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Extended Finite Element models of introcortical porosity and heterogeneity in cortical bone

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Abstract

Due to changes in the bone quality during ageing the fracture risk increases. The influence of the different parameters affecting bone quality is not well understood. The Finite Element method offers the opportunity to determine the individual contribution of a parameter by changing single parameters.

In this study, the ABAQUS extended Finite Elements Method (xFEM) was applied to simulate the crack propagation in compact bone samples using the quadratic nominal stress as crack criterion. Micro computed tomography images of compact-tension samples machined from a 19 and an 81 years old donor were used to generate Finite Element meshes consisting of linear tetrahedrons via Mimics. Cavities were modelled only in the estimated crack area to avoid a high number of degrees of freedom. Crack area was meshed with a higher number of smaller elements. The other areas were meshed with a small number of larger elements. The changes in the material constants due to the simplification of the model were taken into account by using effective material parameters in these partitions. Our results show that age-related loss in bone toughness results from increased porosity and loss in heterogeneity of material level properties.

Keywords

xFEM; Crack propagation; Fracture toughness; Compact bone

1. Introduction

Fracture risk of bone increases with ageing [1], due to changes in the microstructure, bone loss and changes in the material quality [2–4] of bone. However the influence of each variable on fracture of bone is not well understood.

Bone adapts very well to applied loadings. Changes in the normal loading cycle lead to alterations in bone architecture. Such changes can be seen at all levels of bone hierarchy. Bone has a compact shell at the surface called compact bone and a sponge like inner

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structure called trabecular or cancellous bone [5]. At the next structural level, bone tissue contains osteons or trabecular packets. The osteons are also referred to as Haversian system. In this system blood vessels and nerves are present. Bone tissue is internally remodelled by osteoclasts and osteoblasts. Osteoclasts excavate tunnels into the compact bone. Osteoblasts refill the holes. They start with the deposition of a thin layer of cement on the excavated surface. Layers of lamellar bone follow the cement deposition. If the tunnels are nearly filled, the process stops. The narrow channel left at the centre contains a blood vessel. In cancellous bone, osteoclasts remove the bone from the surface, while osteoblasts deposit bone on the resorbed surface [6,7]. The lamellar bone deposited by osteoblast contains mineralised collagen fibrils [8]. Weiner and Wagner [6] subdivide the hierarchical structure into seven different levels. On the levels of micro-and nano-structure compact and trabecular bone consist of the same material. At the ultra structural level, fibres of collagen, a soft-polymeric helix, and crystals of hydroxyapatite, a hard brittle mineral material based on calcium, can be found [9]. With ageing the osteoblasts are unable to rebuild bone as quickly as the osteoclasts resorb it. Therefore, the porosity of the bone increases [10].

Fracture and repair of bone influence tissue organisation at the macro, the micro and the nano scale [11,8]. Yeni et al. showed the correlation between fracture toughness and porosity of compact bone, as well as between fracture toughness and osteon density [12]. Other experimental studies showed age related changes in stiffness, strength and toughness of cortical bone [13]. Microcracks occur in bone during normal daily activities. These cracks can be influenced by the micro structure, including the cement lines and the osteons. In some cases microcracks can lead to fracture of bones [14,15].

Fracture toughness is a measure of bone quality. Fracture toughness on bone varies with orientations [16–18]. A number of studies try to have attempted to identify a fracture mechanics-based parameter that is more closely related to bone fracture. Yan et al. state that the J-integral method is a better technique to assess bone's toughness [19]. Vashishth et al. use the *R*-curve to characterise fracture toughness [20]. Zimmermann et al. showed that it is also important to report fracture toughness under mixed mode loading conditions (tensile and shear loading) [21].

A better understanding of the different aspects of bone fracture could help the development of better prevention therapies and treatment strategies [22]. One method to determine the influence of a single bone quality parameter on bone fracture is the Finite Element (FE) Analysis. FE provides an opportunity to change single parameters including the geometry or material properties.

One FE-method to simulate fracture and crack growth in bone is the cohesive FE analysis of the crack area [23–27]. Another approach is the Method of extended Finite Elements (xFEMs).

