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# Combining specimen-specific finite-element models and optimization in cortical-bone material characterization improves prediction accuracy in three-point bending tests

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## ABSTRACT

Although the beam theory is widely used for calculating material parameters in three-point bending test, it cannot accurately describe the biomechanical properties of specimens after the yield. Hence, we propose a finite element (FE) based optimization method to obtain accurate bone material parameters from three-point bending test. We tested 80 machined bovine cortical bone specimens at both longitudinal and transverse directions using three-point bending. We then adopted the beam theory and the FE-based optimization method combined with specimen-specific FE models to derive the material parameters of cortical bone. We compared data obtained using these two methods and further evaluated two groups of parameters with three-point bending simulations. Our data indicated that the FE models with material properties from the FE-based optimization method showed best agreements with experimental data for the entire force-displacement responses, including the post-yield region. Using the beam theory, the yield stresses derived from 0.0058% strain offset for the longitudinal specimen and 0.0052% strain offset for the transverse specimen are closer to those derived from the FE-based optimization method, compared to yield stresses calculated without strain offset. In brief, we conclude that the optimization FE method is more appropriate than the traditional beam theory in identifying the material parameters of cortical bone for improving prediction accuracy in three-point bending mode. Given that the beam theory remains as a popular method because of its efficiency, we further provided correction functions to adjust parameters calculated from the beam theory for accurate FE simulation.

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## 1. Introduction

Bone is a complicated composite material that consists of 65% minerals (carbonated hydroxyapatite), 25% proteins (mostly collagen-I, with a small amount of non-collagenous proteins) and 10% water (Manilay et al., 2013). Due to this composition, bone exhibits viscoelasticity, anisotropy and inhomogeneity (Huang et al., 2010). However, accurate identification of each of these material parameters of bone remains technically challenging. The constitutive model of elastoplastic material is simple and can simulate the biomechanical response of bone well, and thus, it is widely used in skeleton finite element (FE) models (Klein et al., 2017; Untaroiu et al., 2005).

Due to the relatively low requirements in terms of the shape of the sample and minimal mechanical processing, three-point bending tests are widely used to characterize bone material and determine the biomechanical properties of long bones (Akhter et al., 2000; Kerrigan et al., 2003; Turner and Burr, 2001; Untaroiu, 2010). There are two ways to obtain material parameters based on a three-point bending test, classic beam theory (Albert et al., 2012; Cuppone et al., 2004; Goodyear and Aspden, 2012; Turner and Burr, 2001; Unger et al., 2010) and optimization methodology with specimen-specific FE models (Guan et al., 2011; Untaroiu et al., 2006; Zhang et al., 2016). Beam theory assumes bone exhibits linear elastic behavior, with perfect rectangular or cylindrical shape in uniform cross-section and is composed of homogeneous material (Cordey et al., 2000; Van Lenthe et al., 2008). Obviously, these assumptions may lead to inaccurate identification of material parameters of bone because of its non-linear properties. On the other hand, the optimization approach has been used to derive

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material parameters in relatively recent years (Guan et al., 2011; Hu et al., 2009; Krone and Schuster, 2006), which may generate accurate material properties due to its consideration of geometry, boundary condition, and dynamic effects (Hu et al., 2009). However, beam theory is still largely used due to its efficiency in solving simple mathematical equations to calculate material parameters. It is unclear how large of errors one can make in applying beam theory to obtain material parameters with three-point bending test data (Van Lenthe et al., 2008). If the error is small, beam theory remains a reasonable approach, given that the FE optimization method is computationally time consuming (Untaroiu and Lu, 2013). As such, beam theory can be found in many well-designed studies, which estimate the material properties of cortical bone of long bones (Albert et al., 2012; Kourtis et al., 2014; Ramezanzadehkoldeh and Skallerud, 2017; Unger et al., 2010).

However, Van Lenthe et al. (2008) found that the tissue modulus was underestimated by 29% when using beam theory in three-point bending tests, with geometry and size having strong effects on beam theory-derived tissue moduli (Van Lenthe et al., 2008). Furthermore, Guan et al. (2011) reported lower elastic moduli obtained by beam theory than that determined by the optimization approach (Guan et al., 2011). However, the bone specimens used in both studies were either whole bones (Van Lenthe et al., 2008) or skull bones (Guan et al., 2011). The whole bones were a structure with complex geometry and material properties, and the machined skull bones were not a perfect beam because of internal porosity, curvature, and change of thickness. Therefore, one may reason that beam theory may lead to erroneous results in whole bone and skull bone specimens, but it could provide accurate findings for cortical bone of the femur, which is denser and can be machined to a nearly perfect rectangular or cylindrical shape.

The aim of this study was to study determine the discrepancy caused by beam theory in three-point bending tests can be ignored when developing accurate FE models. Thus, we designed a study to assess the accuracy of using beam theory in three-point bending test. We compared the beam theory-derived material parameters of bovine femur bone with those determined by the specimen-specific FE-based optimization method. We then performed FE simulations with these two groups of material parameters and compared the model predictions to experimental measurements.

