# Relationships Among Microstructural Features and Crack Propagation in Osteonal Bone Identified Using Finite Element Analysis

E.K. Oneida,[1] M.C.H van der Meulen,[1] A.R. Ingraffea[1]
[1] *Cornell University, Ithaca, USA*
E-mail: *eko4@cornell.edu*

Abstract

At the microstructural length-scale, osteonal bone is highly heterogeneous, and experimental observations have demonstrated that relationships exist among microstructural features, such as cement lines, and crack propagation. An improved understanding of the roles played by lamellar layers, cement lines, and Haversian canals during damaging processes can be obtained through computational modeling. In this study, these relationships are explored by first developing complex, representative, finite element models of microstructural features contained in osteonal cortical bone and subjecting them to simulated tests. Cracks are then incorporated into the models by explicitly modeling geometric discontinuities, and parameterization studies are performed to explore how variations in microstructural feature properties promote or inhibit crack propagation. Overall, this study allows for an understanding of how crack propagation behavior can be directly influenced by specific material and microstructural properties.

## 1. Introduction

In a single year, more than 2 million people in the U.S. aged 50 and older will experience a skeletal fracture [1], which leads to increased mortality [2], and financial costs of more than $17 billion [1]. Bone is a complex, hierarchical material [3], and by understanding the behavior of *in vivo* damage at the microstructural length-scale, better treatments for preventing large-scale fracture can be developed.

Bone is a heterogeneous living material that takes on different forms depending on its anatomical location. Osteonal cortical bone is a dense tissue that is composed of longitudinal cylindrical osteonal structures. In newer bone, primary osteons are present. Through remodeling, the primary osteons are replaced by new structures known as secondary osteons (200-250 μm in diameter [4]), which are composed of lamellar layers (3-7 μm thick) [5] concentrically arranged around a 50-90 µm (diameter) Haversian canal [5]. Unlike primary osteons, secondary osteons are surrounded by a thin interface (1-5 µm thick) known as a cement line [5]. The tissue surrounding the secondary osteons can contain older primary bone and remnants of osteons and is referred to as interstitial bone.

Material properties vary considerably across this heterogeneous microstructure. Nanoindentation techniques have identified interstitial bone as being stiffer than intra-osteonal tissue [6]. Significant modulus differences also exist between different lamellae in osteons [6]. The cement line properties are not well understood, but they are known to differ compositionally from adjacent tissue [7].

Microcracks are present throughout bone, with the majority located in the older interstitial bone [8]. Geometrical features and material properties affect crack propagation behavior, such as when a crack encounters a secondary osteon and either arrests at, deflects around, or penetrates it depending on the length of the crack [9]. Understanding how each microstructural feature and its associated properties either inhibit or promote crack propagation and contribute to macroscopic behavior would be beneficial to human health.

Finite element modeling, coupled with experimental data, can be used to explore the connections between variations in geometry and material properties and whether microcracks will evolve to the point of causing large-scale failure. Developing three-dimensional finite element model geometries with locally varying material properties, and identifying and implementing accurate crack growth criteria, will allow a thorough study of the relationships at play during damage propagation. Realistic experimental loading scenarios could be simulated at the macroscale, and microdamage evolution could be predicted at the microscale.

The overall objective of the present study is to explore the relationships among geometrical features and their associated material properties and crack propagation through the use of realistic and simplified, three-dimensional finite element models of the microstructure of osteonal cortical bone. In the future, crack propagation experiments and detailed microstructural characterizations will be conducted to provide data for model development and the evaluation of different crack growth criteria. Using the most appropriate crack growing criteria, parameter studies exploring the full roles of each microstructural feature and the effects that variations in each feature’s material properties or geometry has on microcrack propagation will be evaluated. The initial phase of this project will be presented in this paper, as will a description of the work that is anticipated to be completed prior to July 2009.

## 2. Methods

To date, a microstructural geometry model creation code that assigns region-specific material properties has been created. Additionally, currently available crack modeling tools were evaluated to illustrate the basic crack modeling methodology that will be used in the future.