The implementation of (xFEM) in commercial FE software offers new possibilities to study crack growth and crack resistance. In contrast to cohesive elements, xFEM does not require the user to pre-define the crack path. Abdel-Wahab et al. used xFEM to simulate crack propagation within 2D models of compact bone. In their study, using light microscope

pictures, 2D models of the osteons within a specimen were generated. Different material parameters for bone matrix, cement line and osteons were chosen to determine the influence of cement lines on the crack propagation [28]. Budyn et al. [29] calculated multiple cracks within a bone sample using xFEM.

In this study we combine xFEM approach with microCT imaging technology to determine the influence of porosity on bone toughness.

2. Materials and methods

xFEM within ABAQUS 6.10–3 was used to study the influence of the age related changes in bone porosity on the fracture toughness of compact bone. MicroCT data from previously tested compact tension specimens from two human male tibiae, donors age 19 and 81 years old, were used to generate the Finite Element meshes. The crack propagation directions of the samples were oriented parallel to the osteonal direction. The samples were scanned using a vivaCT 40 from Scanco Medical ASG with a resolution of 21 μm (see Fig. 1).

2.1. Mesh generation

To simulate crack propagation with xFEM it is necessary to generate smooth surfaces. Voxel based FE meshes have sharp corners on the surfaces, therefore it was not possible to use them for the simulations. Mimics[®] by Materialise was used to generate FE meshes from the microCT data. To include smaller cavities, a lower threshold of 1300 was utilised. The software uses triangles for surface meshes and tetrahedrons for volume meshes. Every third slice of the microCT scans was used for the mesh generation. Due to the resolution and the limitations of the surface triangles it was not possible to take very small cavities into account. To reduce the number of elements, the bottom and the top areas were meshed with large elements and the cavities in these areas were neglected.

Modelling of cavities without any connection to the surface was an additional challenge. Mimics models such cavities as sub-volumes. However sub-volumes cannot be taken into account for the main mesh. To address this issue we divided the middle of the sample as overlapping slices. Each slice had a thickness of five layers. Two neighbouring slices had an overlap of two layers. Starting at the centre, the neighbouring slices were subtracted from each other by Boolean operations. After creating valid surface meshes the slices were separated again. Volume meshes were generated for each slice using linear tetrahedrons of the type C3D4. All parts were imported into ABAQUS CAE and merged together with Boolean operations.

2.2. Boundary conditions

For realistic simulations of fracture tests, the samples were loaded via pins. These pins were simulated as rigid bodies and restricted to move only in x -direction (Fig. 2). Rotation was prohibited. Contact between samples and pins was simulated as a hard contact in normal direction (and frictionless in tangential direction). Over the whole thickness of each sample a small area, opposite to the crack tip, was fixed. To load the samples reference points of the pins were moved apart.

2.3. Mechanical properties

During the ageing process, both the mechanical properties and the porosity of bone change. The aim of this study is to determine the influence of the changes related to porosity. Therefore, both models were simulated with the same material properties. In order to determine the effect of porosity on fracture properties, both samples were modelled with a linear elastic orthotropic material. The set of orthotropic material properties was taken from Ural et al. [24] (Table 1).

To determine the influence of the simplified geometry, crack propagation toughness was calculated using one set of material properties. Each model was then divided into three parts. The material properties for the middle part were assigned as before and the effective material properties were calculated by homogenisation techniques using representative volume elements [30] for the outer parts. These different areas are shown in Fig. 2. The light grey elements in Fig. 2 represent the area with the original material properties. The darker areas in Fig. 2 have homogenised material parameters. For homogenisation, five cubes with an edge length of 1 mm were cut out of each sample randomly. The cubes were wrapped with a window. The wall thickness was 25% of the cubes edge length. The areas of the cavities within the cubes were also meshed (Fig. 3).

The material properties for the cubes were chosen based on the material properties used for the first simulations. The cavity areas were simulated with a Young's modulus of 1 N/mm² and a Poisson ratio of 0.1. Each cube was simulated under six different loading conditions. At first, tension tests for the *x*-, *y*- and *z*-direction were performed. Additionally shear tests for three different directions were simulated. On the basis of these results, the effective material properties for the whole system consisting of the cube, the window and the cavity areas were calculated. In the next step the new material parameters were assigned to the window. This procedure was repeated until no more changes in the parameters occurred.

