

Propagation of bone micro fracturing: a numerical approach

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Abstract. Fracture mechanics can be understood as the area of science that studies the propagation of fractures, cracks, slits, and other flaws from mechanical processes that may negatively affect the strength of the material. Traditionally, the concepts on which the strength of the materials are based do not consider the toughness to fracture of the material, which can be defined as the property that quantifies the resistance to crack propagation. The essence of these studies can be applied to any type of material, such as in the medical field when studying the behavior of bone fractures. This type of fracture usually arises through high-energy trauma. Bone, under normal conditions, can support loads and absorb this energy. However, if there is a high level of energy associated with the trauma, the bone cannot support it and ends up suffering a fracture. This paper aims to develop a numerical microscale analysis of a bone fracture using the Extended Finite Element Method (XFEM). This paper will study Two-dimensional simulations of the initiation and propagation mechanisms of an initial fracture in a compact bone unit called the osteon, which is bounded by the cement line, a zone that is low in type 1 collagen. In this way, it will be possible to understand the influence of the cement line on the propagation of the microscale fracture.

Keywords: Microscale, Osteon, XFEM, Crack propagation

1 Introduction

Fracture mechanics concepts can be applied to a multitude of materials. Although bone has a simple appearance, its structure is heterogeneous, complex and dynamic, so trying to predict the behavior of a fracture in living tissue such as bone is hard work. Bone fracture is an important clinical problem. The risk depends on several factors such as: age, genetics, or even diet. Fracture toughness is the property of how much the material will resist crack propagation (Callister and Rethwisch [1]). Understanding bone fracture resistance is important for diagnosing bone diseases and evaluating treatments. Mechanisms for increasing fracture toughness are found at all bone length scales (Launey et al. [2]; Wang and Gupta [3]). However, the most powerful mechanisms are found at the microscale, where propagating cracks are deflected or interrupted by weak interfaces (Koester et al. [4]; Mohsin et al. [5]).

On a microscale, compact or cortical bone tissue is characterized by a set of fibers organized around the central canal, through which blood capillaries and/or nerves pass. This arrangement is called the Haversian System, which is composed of the interstitial bone matrix, osteon, and the Havers canal (Wang and Gupta [3]).Microfracture in the osteon can occur in three different ways: the first is in the longitudinal form, which occurs when a crack propagates parallel to the bone axis; the second is transversely, when propagation occurs perpendicularly to the axis; and the third is radial, which occurs when a fracture develops radially to the bone axis (Li et al. [6]). Figure 1 outlines the view of the bone at different scales, exemplifying the Havers System on a microscale. Normally, the osteon-matrix interface is through a layer of cementing substance poor in type 1 collagen (Skedros et al. [7]).

Computational models can be used to study compact bone fracture behavior by evaluating the effect of structural properties and fracture strength (Fratzl et al. [8]; Sabet et al. [9]). One of the most used models for crack propagation is based on the extended finite element method (XFEM), as it does not require a predefined crack path (Belytschko and Black [10]; Melenk and Babuška [11]). XFEM models using the maximum principal strain criterion (MAXPE) are commonly used to model the onset of damage in crack propagation (Abdel-Wahab et al. [12]; Idkaidek and Jasiuk [13]). However, this criterion alone does not bring satisfactory results for the crack trajectory in the matrix/osteon interface. Thus, it is necessary to use an interface damage model that is capable of capturing the deflections along the cement line (Gustafsson et al. [14]).

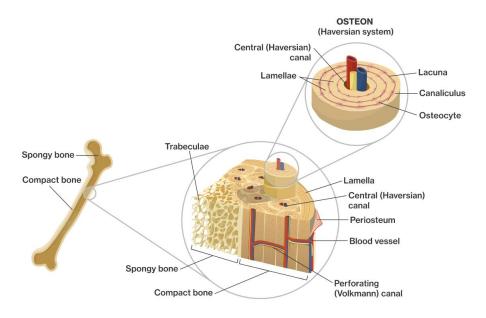


Figure 1. Representation of the Haversian system

In this article, a 2D microscale model of a cortical bone submitted to the MAXPE criterion was simulated using XFEM within the commercial software ABAQUS, in order to understand the crack propagation mechanisms and the role played by the mechanical properties of microstructural and , in particular, by the cement line, considering the finite element mesh density, analysis increment size and boundary conditions.