### *2.1 Geometry Model Creation*

The primary objective of this first phase of the overall research project was the development of a finite element model geometry creating capability that allows for the semi-automatic construction of a simplified or realistic representative model. Two geometry building approaches have been taken thus far, both involving the development of MATLAB [10] code to generate a Python [11]-language script, which is then used by a finite element program, Abaqus [12], to create the desired geometry model.

The first model development approach involves the creation of a simplified representative geometry. Cylindrical regions are used to represent osteons, intra-osteon lamellar layers, and cement lines. Many different geometric models can be easily created using this code. Throughout the model, each osteon can be created with unique (or the same) geometric values for the outer radius, canal radius, and lamellae and cement line thicknesses. The locations of each osteon can be selected. Different isotropic, linear elastic material property values can also be assigned to each region, including the background interstitial bone. An additional model generation option involves the specification of the outer osteon radius, Haversian canal radius, porosity, percent area of the microstructure covered by secondary osteons, lamellar and cement line thicknesses, and material properties. A model satisfying all of the input parameters can then be created.

A second model development approach involves the creation of a finite element geometry model that contains features created from images of bone. This procedure requires the user to trace visible geometry and specify elastic material properties for each region. The traced boundaries are extruded to create a specimen of a length specified by the user.

After entering the geometric and material property values, a script to generate the corresponding geometry model in Abaqus can be easily generated. The complete process is shown in Figure 1.

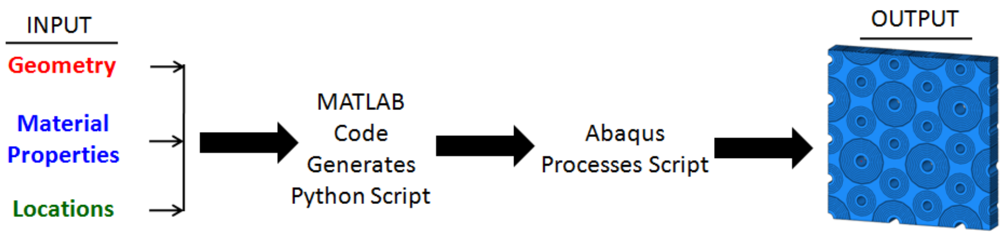


Figure 1. Illustration of model creation procedure

After developing a model that captures the desired geometric features and material properties, a target volume can be carved from the base model using Abaqus tools. This volume can have dimensions matching an experimental specimen cut from real bone. A quadratic, tetrahedral mesh can be easily created and boundary conditions simulating an experimental set-up can then be applied.

*2.2 Modeling Crack Propagation*

After a representative finite element model is completely developed, it is then possible to explore crack propagation through the microstructure. To study crack evolution, cracks are explicitly represented as geometric discontinuities in the finite element model using a program developed in-house—FRANC3D/NG [13]. Cracks can be grown step-by-step according to rules included in the software package or by using user-supplied criteria. For each step, after the new crack geometry is inserted into the model, automatic re-meshing occurs.

The developed tools will soon be used to perform a complete parameter study examining the specific effects that each microstructural component might have on crack propagation behavior. Different material models for bone and different crack growth rules will be explored. Initially, small bone models containing cylindrical representations will be studied. An example of a created model is described below.

*2.3 Example Study*

A geometry model of osteonal bone containing explicitly represented microstructural level information was created. The first step involved the generation of the model building script for Abaqus. From the literature, values were calculated for the average porosity (5.5% [14]), Haversian canal diameter (58.8 μm [15]), percent of the area covered by secondary osteons (41.0 % [14]), secondary osteon modulus (21.6 GPa [14]), and interstitial elastic modulus (24.1 GPa [14]) for seven, male, human mid-diaphysis femoral bone specimens (aged 40 to 75). An average secondary osteon diameter for 23 human mid-diaphysis femoral bone specimens aged 58-88 was found to be 246.8 μm [16]. Poisson's ratio was assumed to be 0.3. The secondary osteons in the model were assigned the identified modulus, and the remainder of the solid tissue was assigned the interstitial modulus. For the present example, the cement lines were treated as part of the secondary osteons and assigned the same material properties. A cylinder with a diameter of 1 mm and a length of 0.125 mm was removed from the base material for study, with the center of the cylinder aligned with the center of an osteon.

