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Frontiers of micro and nanomechanics of materials: Soft or amorphous matter, surface effects

A stochastic homogenization approach to estimate bone elastic properties

Une approche d'homogénéisation stochastique pour estimer les propriétés élastiques de l'os

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ABSTRACT

The mechanical properties of bone tissue depend on its hierarchical structure spanning many length scales, from the organ down to the nanoscale. Multiscale models allow estimating bone mechanical properties at the macroscale based on information on bone organization and composition at the lower scales. However, the reliability of these estimates can be questioned in view of the many uncertainties affecting the information which they are based on. In this paper, a new methodology is proposed, coupling probabilistic modeling and micromechanical homogenization to estimate the material properties of bone while taking into account the uncertainties on the bone micro- and nanostructure. Elastic coefficients of bone solid matrix are computed using a three-scale micromechanical homogenization method. A probabilistic model of the uncertain parameters allows propagating the uncertainties affecting their actual values into the estimated material properties of bone. The probability density functions of the random variables are constructed using the Maximum Entropy principle. Numerical simulations are used to show the relevance of this approach.

RÉSUMÉ

Les propriétés mécaniques du tissu osseux dépendent de sa structure hiérarchisée, de l'échelle de l'organe à celle de ses constituants élémentaires (nano-échelle). En se basant sur la connaissance de la morphologie, de l'organisation et des propriétés mécaniques de ces derniers, des modèles multi-échelles permettent d'estimer les propriétés mécaniques d'ensemble du tissu osseux. Cependant, ces informations sont souvent partielles ou incertaines, rendant peu fiables lesdites estimations. Dans cet article, nous proposons une stratégie originale permettant de prendre en compte ces difficultés de façon efficace. Plus précisément, un modèle multi-échelles du tissu osseux basé sur la théorie de la micromécanique des milieux continus est associé à un traitement probabiliste de certaines des variables du modèle (notamment, les propriétés mécaniques des constituants

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élémentaires du tissu osseux). Le modèle multi-échelle permet de prendre en compte la microarchitecture et l'organisation du tissu osseux aux petites échelles pour estimer les coefficients élastiques de l'ultrastructure osseuse (la matrice solide du tissu osseux). Les incertitudes sur les variables d'entrée sont prises en compte en construisant des lois de probabilités pertinentes basées sur le principe du maximum d'entropie. Quelques résultats numériques sont montrés pour étayer l'intérêt de cette approche.

1. Introduction

Bone is a biocomposite material showing several levels of microstructural organization [1]. In mature bone, two types of tissues can be distinguished: cortical tissue—a dense material forming the outer shell of bones—, and trabecular tissue—a spongy material located inside the bone. Both cortical and trabecular tissues are porous materials. Pores in cortical bones are pseudo-cylindrical canals (Havers' and Volkmann's canals), whereas, in trabecular bone, pores are irregularly shaped cavities. Despite the very different pore morphology, the solid matrix of both cortical and trabecular tissues, hereafter referred to as bone *ultrastructure*, is nearly the same. Bone ultrastructure is an assembly of mineralized collagen fibrils (MCF). MCF are bunches of collagen molecules embedded in a mineral-rich matrix. This latter is made of hydroxyapatite mineral and constitutional water.

Understanding bone mechanical properties requires accounting for its hierarchical structure down to the lowest levels of this hierarchy [2,3]. Multiscale modeling and simulation turns out to be a powerful tool for explaining bone mechanical properties while accounting for its inner organization.

Several authors studied bone focusing on several levels of its hierarchical structure by means of multiscale modeling approaches [4–7]. Modeling studies rely on the experimental characterization of bone microstructure obtained through different experimental techniques (ultrasounds, X-ray microtomography (micro-CT), X-ray synchrotron radiation, etc.) aiming at relating the available clinically relevant information to bone mechanical properties. Several experimental studies highlighted the relevance of porosity and mineralization in determining the mechanical properties of bone and the associated fracture risk [8–15]. Recently, the heterogeneous distribution of bone elastic coefficients in the inferior human femoral neck was described using a continuum micromechanics model based on 3D mappings of porosity and Tissue Mineral Density (TMD) obtained through high-resolution synchrotron radiation [16,17,7].

A critical point for clinical application of biomechanical models of bone is the incomplete knowledge of patient-specific information on bone microstructure. Techniques such as ultrasounds and micro-CT, commonly used in in vivo measurements, can hardly inspect bone microstructure at the sub-micrometric scale. Moreover, the information which is actually made available by the different experimental techniques is affected by the resolution and parameterization of the experimental setup. Furthermore, some of the uncertain parameters may be not directly available from experimental measures but have to be deduced by introducing additional empirical relationships. All these issues may affect the accuracy of the modeling parameters used to estimate bone mechanical properties, questioning the reliability of the model predictions.

Uncertainties on the modeling parameters increase with zooming down into the nanostructure of bone. Current experimental techniques cannot provide accurate information about the morphology, spatial arrangement and mechanical behavior of bone constituents. Not surprisingly, modeling assumptions at the nanoscale may be very different. For instance, bone nanostructure has been described as either a mineral-rich matrix embedding collagen molecules [4,5,16] or as a collagen matrix with mineral inclusions [18–22].

We propose to cope with these experimental limitations by developing a novel multiscale model of bone taking into account the uncertainties on bone nanostructure. A multiscale model will make the global elastic behavior of bone emerge by combining models developed at each relevant scale of bone microstructure. A probabilistic model will allow accounting for the uncertainties about the patient-specific microstructure and to propagate them up to the organ scale. In this very first study, we will focus only on the uncertainties affecting the elastic properties of bone constituents.

Similar approaches have been used to model effective mechanical properties of materials with random microstructure (see for instance [23,24]). Nevertheless, to the best of our knowledge, this is the very first contribution to develop a stochastic modeling of bone.

In order to construct the probabilistic model of bone, we combined a multiscale model based on continuum micromechanics [25,26] with a probabilistic representation of the uncertain parameters of the model, based on the Maximum Entropy principle [27,28]. The paper is organized as follows. The multiscale model of bone based on the continuum micromechanics theory is resumed in Section 2. The probabilistic model of the uncertain parameters is described in Section 3. The numerical procedure and some numerical results are presented in Section 4 to highlight the features of this approach. Eventually, the conclusions of this study are drawn in Section 5 opening the way to further research.