The effective material properties of the five cubes per donor were then averaged and assigned to the areas with the simplified geometry.

2.4. Fracture toughness

Crack propagation was only allowed in the middle part of the samples to reduce the calculation time. Similar to the experiments where a small cut is made with a razor blade at the crack tip to ensure crack initiation, a small plate was introduced in the middle of the crack tip and used as the crack initiation site (Fig. 1).

Similar to a previous study by Ural and Vashishth [26], the quadratic nominal stress criterion with a nominal stress of 57 MPa for σ_n^o , σ_s^o and σ_t^o was used for this study.

$$f = \left(\frac{\sigma_n}{\sigma_n^o} \right)^2 + \left(\frac{\sigma_s}{\sigma_s^o} \right)^2 + \left(\frac{\sigma_t}{\sigma_t^o} \right)^2 \quad (1)$$

Because of the crack criterion, the crack propagation direction was defined parallel to the 1-direction, the displacement at failure was considered to be 3.94%.

The crack growth resistance was calculated by the following equations [31]:

$$k_r = \frac{PY_2}{B\sqrt{W}}, \quad (2)$$

$$Y_2 = \frac{2 + a/W}{\sqrt{(1 - a/W)^3 * (0.866 + 4.64a/W - 13.36(a/W)^2 + 14.72(a/W)^3 - 5.6(a/W)^4)}}, \quad (3)$$

where P is the load; a is the length of the crack from the load line to the crack tip; W is the width of the specimen from the load line and B is the thickness. The load and the crack length were taken from the FE simulations and used to calculate K_r . K_r is plotted as a function of the square root of crack extension (R -curve). Linear regression was used to obtain the R -curve slope. Similar to experimental procedures the R -curve slope was calculated for crack extensions less than 2.25 mm. Crack length was determined as the distance between the load line to the crack tip on the surface of the specimen.

3. Results

The results for the mesh generation for the middle slice are shown in Fig. 4. The meshes show the higher porosity of the 81 year old donor.

The orthotropic material stiffness matrix, calculated from the engineered material properties from Table 1, according to the ABA-QUS manual [32] is:

$$\underline{\underline{C}}_{bone} = \begin{bmatrix} 20.5 & 3.7 & 3.1 & 0 & 0 & 0 \\ & 9.5 & 2.1 & 0 & 0 & 0 \\ & & 7.7 & 0 & 0 & 0 \\ & & & 4.9 & 0 & 0 \\ sym. & & & & 3.6 & 0 \\ & & & & & 2.4 \end{bmatrix} GPa.$$

The effective anisotropic material properties after the homogenisation for the 19 year old donor are:

$$\underline{\underline{C}}_{19effective} = \begin{bmatrix} 19.6 & 3.3 & 2.9 & 0.02 & 0.03 & -0.04 \\ & 8.6 & 1.9 & 0.008 & -0.001 & -0.07 \\ & & 7.2 & 0.01 & 0.005 & -0.07 \\ & & & 4.6 & -0.03 & 0.007 \\ sym. & & & & 3.4 & 0.002 \\ & & & & & 2.3 \end{bmatrix} GPa.$$

And for the 81 year old donor they are:

$$\underline{C}_{81effective} = \begin{bmatrix} 16.7 & 2.3 & 2.1 & -0.3 & 0.1 & 0.01 \\ & 6.3 & 1.4 & -0.02 & 0.002 & 0.04 \\ & & 5.4 & 0.02 & 0.03 & 0.03 \\ & & & 3.6 & 0.01 & 0.01 \\ sym. & & & & 2.8 & 0.01 \\ & & & & & 1.8 \end{bmatrix} GPa.$$

Fig. 5 shows the crack in the sample obtained from the 19 year old donor. The crack has different length on both sides of the sample.

The crack growth resistance versus the square of the crack length curve obtained from the simulation is shown in Fig. 6. The slopes of the linear regression line of the different simulations are presented in Table 2. Fig. 7 shows the loads which were necessary to crack the specimens.