Using Abaqus, one-quarter (containing 101,205 quadratic, tetrahedral elements) of the final geometry model was used for subsequent study. Symmetry plane boundary conditions were used on two faces, one side was fixed, and the final side was displaced by 0.01 mm (Figure 2a). To explore the currently existing crack insertion and growth capabilities of FRANC3D/NG, a penny shaped crack with a radius of 0.02 mm was inserted into the model (Figure 2b).

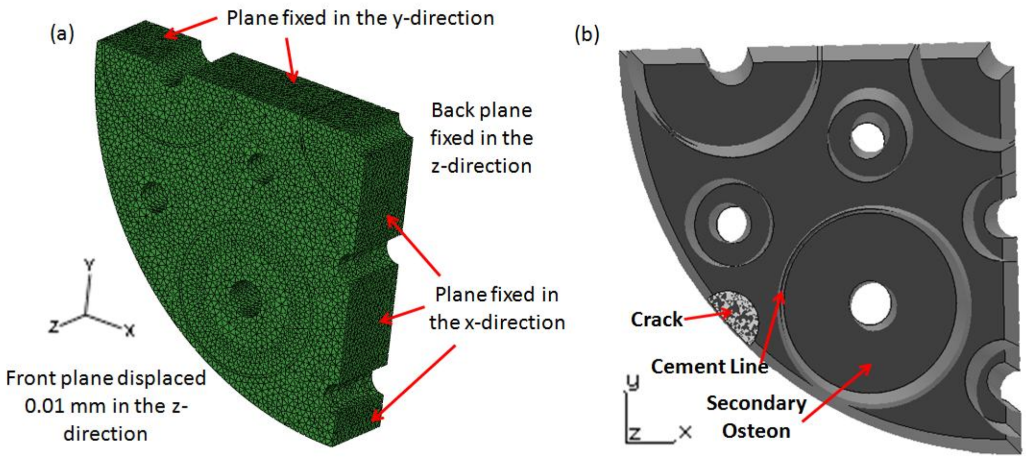


Figure 2. (a) Model with description of boundary conditions. (b) Model showing an inserted crack (image is depicting internal model conditions)

A finite element analysis was performed on a desktop computer (using Abaqus), and stress intensity factors were calculated at the crack front by using capabilities in FRANC3D/NG. All points along the crack front were assumed to grow, and the direction of crack growth was determined by FRANC3D/NG according to the maximum tensile stress criterion. A Paris-like rate equation (Eq. 1) was then used to predict the crack growth at each crack front point.

$$\Delta a_i = \Delta a_{mean}\left(\frac{K_i}{K_{mean}}\right)^n, \qquad \text{(Eq. 1)}$$

where $n$ was set equal to 2, $K_i$ represents the mode I stress intensity factor value at each of the different crack front points, $K_{mean}$ is the mean of the mode I stress intensity factors, $\Delta a_{mean}$ represents the mean crack growth increment that was chosen for each propagation step, and $\Delta a_i$ corresponds to the growth increment for each crack front point.

The crack was propagated one step at a time. First, it was grown according to the values calculated using the power law (and in the direction determined by using the maximum tensile stress criterion), noting that for each step, a $\Delta a_{mean}$ value was chosen. Automatic re-meshing was then performed, followed by a new stress analysis. The crack growing process was then repeated. The crack was grown two times using a $\Delta a_{mean}$ value of 0.01 mm. The crack growth methodology used for this example serves to illustrate the basic framework of how crack propagation in different models could be performed during a parameter study, but it is not necessarily ideal for bone. Criteria controlling crack growth behavior still need to be evaluated at this time.

