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MODELLING POROUS HYDROXYAPATITE MATRIX BASED BONE MICROSTRUCTURE

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Abstract: *This contribution covers the prediction of the stiffness tensor for a microelastic model of the bone based on a three-step homogenization scheme. A micromechanical approach of the elastic properties of bone is being approached via a step-by-step homogenization concept developed around a more general, realistic hierarchical structure of the bone. The homogenization steps were done at: nanoscale – hydroxyapatite foam (extrafibrillar space), microscale (5-10 μm) – collagen and hydroxyapatite network (fibril), microscale (5-10 mm) – bone microstructure. The stiffness tensor will be evaluated for each step of the homogenization process as function of different porosities volume fraction meaningfully from bone structure point of view. The same concept was applied for the volume fractions of the major bone constitutive, the hydroxyapatite crystals (35%) and collagen molecules (30%).*
Keywords: *elastic properties, bone, stiffness, hierarchical approach, micromechanics*

1. INTRODUCTION

It is well acknowledged the role of bone as the most important biological tissues designed by nature for mechanical support, protection and locomotion both in humans and animal reign. Despite of the technological evolution, emerging theories ranging from macro to nanoscale, nature reveals hardly its rules or hierarchical organization. It takes time and other types of approaches to step inside into the beauty of its structure due to the fact that "no one has developed a theory of bone that can satisfactorily explain its mechanical behaviour on the basis of its internal structure and composition" [2]. Consequently, it became a major challenge for material scientist to relate the bone's macroscopic properties with its hierarchical microstructure to serve as a tool for designing of new bone implants and bio inspired nanocomposites.

Micromechanically based theoretical models have been developed during the lat decade with the purpose of getting an inside approach of the bone structure and aid its characterization and elastic constants prediction. The Reuss and Voigt bounds are left far beyond at this level of microscopic scale, even recently scientific papers are using it only for comparison purposes [4]- [6], [7]. The Milton and Torquato developed theoretical models, as well as Hashin-Shtrikman bounds were used in the hierarchical step-by-step homogenization concept developed by Nikolov and Raabe that used these to prove a realistic approach in the bone characterization attempts [5].

The hierarchical organization of the bone – according to the outstanding contributions in the field [1]&[2] – can be summarized in the following levels: macroscale – from several mm to few cm – where one can distinguish the cortical (i.e. compact) and trabecular (i.e. spongy) bone types; microscale – several 100 μm to several mm – cylindrical shaped elements such as osteons and trabecular struts build up cortical and trabecular bone, respectively; nanoscale – several 10 nm – elementary components of mineralized tissues can be distinguished.

The herein contribution aims to approach the bone structure in terms of continuum micromechanics representation as three step homogenization procedure: step I – "composite" made up of hydroxyapatite crystals and ultrastructural water mixed with non-collageneous organic matter; step II – solid bone matrix made up of connected hydroxyapatite polycrystal matrix with cylindrical inclusions of collagen; step III – microstructure made up of connected hydroxyapatite polycrystal matrix with cylindrical inclusions of collagen and cylindrical micropores representing Haversian and Volkmann canals or the intertrabecular space.

None of the references cited provide the full set of the anisotropic elastic constants of the bone structure except the work of Hellmich and Ulm (2008). This paper will lead to a transversely isotropic stiffness matrix as a consequence of the homogenization step-by-step procedure adopted herein. The predicted data will be compared with similar data from literature in order to debate the "realistic" look like adopted approach.

2. MODEL DESCRIPTION

The elastic properties of the bone constitutive, hydroxyapatite and collagen minerals, as were used in the micromechanical approach, are indicated in Table 1 and represents mean values that were reported in the literature. As a simple observation, the other elastic coefficients, such as shear and bulk moduli, can be estimated with the aid of the well known relationships for isotropic elastic materials.