2 Material and Methods

2.1 Specimen geometry and material parameters

A 2D model of a single radial osteon with base developed by Gustafsson et al. [14] was developed. The model has external dimensions of 0.5 x 0.5 mm, in the center of the interstitial matrix is the representation of the osteon and the Haversian canal, which has diameters of 300 μ m and 100 μ m, respectively, and an osteon-matrix interface it is 5 μ m thick. Initially, for the analysis, inherent parameters of the material such as Young's modulus and Poisson's ration are needed, in addition to the separation law, which for this article used the maximum principal strain criterion (MAXPE). In this criterion the value the critical damage initiation strain and the energy release rate are initially assigned. Based on review Gustafsson et al. [15], Gustafsson et al. [14] separated the best values for the properties, as can be seen in Table 1. The boundary conditions and specimen measurements are exemplified in Figure 2.

Table 1. Material	narameters	for specimen	components
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	Interstitial Matrix	Osteon	Haversian Canal	Cement Line
E (GPa)	15	12	0.1	18
ν	0.3	0.3	0.3	0.3
ε_{max}^{0}	0.004	0.004	0.004	0.004
$G (kJ/m^2)$	0.2	0.2	0.001	0.2

Two models were created, one with the cement line and the other without it. In all models, 4-node bilinear quadrilateral elements with reduced integration (CPE4R) and structured mesh were used. The complete models contains 10852 and 9700 elements, respectively.

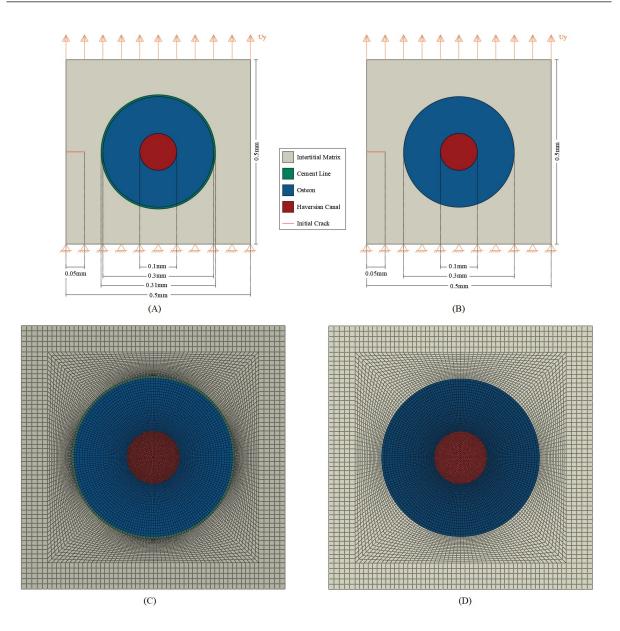


Figure 2. Two-dimensional cortical bone model: (A) Model with Cement Line. (B) Model Without Cement Line. (C) Model mesh with Cement Line. (D) Model mesh without Cement Line

2.2 Finite Element Analysis

Assuming, as a hypothesis, that the Principle of Virtual Work represents the behavior of fractured materials without selecting the faces belonging to surfaces. Belytschko and Black [10] developed the Extended Finite Elements Method (XFEM), based on the partition of unit method proposed previously by Melenk and Babuška [11]. In this way, according to Martínez Concepción [16], it is possible to model the singularity and its discontinuities independently of the mesh. The X-FEM method is an extension of the conventional finite element method, which allows the presence of discontinuities in an element, by local enrichment functions. The displacement approximation for a cracked domain is defined as eq. (1):

$$u(x) = \sum_{i=1}^{m} u_i N_i + (x) \sum_{i=1}^{m} c_i N_i(x) H(x) + \sum_{i=1}^{k} N_i(x) \left(\sum_{l=1}^{4} c_i^a F_a(x) \right).$$
(1)

where u, the displacement vector, N, the shape functions, u_i , the nodal displacement vectors, H(x) and $F_a(x)$ the Heaviside function and the crack tip enrichment function, respectively, c_i and c_i^a are the nodal enriched degrees of

freedom.

