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Crack propagation in cortical bone: a numerical study

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Abstract

The fracture behavior of human bone is an interesting field of research for medical scientists, which are interested in predicting the fracture risk, but also for engineers, which are interested in mimicking bone structure in the design of new materials. To understand this phenomenon and to be able to make predictions, many numerical techniques are currently adopted, with the goal of reaching different length scales. In this paper we present a numerical study of the microstructure of human bone, via a cohesive-based X-FEM approach. A single osteon model is developed to investigate the mechanisms of crack propagation and the role played by the mechanical properties of the micro-structural constituents, and in particular by the cement line. The latter has shown to strongly affect the crack path, by acting as a barrier and arresting or preventing a continuous crack propagation, and causing a deviation, leading to an increase in the fracture energy.

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Keywords: cortical bone, microstructure, crack propagation, osteon, X-FEM

1. Introduction

Bone is a structural hierarchical composite, mainly made of hydroxyapatite crystals and collagen matrix, and showing a complex organization at different length scales. It is well-known for its optimal combination of mechanical properties, and in particular for its remarkable toughness, explaining why it provides supports for many organisms. Thanks to its outstanding mechanical properties, combined with a low weight, bone constitutes a source of inspiration for the design of new tough nanocomposites. The fracture behavior of human bone is an interesting

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field of research for medical scientists (Nalla, Kinney, & Ritchie, 2003; Ritchie, Kruzic, Muhlstein, Nalla, & Stach, 2004), which are interested in predicting the fracture risk, but also for engineers, which are concerned in mimicking bone structure (Espinosa, Rim, Barthelat, & Buehler, 2009) in the design of new materials. Indeed for the clinicians, predicting fracture risk for individual patients is crucial. Many researchers found a correlation between bone fracture risk and bone strength. However, bone strength is largely influenced by bone quality, which is in turn dependent on several factors (*i.e.* genetic disorders, ageing). The prediction of bone fracture is a major challenge. This is due to the high variability of the available data, being bone a living tissue involved in a continuous remodeling process. Bone fracture is largely influenced by the remodeling process, which strongly affects its internal arrangement. In particular, the microstructure of cortical bone, originates from remodeling. Indeed, primary bone is characterized by few osteons, which are smaller and shorter in size, and without the presence of cement lines. Secondary osteons, instead, originate from the osteoblast-osteoclast combined activity, consisting in replacing old tissue with a new one. Secondary osteons have a circular-to-ellipsoidal shape with a 100-300 μm diameter and 1-2 mm length. Each osteon consists of several circumferential lamellae around a central canal (*i.e.* Haversial canal) and an outer boundary called cement line, 1-5 μm thick, whose properties are rather difficult to be determined. Recent studies (Skedros, Holmes, Vajda, & Bloebaum, 2005) based on quantitative backscattered electron (BSE) imaging and energy dispersive X-ray (EDX) spectroscopy dispute historical observation of a tissue characterized by higher mineralization, attributing this statement to unrecognized artifacts that may arise during scanning electron microscopy. The microstructure of cortical bone is characterized by several osteons embedded into the interstitial matrix, consisting of several lamellae. The noticeable toughness of bone is thought to be the result of different mechanisms, activated at different length scales. Launey et *al*. (Launey, Buehler, & Ritchie, 2010) defined intrinsic and extrinsic mechanisms, the former (e.g. fibrillar toughening) activated at subnanoscale, and the latter (e.g. crack deflection) at micro-scale. According to Nalla et *al.* (Nalla, et al., 2003) a main role is played by crack deflection, which largely increase bone toughness by increasing the work of fracture. This mechanism is induced by the osteon and cement lines, along with their size and density, acting as barriers and causing change in the crack path, by altering the crack angle from the minimum energetic configuration (Meyers, Chen, Lin, & Seki, 2008).

Recently, the study of the microstructural level is receiving an increasing attention. To understand this phenomenon and to be able to make predictions, many numerical techniques are currently adopted, with the goal of reaching different length scales. Single osteon computational studies have been carried out by Prendergast and Huiskes (Prendergast & Huiskes, 1996) to investigate the effect of micro-damage on the local strain field in bone microstructure. Hogan et *al.* developed a fiber-reinforced composite (FRC) like model of the haversian systems, where the osteons, are considered to as fibers, the interstitial lamellae as matrix, and the cement line as the fiber/matrix interphase (Hogan, 1992). Recently, other microstructural finite element FRC-likes model have been developed using the software FRANC2D for bone (Raeisi Najafi, Arshi, Eslami, Fariborz, & Moeinzadeh, 2007) and bone-like composite (Huang, Rapoff, & Haftka, 2006). A recent approach to model crack propagation, based on extended finite element method (X-FEM) has been recently proposed by some authors: Budyn and Hoc (Budyn & Hoc, 2007), who developed a multi-scale method to simulate multiple crack propagation across osteons in a three-dimensional finite element model of cortical bone under tensile loading, and Abdel-Wahab et *al.* (Abdel-Wahab, Maligno, & Silberschmidt, 2012)