A comparison of the slopes of the R -curves obtained by assuming one set of material properties for the whole model and the calculations with a homogenised material properties in the areas with the simplified geometry shows, that they are nearly similar in more porous 81-year sample. In the case of the 19 year old donor sample with the homogenised material properties, the Fe-estimated slope is 86.9% of the slope obtained by assuming only a single set of material properties.

If the changes in the material properties obtained by neglecting the cavities are not taken into account, the slope of the R -curve of the 81 year old donor is 69.7% of the slope of the 19 year old donor. In the case of the effective material properties the slope of the 81 year old donor versus the 19 year old donor is 79.9%.

4. Discussion

The simulation results show that xFEM can capture the fracture behaviour of compact bone successfully without a predefined crack path. In particular the quadratic nominal stress criteria results in a straight crack. This crack criterion allows crack growth to occur only in one direction. The straight path allows to compare the results of this study with previous results obtained using cohesive zone models [26]. The K_r value in the xFEM simulations obtained using quadratic crack criteria is less than in values reported in the literature [26]. The decrease of the fracture propagation toughness without the effective material properties for the simplified geometry is within the reported range.

We found that the porosity had significant influence on the fracture toughness of bone. The load necessary to induce a crack growth of 2.25 mm in the 19 year old sample was nearly twice the load needed in the case of the 81 year old sample. Thus samples with a high porosity can crack without large deformations outside the crack area. Relatively high forces are necessary for the same crack propagation in samples with a low porosity and these forces lead to deformations outside the crack area.

The comparison of R -curve slopes, obtained using one set of material parameters versus effective material properties obtained via the homogenisation process, allows us to

determine the effect of inherent variation of material properties in high versus low porosity samples. In comparison to the standard set, the effective material properties showed a decrease of 5–10% in the young donor, and a 20–35% decrease in the older donor. Inclusion of these decrease into the xFEM model of the younger and older donors resulted in 13% and 0.3% change in R -curve slopes, respectively. These results suggest that age-related loss of fracture toughness could be partially explained by loss of heterogeneity in material properties with age.

Because of the time consuming generation and iteration, only five RVs were used to determine whether effective material parameters for the simplified areas have an influence on the simulated fracture toughness. To get more realistic effective material properties we recommend the use of more RVs

5. Conclusion

In this study an xFEM approach was developed to predict fracture toughness of cortical bone from microCT images. Application of this approach to young and old human cortical bone demonstrated that age-related loss on bone toughness results from increased porosity and loss in heterogeneity of material properties.

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References

- [1]. Cummings SR, Melton LJ, III, Lancet 359 (2002) 1761–1767. [PubMed: 12049882]
- [2]. Hogan HA, J. Biomech 25 (1992) 549–556. [PubMed: 1592860]
- [3]. Wang XD, Masilamani NS, Mabrey JD, Alder ME, Agrawal CM, Bone 23 (1998) 67–72. [PubMed: 9662132]
- [4]. Yeni YN, Brown CU, Norman TL, Bone 22 (1998) 79–84. [PubMed: 9437517]
- [5]. Wolff J, Das Gesetz der Transformation der Knochen, Hirschwald, 1892.
- [6]. Weiner S, Wagner HD, Ann. Rev. Mater. Sci 28 (1998) 271–298.
- [7]. Robling AG, Castillo AB, Turner CH, Ann. Rev. Biomed. Eng 8 (2006) 455–498. [PubMed: 16834564]
- [8]. Vashishth D, Int. J. Fatigue 29 (2007) 1024–1033. [PubMed: 18516216]
- [9]. Taylor D, Hazenberg JG, Lee C, Nat. mater 6 (2007) 263–268. [PubMed: 17401419]
- [10]. Chen H, Zhou X, Shoumura S, Emura S, Bunai Y, Osteoporos. Int 21 (2010) 627–636. [PubMed: 19543764]
- [11]. Taylor D, J. Mater. Sci 42 (2007) 8911–8918.
- [12]. Yeni YN, Brown CU, Wang Z, Norman TL, Bone 21 (1997) 453–459. [PubMed: 9356740]
- [13]. Zioupos P, Currey JD, Bone 22 (1998) 57–66. [PubMed: 9437514]
- [14]. O'Brien FJ, Taylor D, Lee TC, J. Biomech 36 (2003) 973–980. [PubMed: 12757806]
- [15]. O'Brien FJ, Taylor D, Lee TC, J. Orthop. Res 23 (2005) 475–480. [PubMed: 15734265]
- [16]. Feng Z, Rho J, Han S, Ziv I, Mater. Sci. Eng. C 11 (2000) 41–46.
- [17]. Behiri JC, Bonfield W, J. Biomech 22 (1989) 863–872. [PubMed: 2613722]
- [18]. Peterlik H, Roschger P, Klaushofer K, Fratzl P, Nat. Mater 5 (2006) 52–55. [PubMed: 16341218]