The maximum principal strain criterion (MAXPE) was adopted in this study to model crack propagation in the interstitial matrix, osteon and Haversian canal. The fracture criterion f is defined as eq. (2) and damage is initiated when $f_{MAXPE} > 1$ and the maximum principal orientation is used as normal vector for the crack propagation (Gustafsson et al. [14]).

$$f_{MAXPE} = \left\{ \frac{\langle \varepsilon_{max} \rangle}{\varepsilon_{max}^0} \right\}.$$
 (2)

where ε_{max} is the maximum principal strain and ε_{max}^0 is the critical damage initiation strain. All the simulations were performed in displacement control mode using $u_y = 0.004$, can be seen schematically in the Figure 2.

3 Results and Discussion

Initially, a simulation was carried out in order to verify the location of the concentration of stresses and the distribution of strains without the presence of an initial arbitrary fracture. As expected, the stress concentration occurred in regions close to the Haversian Canal, and because it is in an area with a low modulus of elasticity, all the elements present in the canal deformed faster than the others (Figure 3 (B)). In terms of stress distribution, the maximum stress is about twice as high as the average stress (Figure 3 (A)). However, it should be noted that the model created is a microscale simulation of a compact bone, and factors such as porosity and the presence of Volkmann Canals were not considered.

When simulations incorporating an initial fracture were performed, it was noted that the path taken by the fracture was similar for the models with Cement Line (Figure 3 (C) - (D)) and without Cement Line (Figure 3 (E) - (F)).

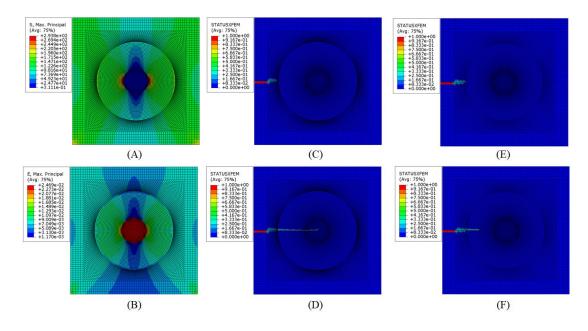


Figure 3. Analysis Results: (A) Maximum Principal Strain for initial simulation. (B) Maximum Principal Stress for initial simulation. (C) Crack propagation before Cement Line. (D) Crack propagation after Cement Line. (E) Crack propagation before Osteon. (F) Crack propagation after Osteon.

From the stress-strain curve (Figure 4), it can be inferred that the cement layer, witch is poor in collagen type 1, offers the model the ability to resist higher stresses and strain levels for microcracks, taking into account that the cement line directly influences the propagation of cracks in the microscale cortical bone.

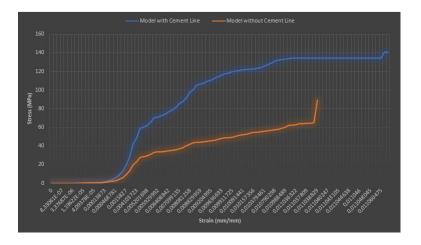


Figure 4. Stress-strain behaviour of two studied models

4 Conclusions

It is possible to find, in this article, a preliminary study on the propagation of cracks in the microstructure of cortical bone, using an X-FEM approach with MAXPE criterion. For this, a simple geometric model of a radial osteon was considered, to investigate the effect of different parameters. A clear effect of the cement lines was observed, which play a fundamental role in the propagation of cracks, acting as a barrier and preventing or retarding the growth of cracks.