In the following we present a single osteon numerical study, via a cohesive-based X-FEM approach implemented in Abaqus 6.12 (ABAQUS, 2012). A simple 2D model is developed to provide an insight into the mechanisms of crack propagation and the role played by the mechanical properties of the micro-structural constituents, and in particular by the cement line.

2. Methods

2.1. Model geometry and materials properties

We built a 2D single osteon model and we considered it as transversely isotropic. Indeed, being the osteons longitudinal and having an approximately circumferential cross section, we assumed them similar to continuous fibers in the transversal plane, embedded into a matrix. To reduce the computational costs we simplified the geometry by considering the osteon as a hollow cylinder, neglecting the Haversian canal and the porosity, and we modeled only a quarter, due to the axisymmetric structure. The dimensions of the models are 0.108 × 0.108 × 0.108 mm, with an approximate 67% osteon volume ratio. The dimensions of all the components are listed in Table 1, whereas the geometry and boundary conditions are represented in Fig. 1. In all the simulations we assumed plain strain conditions and we defined an initial micro-crack of 0.01 mm, represented by a red line in Fig. 1. We also varied the crack site, to investigate the effect of different positions.

To study the effect of the cement line, we considered a two phase model, including only osteon and interstitial matrix, and a three phase model, also accounting for the cement line. The geometrical parameters and mechanical properties used in this study are considered as average values derived from the literature. Indeed, there is a large variation of the data available in the literature, being bone properties affected by several factors, firstly bone type (*e.g.* human, bovine, ovine) and bone anatomical location (e.g. femur diaphysis, femur neck, tibia). Besides, other factors such as age, gender, and genetic diseases (Busse, et al., 2013; Carriero, et al., 2014) may further affect the bone density and quality, hence the structure and properties. The mechanical characteristics of osteons and interstitial matrix are generally measured by means of nanoindentation (Rho, Roy, Tsui, & Pharr, 1999; Rho, Tsui, & Pharr, 1997; Turner, Rho, Takano, Tsui, & Pharr, 1999). To measure the mechanical properties of the cement line is rather more difficult. Some authors considered this tissue softer than the surrounding ones and reported in their study the characteristics of the cement line as average values between those of the boundary constituents (i.e. osteons and interstitial matrix), reduced by approximately 25-30%. Other authors instead, considered the cement line as stiffer tissue, characterized by higher mineralization.

In this study we adopted the mechanical properties of bovine cortical bone as given by Abdel-Wahab *et al.* (Abdel-Wahab, et al., 2012) and by Budyn *et al.* (Budyn & Hoc, 2007) and we compare the results. In both cases the cement line was considered softer than the surrounding tissues, with an elastic modulus 25% lower than that of the osteon. All the components were considered transversely isotropic, hence isotropic in *xy*-plane. The mechanical properties of the bone components in the transversal direction adopted in this study are given in Table 1.

Table 1. Geometry and transversal properties of microscopic components of haversian bone tissue (Abdel-Wahab, et al., 2012; Budyn & Hoc, 2007).

Component	Dimension	Elastic Modulus (GPa)	Poisson's ratio	Strain energy-release rate (N/mm)
Haversian canal	diameter = 0.06 mm			
Osteon	diameter = 0.2 mm	9.130* 11.510**	0.170	0.860
Cement line	thickness = 0.003 mm	6.850* 8.632**	0.490	0.146
Interstitial matrix		14.122* 12.660**	0.153	0.238

*case study 1; **case study 2.

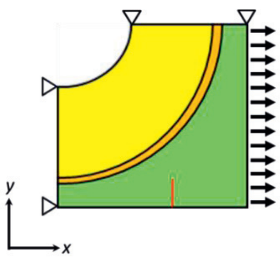

Fig. 1. Micromechanical model of Haversian cortical bone: osteon quarter: loading and axisymmetric boundary conditions. The initial microcrack is represented by a red line.

