction and orientation of fibrils at the sub-microscale level, and the porosity, pore size distribution, connectivity of microstructure, and thickness of trabeculae at the microscale level. We also store the digitized images of bone structures at each scale for use in numerical simulations. SEM and TEM investigations provide us with the two-dimensional data. In addition, we use the x-ray micro- and nano-computed tomography (micro-CT and nano-CT), which gives three-dimensional details of bone structure. The chemical composition of bone is characterized by using Raman spectroscopy and Fourier Transform Infrared Spectroscopy. In addition, the SEM used in a backscattered mode provides us with quantitative information on mineral content. These measurements are complemented by ash content measurements and imaging using dual-energy x-ray absorptiometry. Finally, the measurements of mechanical properties are done using compression test and nanoindentation. We use an MTS testing machine to determine the constitutive response of bone at mesoscale (5-10 mm samples). We employ the nanoindentation apparatus (Hysitron) to determine bone's mechanical properties (elastic modulus and hardness) at lower scales. These experimental results along with those reported in literature are used as inputs and validation of modeling approaches.

[a)] Corresponding author. Email: ijasiuk@illinois.edu.

MODELING OF TRABECULAR BONE AS A HIERARCHICAL MATERIAL

Following the characterization and testing of bone, the theoretical mechanics analysis of trabecular bone is conducted. Inputs reflecting structural features at different scales are rectified with our experimental observations obtained by methods described in the previous section. Material responses at each structural level defined in the Introduction section and shown in Fig. 1, are obtained either analytically (using micromechanics or composite laminate theories) or computationally (using finite element method). Bone's structure is analyzed in an "ascending" order by starting with the nanoscale and moving up the scales to the mesoscale. The results obtained at a lower scale serve as inputs for a higher scale. At the nanoscale level, apatite crystals are represented as plate-like or ellipsoidal inclusions, which are embedded in collagen fibrils (matrix). Alternatively, apatite crystals and collagen are treated as interpenetrating phases. First, micromechanics effective medium theories are used, for simplicity, and then numerical simulations are conducted to account for a discrete (molecular) structure of bone at that structural level. At the next higher up scale (sub-microscale), a single lamella consisting of aligned collagen fibrils reinforced with extrafibrillar apatite crystals is modeled using micromechanics. At the microscale level, involving a lamellar structure of a single trabecula, a laminate theory from mechanics of composite materials is used. The challenges at this scale include curved, crescent like geometry of trabecular packets, made of several lamellar layers stacked at different orientations, which form trabecular struts. At the mesoscale level, trabecular bone consists of a random porous network of struts or plates. The trabecular structure poses modeling challenges because of its complex and irregular geometry. Initially, this structure is modeled by assuming periodicity in the pores' arrangement and then this material is represented as a micropolar one. This higher order theory allows us to account for microstructural features such as pore geometry via characteristic lengths. Then, we conduct large scale finite element computations accounting for the actual geometry and random structural features of trabecular network. At this scale, the inputs on geometry are taken from a micro-CT digitized data of actual bone samples. Computational results are compared with experimental ones obtained by compression testing of digitized bone samples.

RESULTS

In the numerical simulations, due to uncertainty, especially at nanoscale, and the stochastic nature of the problem at different scales, we consider a range of parameters and possible geometries in order to build a stochastic model of the elastic moduli and strength of trabecular bone. The theoretical results, showing a range of values, are in good agreement with our experimental data using compression test at the mesoscale and nanoindentation at the micro- and sub-microscale and those reported in literature. Preliminary results, involving theoretical predictions of elastic moduli of trabecular bone using multiscale analysis, are given in ref. [1].

CONCLUSIONS

We characterized, tested, and modelled trabecular bone as a hierarchical material. Good agreement was found between theoretical and experimental predictions, considering the complexity of bone's hierarchical structure and the idealizations used in modelling of each structural level. The approach taken presents a framework for studying other biological materials with complex hierarchical structures.

References

[1] Hamed E., Jasiuk I., Yoo A., Lee Y., Liszka T.: Multiscale Modeling of Elastic Moduli of Trabecular Bone. *J. R. Soc. Interface*, In Press.

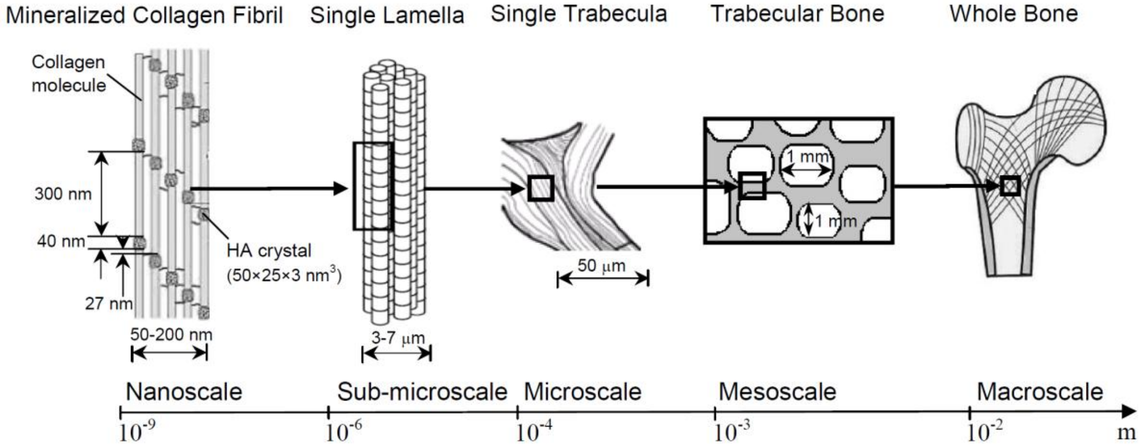

Fig.1 Schematic of a hierarchical structure of trabecular bone (taken from ref. [1]).