Experiments studying crack growth through the microstructure during three-point bend tests will be conducted in conjunction with the presented modeling study to gain additional information and data for developing improved models. Thorough characterizations of the microstructure will be performed, and the propagation behavior of cracks will be analyzed. This information will allow for realistic and simplified cylindrical three-point bend models to be developed and for different crack growth rules to be evaluated. The models will contain millions of degrees-of-freedom and will be analyzed using an in-house finite element program and a computer cluster with hundreds of processors.

## 3. Results

The developed code and methodology allowed for the quick creation of four different examples of microstructural models, Figure 3. Most of the Abaqus scripts were over 15,000 lines long, and each one was generated in less than 5 seconds using a Dell XPS 720 (Intel® Core™ 2 Quad CPU, 2.67 GHz). Processing each script in Abaqus took fewer than 5 minutes.

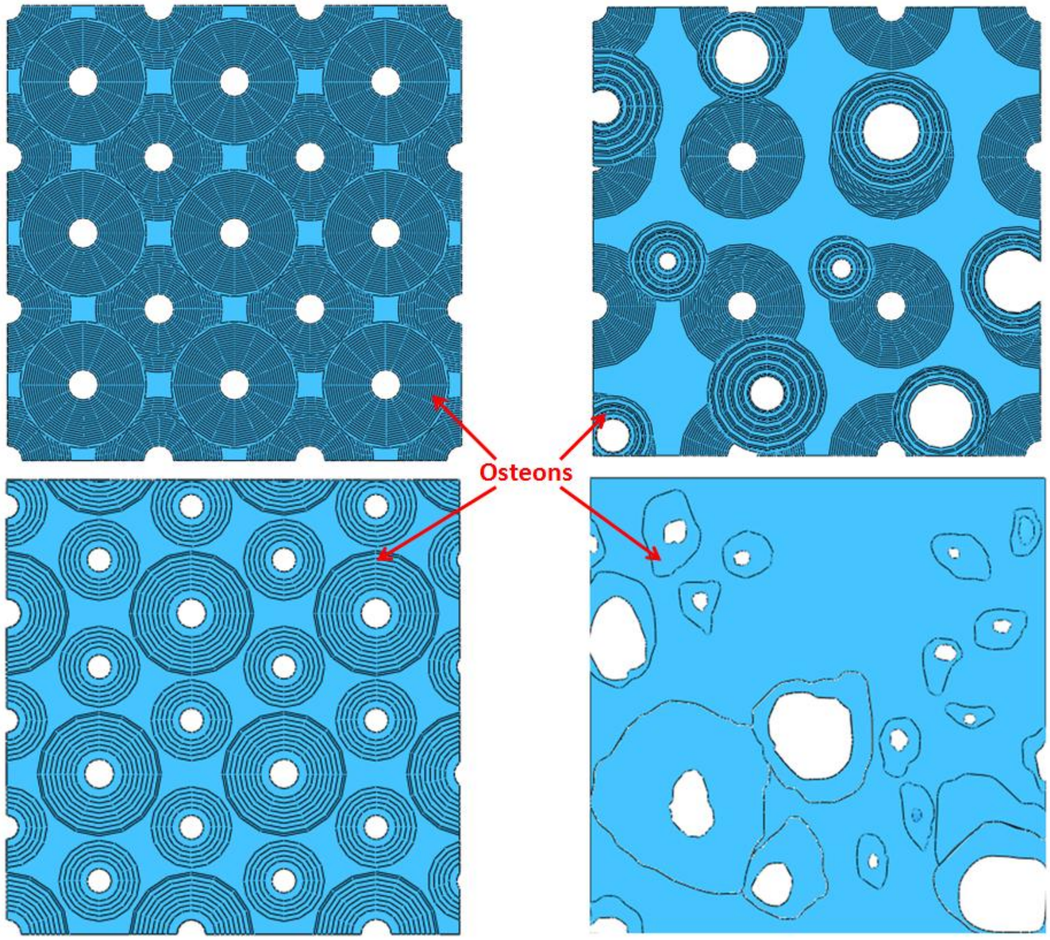


Figure 3. Four different geometry models (extruded to a depth of 0.125 mm) created using the developed code and Abaqus. The code allowed for desired material properties to be assigned to each region. Each model shown measures 0.9 mm across.

