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Mechanical Properties and Structural Behavior of Bone at Nano Scale with Cohesive Element

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ABSTRACT: Bone is a biological tissue whose main components are different from the mechanical aspect. Some of the bone diseases are due to mutations in the bone structure at the nano scale, while their clinical symptoms appear at the macro scale. Therefore, the evaluation of bone at micro and nano scales is important. In the current study, the finite element modeling is performed to evaluate the mechanical properties and behavior of bone at the nano scale and the cohesive element is applied. After its verification, the stress distribution and elastic properties are compared with the analytical model. Limited studies are available on strain ratio and it is presented for different cohesive elements in the current study. The influence of mineral volume fraction and mechanical properties of collagen is investigated. The comparison between finite element models and the other ones demonstrate an excellent agreement. The collagen- hydroxyapatite interface with unknown mechanical properties is the most important parameter in the model and the thick water layer with Van der Waals interaction and viscous shear is determined as the most probable cohesive layer. The parametric studies indicate the significant effect of nonlinear collagen on the model. To decrease the calculation in models, the proposed unit cell with periodic boundary conditions could be employed.

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1. INTRODUCTION

Bone is a connective tissue that stores minerals, produces blood cells and protects vital internal organs [1]. The mechanical properties and behavior of bone are different at the nano to the macro level and the result of each level can be used as an input for the upper level.

Numerous methods are used to model the multi-scale mechanical properties of bone such as continuum and structural mechanics [2-4], micromechanics [5-7], finite element analysis [8-11] and molecular dynamics [12-14].

In the current study, the numerical model of bone at the nano level is investigated in Abaqus. After verification the results with other numerical and analytical research, the stress distribution in different layers, load transfer mechanisms and elastic modulus are compared with the shear-lag model. The strain ratios of hydroxyapatite platelets versus mineralized collagen fibril with three different collagen-hydroxyapatite interfaces are determined and the limitation of the shear-lag model is investigated by comparing the numerical results of different hydroxyapatite volume fraction with analytical ones. Besides, the effect of collagen mechanical properties on the behavior of the model is presented.

2. MATERIALS AND METHODS

The mineralized collagen at the nano level is numerically modeled by the staggered arrangement of collagen layers, hydroxyapatite platelets and cohesive zone in collagen-hydroxyapatite interaction and potential fracture sites in mineral layers and also some links between collagen materials. Five different models including strong collagen-hydroxyapatite interaction, intermediate and weak ones and also perfectly bonded interfaces (without any cohesive zones) and pure hydroxyapatite are studied.

The hydroxyapatite materials are assumed with isotropic elastic elements and both elastic and hyperelastic material properties are used for modeling the collagen layers. The strain energy potential is utilized for modeling the hyperelastic collagen materials and also the exponential traction-separation laws are used in modeling the cohesive zones. Moreover, maximum stress criterion and energy are considered as damage initiation and evolution parameters.

3. RESULTS AND DISCUSSION

The numerical results of the presented mineralized collagen model are compared with other research as shown in Fig. 1 and Fig. 2. Besides, the comparison between current numerical results and molecular dynamic method are presented in Table 1.

The stress-strain results of mineralized collagen fibrils with hyperelastic and elastic collagen properties with different links for strong hydroxyapatite - collagen interactions are presented in Fig. 3.

4. CONCLUSION

The comparison between current numerical results and

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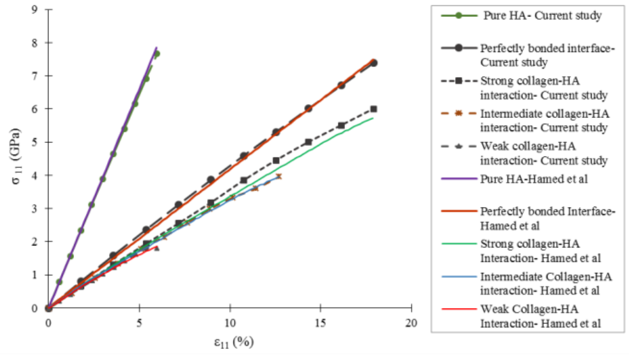

Fig. 1. Stress-strain diagram of models with hyperelastic collagen properties in current study and comparison with Hamed et al [15]

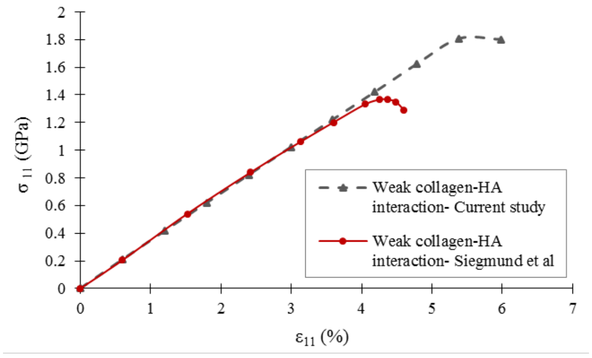

Fig. 2. Stress-strain diagram of weak collagen- hydroxyapatite interaction models with hyperelastic collagen properties and

Table 1. Comparison between strength and ultimate strain results of mineralized collagen models in current research and other molecular dynamics studies

Items		Ultimate strength (GPa)	Ultimate strain
Numerical method (current study)	Strong interaction	5.93	17.9
	Intermediate interaction	3.96	12.68
	Weak interaction	1.80	5.97
Molecular dynamic method	Buehler [13]	0.6	6.7
	Dubey and Tomar [14]	3	6

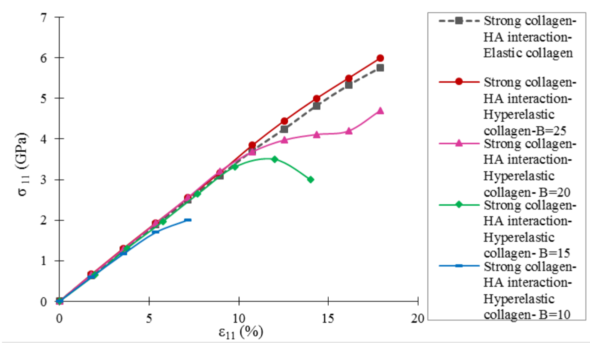

Fig. 3. Stress-strain results of mineralized collagen fibril with strong collagen-hydroxyapatite interaction with hyperelastic and elastic collagen properties with different

the other numerical and analytical studies indicate a good agreement between them. Besides, the stress distribution and load transfer mechanism confirm the shear-lag model in which the hydroxyapatite phase is responsible for normal stress and the shear stress between layers is carried by collagen. The zero stress in the cohesive layer demonstrates the debonding in layers between the hydroxyapatite-collagen interface.

The strain ratio of hydroxyapatite platelets versus mineralized models in different hydroxyapatite-collagen interactions is presented and the strain ratios in weak interaction coincide well with experimental results.

The numerical and analytical results of different hydroxyapatite volume fractions are compared and the limitation of the shear-lag method is investigated. The cover length and the longitudinal distance between hydroxyapatite crystals are the two main parameters that should be considered in numerical models.

The nonlinear behavior of collagen material has a significant effect on the mechanical behavior of mineralized collagen fibril. Moreover, the two-unit cell models proposed in the current study are compatible with the whole model results and could be used with periodic boundary conditions in future studies.

The results of different numerical and analytical studies in current research show that the weak collagen- hydroxyapatite interaction is the most probable case among others.

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