## 2. Materials and methods

### 2.1. Specimen preparation

Ten fresh male bovine femur bones (approximately 24 months old) were collected from a local slaughterhouse. To ensure there were no bones with diseases or damaged, a CT scan (Philips Brilliance 64 CT Scanner, Philips Medical, Cleveland, Ohio) was performed. Cortical bone has anisotropic or transversely isotropic properties (Martin et al., 2015; Novitskaya et al., 2011), as such previous research prepared axial and transverse specimens to study cortical bone anisotropy (Li et al., 2013; Ritchie et al., 2005; Sanborn et al., 2016). Therefore, we collected 40 specimens along the longitudinal direction and 40 specimens along the transverse direction from ten bones. We cut the mid-diaphysis of the fresh femur bones into two cross-sectional segments with a junior hacksaw (Fig. 1). Then, we randomly obtained four rectangular specimens along the longitudinal direction of bone from one of the two segments, and we obtained four rectangular specimens along the transverse direction randomly from the other segment. The dimensions were targeted as 12 mm × 2 mm × 0.5 mm for all 80 specimens. All specimens were under constant irrigation with 0.9% saline solution during cutting and were frozen at −20° (Saffar et al., 2009). Before testing, all specimens were thawed in

a 0.9% saline solution at room temperature for 2 h (Granke et al., 2014; Linde and Sorensen, 1993). All mechanical tests were conducted within 3 days of harvesting the bovine femur cortical bone specimens.

### 2.2. Mechanical test

Detailed dimensions of each specimen were obtained using a digital caliper with 0.02 mm accuracy immediately prior to mechanical testing (Zhang et al., 2016). The average lengths, widths, and thicknesses were calculated by averaging the three corresponding measured values. The destructive three-point bending testing was conducted at room temperature with a material testing machine (INSTRON 5985, Instron Corp., Canton, MA) (Fig. 2(a)). The distance between the two supports (1 mm diameter steel cylinders) was set at 10 mm, giving a span/depth aspect ratio of 20, to ensure that the impact of shear stress on the bending deformation was minimal (Turner and Burr, 1993). Specimens were loaded by a 1-mm-diameter steel cylinder with a constant speed of 0.02 mm/s. The bending force-time curves were recorded by a load cell with a capacity of 45 N (WMC-10-38, Interface Inc., Scottsdale, AZ). The displacement sensor of the INSTRON system was used to obtain the displacement-time curves at the loading point. The sampling frequency for the force and displacement data was set as 250 Hz throughout the test.

### 2.3. Identification of material parameters using beam theory

Beam theory (Eqs. (1) and (2)) was used to derive the stress-strain curves from the force-displacement curves produced in the three-point bending tests (Albert et al., 2012; Turner and Burr, 2001). Using 25% of the ultimate stress as the window width (Linde and Ivan, 1987), the stress-strain curve was fitted using a straight line within the window width. The maximum slope of the line was found by moving the window, which was defined as the Young's modulus of the specimen ( $E_{\text{Beam}}$ ). The point of zero strain was defined as the point where the straight line of stress-strain curve corresponding to Young's modulus crossed the zero-stress abscissa (Hvid and Jensen, 1984; Hvid et al., 1985). Strain offset method (0.2%) (Albert et al., 2012; Bayraktar et al., 2004a; Kotha and Guzelsu, 2003; Ohman et al., 2008) was used to obtain the yield stress ( $\text{SIGY}_{\text{Beam}}$ ). Effective failure strain ( $\text{FS}_{\text{Beam}}$ ) was assumed as effective plastic strain at failure. The tangent modulus ( $\text{ETAN}_{\text{Beam}}$ ) was 5% of Young's modulus (Bayraktar et al., 2004a; Ramezanzadehkoldeh and Skallerud, 2017; Yang et al., 2010). These four parameters were automatically calculated by the in-house codes developed using Matlab (Version R2017a, The MathWorks, MA, USA).

$$\sigma = \frac{3FL}{2WT^2} \quad (1)$$

$$\varepsilon = \frac{6T\delta}{L^2} \quad (2)$$

where  $\sigma$  and  $\varepsilon$  are the stress and strain of the loading point, respectively;  $F$  is the loading force;  $L$  is the span of the two supports;  $W$  and  $T$  are the width and thickness of the specimen, respectively; and  $\delta$  is the displacement of the beam at the loading point.

### 2.4. Identification of material parameters using optimization method combined with specimen-specific FE models

A FE baseline model with dimensions of 12 mm × 2 mm × 0.5 mm was created, using the software HYPERMESH 12.0 (Altair Engineering, Troy, MI). The baseline model consisted of eight-layer elements in the thickness direction and was composed of

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