A crack was successfully inserted into and subsequently propagated through part of the example model, Figure 4.

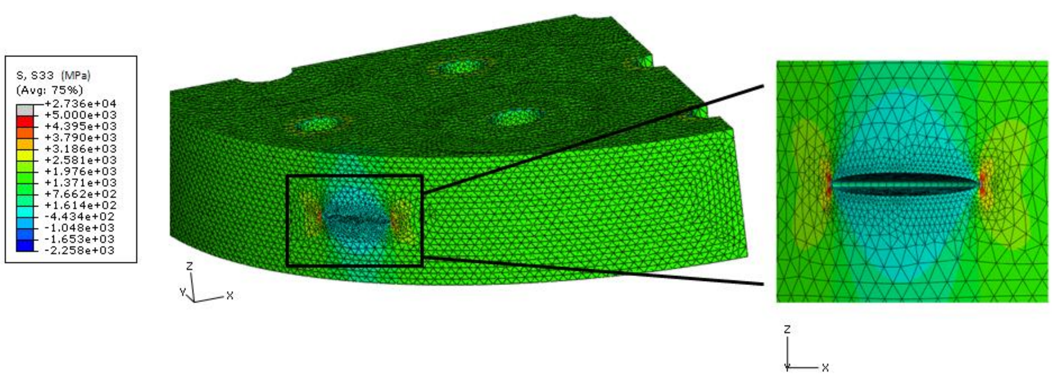

Figure 4. Results from a stress analysis performed on the example microstructural model with the propagated crack (height of quarter cylinder is 0.125 mm)

## 4. Discussion

An efficient model generation code and methodology that allows for the creation of simplified cylindrical representations, as well as more realistic models, was developed. The ease of generating the geometry will allow for the quick creation of many different models during a future comprehensive parameter study.

The ability of the available software to insert and grow cracks according to prescribed rules was illustrated, and an example study following the overall methodology presented in this paper to explore the different roles played by geometric features (and their associated material properties) during crack growth was shown (Figure 4).

In the future, experimental images and data will be used to create realistic models and their corresponding simplified cylindrical models. Analyses will be performed for both types of models and the results will be studied to verify the sufficiency of the simplified models for conducting a parameter study. Additionally, possible criteria for crack growth in bone at the microstructural length-scale need to be evaluated. Experimental studies, coupled with realistic models, should provide information that will be useful for analyzing different criteria. At a larger length-scale, cohesive-zone modeling works well for capturing the effects of crack-bridging toughening mechanisms [17]. This type of model may be necessary for simulating microcrack growth and will be studied if other criteria prove unsatisfactory.

After evaluating geometry model quality and crack growth criteria, a parameter study looking at damage propagation in models with different material properties and geometrical features will be performed. Models can be created to explore variations in the geometry of the osteons, lamellae, cement lines, and other porous spaces, as well as variations in the material properties observed in each of the different regions. Additional material models could also be incorporated into the code for an even deeper investigation. Overall, this study will allow for an assessment of how each of the different microstructural components and properties work together to inhibit or promote crack propagation.

## 5. Conclusions

Detailed finite element modeling can allow for an improved understanding of the relationships among crack propagation behavior and local geometric features and material properties to be obtained. The literature contains characterizations of microstructural features and local properties and details of experimental observations of microcrack propagation at the microstructural length-scale, but only a limited amount of finite element modeling at this length-scale has been performed. This paper illustrates the feasibility of modeling damage propagation at the microstructural length-scale, and it is anticipated that a thorough parameter study will be completed by July 2009.

## 6. Acknowledgements

We are grateful for support from a Ross-Tetelman Fellowship, the Cornell Center for Materials Research (NSF DMR 0089992), and NIH Grant AR 053571.

7. References

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