A simple mechanical model of mineralized collagen fibrils

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***Abstract*—Mineralized collagen fibrils represent the basic building blocks of bone tissues. In this work, a simple model for describing the mechanical response of mineralized collagen fibrils is proposed. The model is formulated by a rheological approach and by introducing parameters that describe well-defined histological and biochemical features only. It accounts for structural arrangement of different fibril constituents, allowing to describe dominant nanoscale mechanisms (elastic and inelastic) and nonlinearities. Some numerical results are presented, showing soundness and effectiveness of present formulation in reproducing experimental data obtained via tensile tests for different mineralization levels.**

***Keywords*—Mineralized collagen fibrils, Bone microstructure, Rheological model.**

I. Introduction

BONE is a complex hierarchical biomaterial mainly composed of collagen protein, hydroxyapatite (HAP), non-collagenous proteins and proteoglycans. From a mechanical point of view, collagen molecules (with a soft response) and HAP mineral (much stiffer) play the fundamental role. As a matter of fact, the biomechanical interactions at the nanoscale between collagen molecules and HAP, as well as the mineral amount, are responsibleof strength and toughness levels in bone tissues [1].

At the microscale, collagen molecules are arranged in staggered arrays, namely collagen fibrils, characterized by the presence of sub-microscopic crystals of HPA. Mineralized collagen fibrils (MCFs) can be considered as the basic building blocks of bone tissues. In MCFs, he HAP crystal platelets nucleate in gap regions between subsequent molecules, growing in length along the main axis of collagen molecules, and in width, along channels [2]. Moreover, for high mineralization levels, HAP crystals significantly occur also into the overlap-zone among parallel collagen molecules [3]. Accordingly, due to such a mineral occurrence and location, different types of interactions between fibril constituents arise, strongly dependent on mineral quantity and highly affecting bone mechanics.

In this work, a simple rheological model for describing the non-linear elasto-damage mechanical response of mineralized collagen fibrils is conceived. The model has been applied to analyze different MCFs characterized by different mineralization levels, highlighting model capability in successfully reproducing some experimental evidence available in literature [4].

II. Material and Methods

The elasto-damage mechanical behaviour of mineralized collagen fibrils is addressed by accounting for dominant mechanical features and mechanisms associated to MCF-constituents. In order to produce a simple model formulation, a rheological description is adopted. Figure 1 schematically summarizes the nano-structural arrangement considered as descriptive of a MCF, and the corresponding rheological scheme that has been conceived.

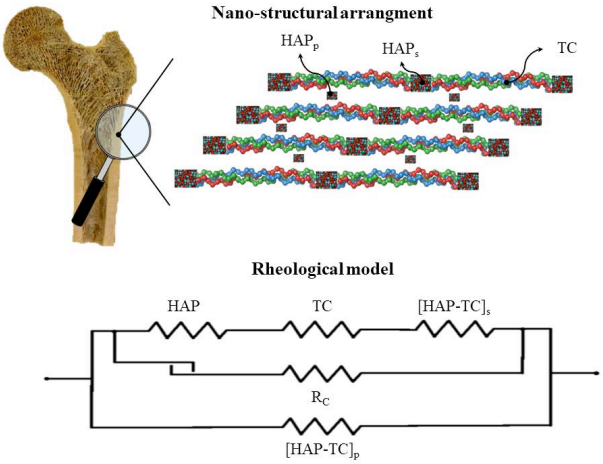

Fig. 1: Schematic representation of: (top) nano-structural arrangement of mineralized collagen fibril constituents, (bottom) the proposed rheological model.

A. Nano-mechanics of MCF constituents

The material bone is a mineral connective tissue that has a complex hierarchical structure. Bone is composed of type I collagen protein, HAP mineral, non-collagenous proteins and proteoglycans.

Type I collagen, the most common type of collagen, is present in many tissue such as bones, teeth, tendons, arterial wall and the cornea. The basic structural unit of collagen molecule is tropocollagen that is made up of three polypeptide strands arranged in left-handed helix. The three helices are twisted together in a cooperative quaternary structure namely triple helix. The triple helix can be regarded as a one-dimensional structure about 300 nm long and 1-2 nm in diameter. The elastic (reversible) response of a collagen molecule is modelled considering an equivalent one-dimensional element [5].

In bone the mineral component is present in form of sub-microscopic crystals of HPA. The crystals are plate-shaped and is characterized from a width of 25 nm, a length of 50 nm and a small thickness of 1,5 - 4 nm. The longest dimension of crystal are oriented parallel to the collagen molecule.

The interfacial interactions between collagen and hydroxyapatite is a key aspect in the modelling of mechanical

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response. The interaction in the hole zone as well as the interaction in overlap region are accounted in the model [6].

B. Rheological model

The behaviour of viscoelastic materials under uniaxial loading may be represented by means of conceptual models composed of elastic and viscous elements which provide physical insight. The developed model accounts: (i) mechanical response of tropocollagen molecule; (ii) mechanical response of HAP cristals; (iii) interaction between tropocollagen molecules and HAP in hole zone; (iv) interaction between tropocollagen and HAP in the overlap region; (v) restraint mechanism.

III. RESULTS

Results are obtained addressing a tensile test. In particular, stress-strain curve are obtained, highlighting the coupled influence of mineralization and of different tropocollagen HAP interaction. Fig. 2 shown the obtained results for two mineralized collagen fibrils, with different HAP content, in comparison with experimental data [4].

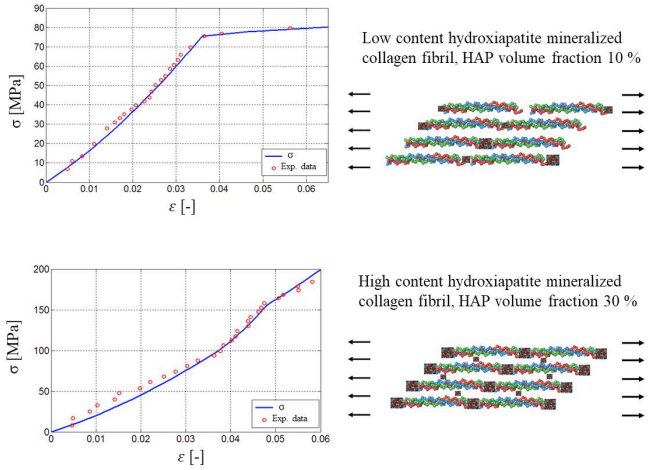

Fig. 2: Stress - strain response resulting from tensile tests for: (top) low content HAP mineralized collagen fibrils, (bottom) high content HAP mineralized collagen fibrils. Comparison between present model (blue line) and experimental data [4].

IV. CONCLUSION

The mechanical response of mineralized collagen fibrils has been addressed by proposing a simple rheological model, based on histological and biochemical features.

Numerical results show the model capability in reproduce the experimental evidence found in literature and is able to reproduce the different behaviour of mechanical responses to external load.

Moreover, the developed model, based on a structurally-motivated description, accounts dominant nano-scale mechanisms in order to understand the interaction between the mineralized collagen fibrils constituents. It is worth to highlighting that the used approach introduces model parameters describing well-defined histological and biochemical features only, thereby opening to a straight-forward model calibration based on clinical/experimental evidence gates.

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