As this is a work in progress, further work will verify the same effect for longitudinal and transverse propagation, in addition to considering the interaction of multiple osteons in the same analysis, to investigate the phenomenon of crack deviation.

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References

[1] D. Callister and D. G. Rethwisch. Magnetic properties. *Materials Science and Engineering, An Introduction, 7th Ed. ed. John Willey & Sons, Inc*, pp. 19–56, 2007.

[2] M. E. Launey, M. J. Buehler, and R. O. Ritchie. On the mechanistic origins of toughness in bone. *Annual review of materials research*, vol. 40, pp. 25–53, 2010.

[3] R. Wang and H. S. Gupta. Deformation and fracture mechanisms of bone and nacre. *Annual Review of Materials Research*, vol. 41, pp. 41–73, 2011.

[4] K. J. Koester, J. Ager, and R. Ritchie. The true toughness of human cortical bone measured with realistically short cracks. *Nature materials*, vol. 7, n. 8, pp. 672–677, 2008.

[5] S. Mohsin, F. J. O'Brien, and T. C. Lee. Osteonal crack barriers in ovine compact bone. *Journal of anatomy*, vol. 208, n. 1, pp. 81–89, 2006.

[6] S. Li, A. Abdel-Wahab, and V. V. Silberschmidt. Analysis of fracture processes in cortical bone tissue. *Engineering Fracture Mechanics*, vol. 110, pp. 448–458, 2013.

[7] J. G. Skedros, J. L. Holmes, E. G. Vajda, and R. D. Bloebaum. Cement lines of secondary osteons in human bone are not mineral-deficient: New data in a historical perspective. *The Anatomical Record Part A: Discoveries in Molecular, Cellular, and Evolutionary Biology: An Official Publication of the American Association of Anatomists*, vol. 286, n. 1, pp. 781–803, 2005.

[8] P. Fratzl, H. S. Gupta, F. D. Fischer, and O. Kolednik. Hindered crack propagation in materials with periodically varying young's modulus—lessons from biological materials. *Advanced Materials*, vol. 19, n. 18, pp. 2657–2661, 2007.

[9] F. A. Sabet, A. Raeisi Najafi, E. Hamed, and I. Jasiuk. Modelling of bone fracture and strength at different length scales: a review. *Interface focus*, vol. 6, n. 1, pp. 20150055, 2016.

[10] T. Belytschko and T. Black. Elastic crack growth in finite elements with minimal remeshing. *International journal for numerical methods in engineering*, vol. 45, n. 5, pp. 601–620, 1999.

[11] J. M. Melenk and I. Babuška. The partition of unity finite element method: basic theory and applications. *Computer methods in applied mechanics and engineering*, vol. 139, n. 1-4, pp. 289–314, 1996.

[12] A. A. Abdel-Wahab, A. R. Maligno, and V. V. Silberschmidt. Micro-scale modelling of bovine cortical bone fracture: Analysis of crack propagation and microstructure using x-fem. *Computational Materials Science*, vol. 52, n. 1, pp. 128–135, 2012.

[13] A. Idkaidek and I. Jasiuk. Cortical bone fracture analysis using xfem-case study. *International journal for numerical methods in biomedical engineering*, vol. 33, n. 4, pp. e2809, 2017.

[14] A. Gustafsson, H. Khayyeri, M. Wallin, and H. Isaksson. An interface damage model that captures crack propagation at the microscale in cortical bone using xfem. *Journal of the mechanical behavior of biomedical materials*, vol. 90, pp. 556–565, 2019a.

[15] A. Gustafsson, M. Wallin, H. Khayyeri, and H. Isaksson. Crack propagation in cortical bone is affected by the characteristics of the cement line: a parameter study using an xfem interface damage model. *Biomechanics and modeling in mechanobiology*, vol. 18, n. 4, pp. 1247–1261, 2019b.

[16] E. R. Martínez Concepción. Modelagem numérica de fraturamento hidráulico via método dos elementos finitos estendido, 2015.