2.2. X-FEM: simulation setup

We performed X-FEM-based cohesive analyses of crack initiation and propagation by using the X-FEM implemented into the finite element software Abaqus 6.12 (ABAQUS, 2012). Indeed Abaqus has introduced, since the 6.9 version, the possibility of modeling cohesive cracks into the X-FEM framework (Belytschko & Black, 1999; Moës, Dolbow, & Belytschko, 1999).–X-FEM method is particularly suitable to treat discontinuities (Hansbo & Hansbo, 2004): strong discontinuities, which are discontinuities in the solution variable, generally induced by cracks, and weak discontinuities, which are discontinuities in the derivatives of the solution variable (*e.g.* biomaterials problems). In this case study both severe and weak discontinuities occur. The X-FEM method is an extension of the conventional FE method based on the concept of partition of unity, allowing the presence of discontinuities in an element, by local enrichment functions. The displacement approximation for a cracked domain assumes the following form:

$$\mathbf{u} = \sum_{i=1}^{N} N_i(x)\left[\mathbf{u_i} + H(x)\mathbf{a_i} + \sum_{\alpha=1}^{4} F_\alpha(x)\mathbf{b_i^\alpha}\right] \tag{1}$$

Where $\mathbf{u}$, the displacement vector, N, the shape functions, $\mathbf{u_i}$, the nodal displacement vectors, $H(x)$and $F_\alpha(x)$ the jump and tip enrichment function, respectively, $\mathbf{a_i}$ and $\mathbf{b}_i^\alpha$ nodal enriched degrees of freedom.

For damage modeling we used a cohesive segment approach, which is similar to those used for cohesive elements, and based on traction-separation laws (ABAQUS, 2012). We assumed an initial linear-elastic behavior, followed by a damage initiation, defined via a maximum principal strain criterion, and an energy-based damage evolution with a linear softening. We set the crack initiation at 0.4% strain value for all the components of the micro-structural model, as described in previous studies (Abdel-Wahab, et al., 2012; Budyn & Hoc, 2007) and fracture energy values as reported in Table 1. First we simulated crack initiation, by means of an X-FEM approach. Then we performed X-FEM simulations of the osteon quarter model, including an edge micro-crack. In all the models we used 4-node bilinear quadrilateral elements with reduced integration (CPE4R). The whole models contains 5449 elements and 5290 nodes. We should point out that in X-FEM the mesh does not need to follow the problem geometry, since there is no need for remeshing during crack propagation. All the simulations were performed in displacement control mode, by applying 0.4-2% strain in *x*-direction at the right-hand side, and constraining the left-hand side and the upper side, in *x*- and *y*-directions respectively, as schematically shown in Fig. 1. To respect the symmetry, we also constrained the rotations around the *y*- and *z*-axes, for the left-hand side and the rotations around *x*- and *z*-axes, for the upper side.

3. Results and discussion

We firstly simulated crack initiation. As we would expect, crack originated in the region of maximum stress concentration, close to the hole, which represents the Haversian canal. Several crack originated in this region and propagated orthogonal to the applied load. Then, by observing the stress distribution, we could notice that the stress is increased by approximately three times in the zone close to the Haversian canal. However, we should point out that our model is a simplification of the real microstructure of cortical bone, since we neglected the presence of the Volkmann's canals and small canaliculi and the local porosity, which may further affect the local stress distribution.

In the models with an arbitrary initial microcrack we noticed a similar crack path in all the simulations, characterized by: *i)* an initial crack propagation into the interstitial matrix, orthogonal to the load direction, *ii)* a small deviation close to the cement line region, *iii)* a crack arrest at cement line, followed by *iv)* a secondary growth into the osteon region. In the latter part, the crack did not show a straight path, but a certain deviation in the direction of the Haversian canal.

By comparing the results of the simulations performed on a two-phase and a three-phase model, we can confirm a clear effect of cement line, which acts as a barrier, dissipating energy and arresting the crack (Fig.2a). In Fig. 2 we depict the final maximum principal stress distribution and crack propagation in the two models, with (a) and without (b) the cement line, for simulations with an applied strain of 0.42 %. We also carried out simulation at higher applied strain (1-2 %) and we found out that crack occurs at higher deformation level. Hence, we conclude that in presence of cement line, more energy is required for crack propagation.