Table 1: Elastic constants (technical) of the collagen and the hydroxyapatite minerals

	Collagen	Hydroxyapatite	Ultrastructural water
E [GPa]	1.2	114	2.7
ν	0.35	0.28	0.47
ρ [kg/m^3]	1410	3140	1000

The homogenization procedure applied in each step was based on the Mori-Tanaka scheme, as an alternative to the classical bounds relationships of Voigt and Reuss or Hashin-Shtrikman as were reported in the literature. As was mentioned in the first section, the first step aimed the homogenization of the hydroxyapatite crystals and ultrastructural water as phases of the generated “composite” embedded into a matrix considered as an “average” of previous both (see Figure 1, left). The hydroxyapatite crystals were embedded into a volume fraction of 35% whereas the water in 15%. Next, at a 10 μm scale, the porous hydroxyapatite polycrystals from the previous homogenization step will be used as matrix of the new composite, collagen platelets being the reinforcements (see Figure 1, center). The volume fraction of the latter was considered as having 30% and has physiological meaning. The retrieved elastic constants will be further used in the last homogenization step were supplementary were added cylindrical micropores representing Haversian and Volkmann canals in case of the cortical bone or intratrabecular space (see Figure 1, right). The volume fraction of the porosities range from 2 to 16 % values that is typical for the cortical bone. With respect to the latter, porosity is the primary parameter for the distinction between the cortical and trabecular bone (50-90%). As a matter of fact, the herein micromechanically predicted bone elastic properties were considered for a perfectly healthy bone, a rather idealized case.

All calculation performed here are based on matrix representations of second and forth order tensors. The micromechanical model has been validated by comparison with estimates from other literature cited works herein.

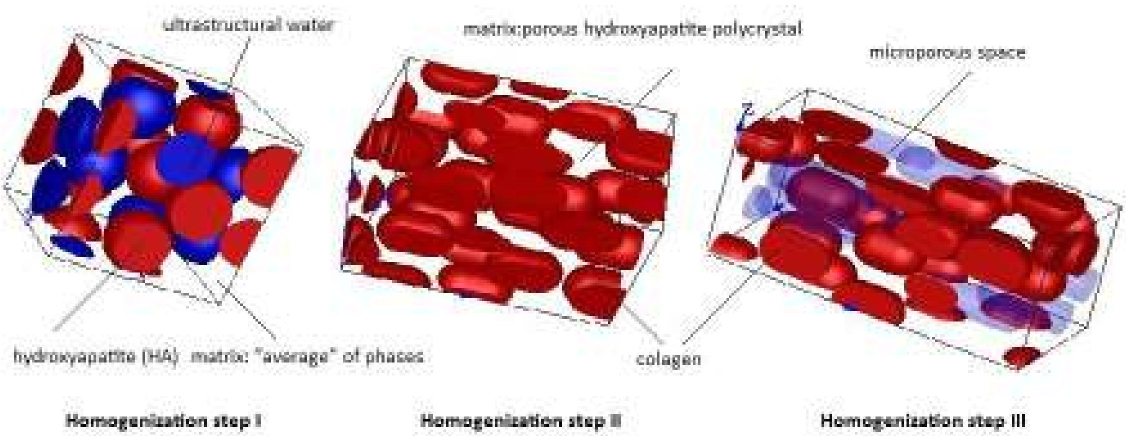

Figure 1: Micromechanical representation of bone by means of the multistep homogenization procedure applied

3. RESULTS AND DISCUSSION

Apart from the first homogenization step were the inclusion were taken as having a random distribution, we believe that the elastic coefficients are best estimated by assuming a periodic distribution of the platelet shaped minerals rather than assuming a random distribution. The approximately transversely isotropic material behaviour of bone represented by the micromechanical model of Figure 1 reduces the number of independent elastic properties of the general anisotropic case to 5 instead of 21 constants to define the stiffness tensor.

In Figure 3 are being plotted the longitudinal and transversal stiffness values predicted for the overall elastic properties of the bone microstructure depicted in the previous section vs. different porosities volume fractions.

