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A multiscale modelling of bone ultrastructure elastic proprieties using finite elements simulation and neural network method

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ABSTRACT

Bone is a living material with a complex hierarchical structure which entails exceptional mechanical properties, including high fracture toughness, specific stiffness and strength. Bone tissue is essentially composed by two phases distributed in approximately 30–70%: an organic phase (mainly type I collagen and cells) and an inorganic phase (hydroxyapatite-HA-and water). The nanostructure of bone can be represented throughout three scale levels where different repetitive structural units or building blocks are found: at the first level, collagen molecules are arranged in a pentameric structure where mineral crystals grow in specific sites. This primary bone structure constitutes the mineralized collagen microfibril. A structural organization of inter-digitating microfibrils forms the mineralized collagen fibril which represents the second scale level. The third scale level corresponds to the mineralized collagen fibre which is composed by the binding of fibrils. The hierarchical nature of the bone tissue is largely responsible of their significant mechanical properties; consequently, this is a current outstanding research topic. Scarce works in literature correlates the elastic properties in the three scale levels at the bone nanoscale. The main goal of this work is to estimate the elastic properties of the bone tissue in a multiscale approach including a sensitivity analysis of the elastic behaviour at each length scale. This proposal is achieved by means of a novel hybrid multiscale modelling that involves neural network (NN) computations and finite elements method (FEM) analysis. The elastic properties are estimated using a neural network simulation that previously has been trained with the database results of the finite element models. In the results of this work, parametric analysis and averaged elastic constants for each length scale are provided. Likewise, the influence of the elastic constants of the tissue constituents is also depicted. Results highlight that intelligent numerical methods are powerful and accurate procedures to deal with the complex multiscale problem in the bone tissue with results in agreement with values found in literature for specific scale levels.

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1. Introduction

Bone is a mineralized biological material which serves, among its other functions, as a structural support for other tissues in the body. The mechanical properties of bone have been naturally designed to fulfil this specific physiological function. In fact, in order to accomplish their biological and mechanical functions, bone hierarchical structure is constituted of many scale levels with specific interactions and a very complex architecture [1]. These structural scales can be distinguished as follows: macro-scale (whole bone), meso-scale (cortical and trabecular bone), micro-scale (single osteon and single trabecula), sub-micro-scale (lamella), nano-scale (microfibrils, fibrils and fibres), and sub-nanoscale (HA crystals and TC molecules) [2,3].

In order to analyse the equivalent mechanical behaviour of bone material, it is important to investigate the mechanical properties of its components and the structural relationships between them at different scales of hierarchical structural organization [4–6].

Many researchers in the literature have addressed this problem by developing analytical and numerical multiscale modelling of the bone mechanical behaviour [3,7–12]. These models use the homogenization and/or finite element technique to describe the mechanical behaviour of bone at certain scale levels. Some of these studies have focused on Mineralized Collagen Microfibrils (MCMs) scale [13–17]. Others have been interested on the second scale level Mineralized Collagen Fibrils (MCFs) [18–21]. There are also works dealing with lamella scale [11,22] and osteon scale [12]. However, to the best of our knowledge, there are no studies focusing on the full multiscale description of bone hierarchical organization using numerical simulation methods.

Previous researchers have tried to approach bone multiscale organization by resorting to homogenization method. Some of them have estimated bone elastic properties. We can cite, as an example and not a limited list, the works of Martinez et al. [7] and Hamed et al. [3]. Others have evaluated fracture properties such as Fritsch and Hellmich [9] while Fritsch et al. [23] have extended their elastic multiscale micromechanical model for elasto-plastic analysis to predict cortical bone fracture toughness. Their findings mention that bone material fracture begins at the nano-scale at HA crystals and is followed by collagen cross-links fracture.

Concerning nano-structural scale levels, a particular attention has been given to the composition and structure of bone at these levels [24–27], the numerical modelling and experimental studies. There are few studies that focused on the MCMs scale level [3,13,15,16,28]. In the work of Barkaoui et al. [13], a finite element geometrical model has been proposed to study elastic mechanical properties and investigate the effect of some mechanical and geometrical parameters on the mechanical behaviour of mineralized collagen microfibril scale.

Scarce studies that have been interested on the study of mechanical properties of mineralized collagen fibres (MCFRS) scale level. Yoon and Cowin [11] have studied mechanical properties of the tissue at the fibre scale by means of the homogenization method.

Most of works have been interested on mechanical behaviour and properties of individual MCF [29–32]. Several mechanical models have been developed in order to estimate the mechanical properties of MCFs and bone tissues [9,33] and to model the 3D orthotropic elastic properties of a single MCF [34]. Nikolov and Raabe [10] proposed a homogenization method to model the elastic properties of bone at the mineralized MCF level from the staggered arrangement of collagen molecules up to an array of parallel MCF. Jaeger and Fratzl [35] proposed a model of MCF with a specific staggered arrangement of mineral particles distributed unequally in the gap and overlap zones of collagen fibrils. This geometric model has served as a reference for almost all the FEM models proposed for modelling bone at nanoscale. Jaeger and Fratzl [35] used this model to explore the effect of the mineral volume fraction and thickness as well as the distance of the HA platelets on the longitudinal elastic modulus, maximum elastic strain, and maximum elastic stress (strength) of the MCF. Kotha and Guzelsu [36] extended the Jaeger–Fratzl model [35] to investigate the effect of interphase and bonding on elastic properties of bone. Ji and Gao [37] used the same model geometry coupled with analytical formulation and a FEM analysis to obtain the transversely isotropic elastic constants of the MCF as a function of mineral aspect ratio. Yuan et al. [18] used a FEM analysis to predict the elastic properties of an MCF both in 2D and 3D and validated their computational results with experimental data obtained by synchrotron X-ray diffraction. They improved the shear lag Jaeger–Fratzl model [35] by incorporating more structural features of the MCF. To the best of our knowledge, this is the first MCF 3D model considering the staggered arrangement of HA crystal within the collagen matrix. Vercher-Martínez et al. [21] used a direct homogenization procedure by means of the finite element method and composite material approaches to estimate the transversally isotropic properties of the MCF by considering the collagen and mineral distribution accordingly to the Hodge and Petrutska model [38]. Molecular dynamics simulations (MD model) [39] have been developed to investigate the mechanical response under uniaxial tension of individual MCF. The results show that the deformation and failure mechanisms of a collagen fibril are strongly influenced by its length and width as well as cross-linking density which, in turn, indicates the size dependence of failure mechanical properties of collagen fibrils.

In this study, we extend our previous models dealing with bone ultrastructure modelling in two aspects: (i) proposition of new 3D FE models to represent MCF and MCFR structures, (ii) development of a multiscale hybrid approach EF/NN of bone ultrastructure composed of three scale levels MCM, MCF and MCFR. This novel multiscale modelling is used to study the elastic properties of different bone tissue levels. Such model provides advantages when studying the effects of some parameters (geometrical or mechanical) related to the collagen, the mineral or the cross-links components on the strength of human bone.

2. Bone ultrastructure

All researchers agreed on the fact that the bone in a nanoscopic scale is essentially formed by two phases: organic phase is mainly composed of collagen type I representing 85–95% [40] of the total protein in bone. The remaining bone organic matter consists of non-collagenous proteins (NCPs) and lipids. Inorganic