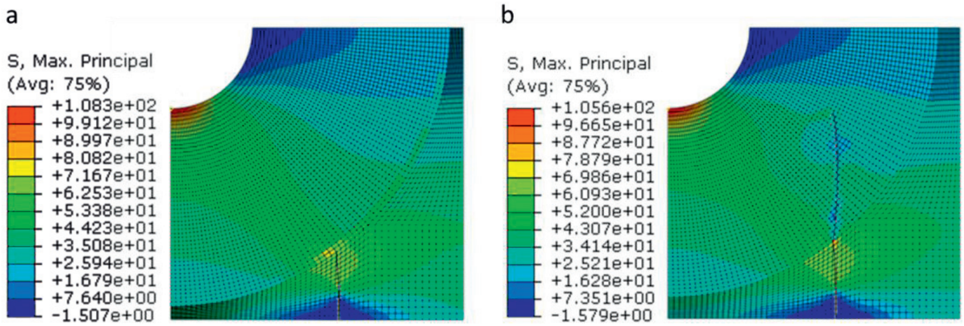

Fig. 2. (a) Three-phase model: crack arrest; (b) Two-phase model: crack propagation. Final crack path in the two models with a 0.42 % applied strain. The presence of cement line (a) affects the final behavior by causing crack arrest.

We also considered different crack positions, to investigate the effect on the crack propagation and the global behaviour. We found a linear relationship between the critical strain for crack propagation into the osteon and the crack position (Fig. 3a): the critical strain linearly increases as the crack is shifted from the middle of the edge the far field. For the crack position we considered the normalized *x*-distance from the left-hand constrained side.

Fig. 3 shows the effect of different mechanical properties, as reported in Table 1. The elastic properties for *case study 1* and *case study 2* are different. However, in both cases the stiffness of the cement line is 25 % lower than that of the osteon, whereas the cement line/interstitial matrix stiffness ratio changes. In particular, in *case study 1* (see Table 1), the cement line elastic modulus is 39% lower than that of the interstitial matrix; in *case study* 2 (see Table 1) instead, the cement line elastic modulus is 32 % lower than that of the interstitial matrix. The results from the second case show a toughness modulus, 10 % higher than that of the first case (see Fig. 3b). We also compared the crack propagation for the two cases. In Fig. 3c we plot the crack length as a function of the applied strain. From the graph we can distinguish three regions: I) crack propagation into the interstitial matrix, II) crack propagation into the cement line and in the external osteon region, and III) crack propagation into the mid-to-internal osteon region. Crack propagation rate in region I is lower than crack propagation rate in region III, and seems to be affected by the close presence of the cement line. Moreover, points of crack arrest are clearly visible from the graph represented in Fig. 3c and correspond to the small steps in the trend, that are clearly visible for the three-phase models.

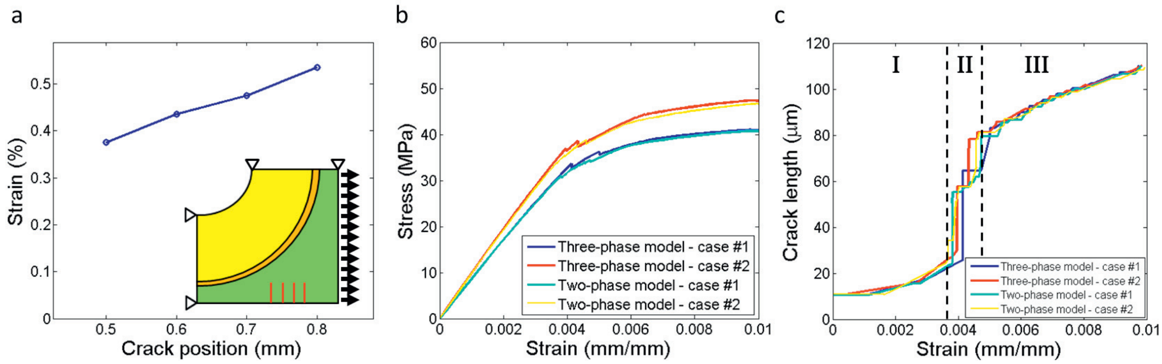

Fig. 3. (a) Strain vs. Crack position: the critical strain required for crack propagation linearly increase by shifting the crack position; (b); Stress vs. Strain behavior of two- and three-phase models with different mechanical properties (case 1 and case 2); (c) Crack length vs. Strain of two- and three-phase models with different mechanical properties (case 1 and case 2)

4. Remarks

In this paper we showed a preliminary study of crack propagation into the microstructure of cortical bone, by means of a cohesive-based X-FEM approach. We considered a simple geometrical model of an osteon quarter, to investigate the effect of different parameters. We could observe a clear effect of cement lines, which play a main role in crack propagation, acting as barrier and preventing or slowing down the crack growth.

In an ongoing work, we are considering also the effect of more osteons, to investigate the phenomenon of crack deviation. As future work we aim to extend the framework to 3D models of cortical bone and compare the results with experimental ones, and validate the models.

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