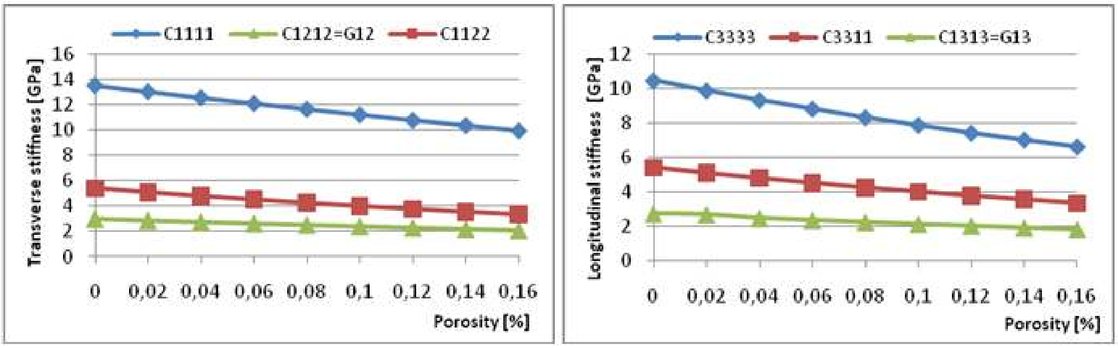

Figure 2: Micromechanically estimated (transversely isotropic) stiffness tensors as functions of porosity for physiologically meaningful volume fractions of hydroxyapatite and collagen

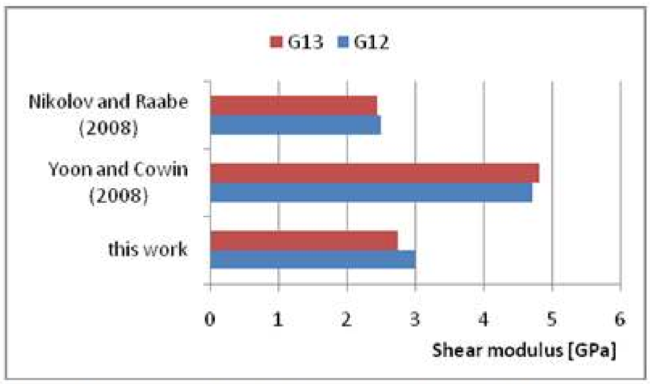

Figure 3: Micromechanically predicted shear moduli comparison: this work and literature

As it can be seen, the stiffness values are experiencing a decrease with the increase of the meaningful porosity volume fractions, that is normal and experimentally validated in mostly all the bone related scientific papers. Furthermore, comparisons of the values predicted in this work with similar constants from the cited papers are being compared in Figure 3 for the shear moduli, for example. As it can be seen, is rather difficult to compare if the bone microstructure do not resemble with the herein presumptions, especially when the models do include supplementary phases such as mineral ash, volatile inorganic fraction, organic components, etc. The herein micromechanically approach lead to predicted values that resemble the model proposed by Nikolov and Raabe (2008) that applied the same Mori-Tanaka concept in the homogenization step with the difference of considering the inclusions in the first homogenization step as having an elliptic shape not spherical as in our case and in the following homogenization steps needlelike inclusions instead of platelet as in ours.

4. CONCLUSIONS AND PERSPECTIVES

The explicit modelling of the microstructure at higher levels of hierarchy within the frame of herein approach is possible but beyond the scope of this work. Here it was used a simple phenomenological model to reproduce the properties of compact bone observed at macroscopic scale. The representative volumes that were defined within this framework were tackled as a step-by-step homogenization procedure and physiologically meaningful volume fraction of the main bone components were considered to predict data similar to those reported in the literature.

The stiffness values recovered by using a well known micromechanical concept developed by Mori-Tanaka and used in all the homogenization steps were plotted against the porosities content within the bone microstructure. A decrease of these values with the increase of micro porous space content were experienced and the elastic coefficients shown similarities with the similar stiffness values from other sources.

The present study serves as a dataset for building a more realistic model that will provide the whole anisotropic stiffness tensor of this “natural composite material” structure and furthermore to develop a poro-micromechanical model that will allow the understanding of the poro-elastic properties such as Biot and Skempton coefficients. Furthermore, these predicted data can be exported to other simulation environments such

is the one based on finite elements method to aid the phenomenological approaches such are the car crushes, human injuries, human locomotion, bone-implants or bone-prosthesis design and compatibilities.
Supplementary, the model can be extended to take into account the different values of densities which lead to a benchmark study where the elasticity-density relationship will be taken as the variable under study.

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