- [19]. Yan J, Mecholsky JJ, Jr., Clifton KB, Bone 40 (2007) 479–484. [PubMed: 17030159]
- [20]. Vashishth D, Behiri JC, Bonfield W, J. Biomech 30 (1997) 763–769. [PubMed: 9239560]
- [21]. Zimmermann EA, Launey ME, Barth HD, Ritchie RO, Biomater 30 (2009) 5877–5884.
- [22]. Ferreira F, Vaz MA, Simões JA, Mater. Charact 57 (2006) 71–79.
- [23]. Cox BN, Yang Q, Eng. Fract. Mech 74 (2007) 1079–1092.
- [24]. Ural A, Vashishth D, J. Biomech 39 (2006) 2974–2982. [PubMed: 16375909]
- [25]. Ural A, Vashishth D, J. Biomech 40 (2007) 1606–1614. [PubMed: 17054962]
- [26]. Ural A, Vashishth D, J. Biomech. Eng 129 (2007) 625–631. [PubMed: 17887887]
- [27]. Buchanan D, Ural A, J. Biomech. Eng 132(8) (2010). 10.1115/1.4001681.
- [28]. Abdel-Wahab AA, Maligno AR, Silberschmidt VV, Comput. Mater. Sci (2011), 10.1016/j.commatsci.2011.01.021.
- [29]. budyn E, Hoc T, Jonvaux J, Comput. Mech 42 (2008) 579–591.
- [30]. Hain M, Wriggers P, Comput. Mech 42 (2008) 197–212.
- [31]. Vashishth D, J. Biomech 37 (2004) 943–946. [PubMed: 15111083]
- [32]. ABAQUS User's Manual; Abaqus/CAE User's Manual. Abaqus Online Documentation: Version 6.10; Dassault Systèmes.

Fig. 1. Slices of fracture toughness samples of (a) 19 year old donor, and (b) 81 year old donor; scanned with a vivaCT 40 from Scanco Medical ASG with a resolution of 21 μm . The samples are approximately 17 mm $\times$ 3 mm $\times$ 16.8 mm (W $\times$ L $\times$ H).

Fig. 2. FE model of the 81 year old donor sample. Different grey values show the different materials. The arrows show the direction of the movement.

Fig. 3.
Embedded reference volume with an edge length of 1 mm. The wall thickness is 0.25 mm.
The cavities are filled with a different material.

Fig. 4. Meshed middle slice of the (a) 19 year old donor, and (b) 81 year old donor.

Fig. 5.
With xFEM calculated crack in the sample of the 19 year old donor.

Fig. 6. Results for K_r [N/mm^{3/2}] for the samples of the (a) 19 year old donor, and (b) 81 year old donor versus square from a [mm^{1/2}]; with a linear regression line.

Fig. 7.
Load P [N] versus the square of the crack length [$\text{mm}^{1/2}$].

Table 1

Orthotropic material properties of human tibia used in the simulations [Knets].

$E_1 = 18.4 \text{ GPa}$	$G_{12} = 4.91 \text{ GPa}$	$\nu_{12} = 0.31$
$E_2 = 8.51 \text{ GPa}$	$G_{13} = 3.56 \text{ GPa}$	$\nu_{13} = 0.32$
$E_3 = 6.91 \text{ GPa}$	$G_{23} = 2.41 \text{ GPa}$	$\nu_{23} = 0.23$

Table 2

R-curve slope of the crack simulations.

	One material	Effective material
19 year old donor	182.24	158.28
81 year old donor	127.07	126.57