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Micromechanical Modeling of R-Curve Behaviors in Human Cortical Bone

Kwai S. Chan* and Daniel P. Nicoletta

Southwest Research Institute, 6220 Culebra Road, San Antonio, TX 78238

Abstract

The risk of bone fracture increases with age because of a variety of factors that include, among others, decreasing bone quantity and quality due to increasing porosity and crack density with age. Experimental evidence has indicated that changes in bone microstructure and trace mineralization with age can result in different crack-tip strain field and fracture response, leading to different fracture mechanisms and R-curve behaviors. In this paper, a micromechanical modeling approach is developed to predict the R-curve response of bone tissue by delineating fracture mechanisms that lead to microdamage and ligament bridging by incorporating the influence of increasing porosity and crack density with age. The effects of age on fracture of human femur cortical bone due to porosity (bone quantity) and bone quality (crack density) with age are then examined via the micromechanical model.

Keywords

age-induced embrittlement; microdamage; R-curve behavior; human femur; crack density; porosity; fracture risk

1. Introduction

The incidence of skeletal fractures in humans increases with age due to a variety of factors that include reduced bone mineral density, impaired balance and reflexes, changes in bone geometry, porosity, architecture, and mineral and organic phases, as well as damage accumulation in the form of microdamage zones or microcracks (Schaffler et al., 1995; Burr et al., 1997; Schaffler and Jepsen, 2000; Parsamian and Norman, 2001; Akkus et al., 2003; Jepsen, 2003; Diab et al., 2006). Experimental evidence suggests that bone mass alone cannot account for changes in the observed fracture risk and that measures of bone mass should be supplemented with measures of bone quality (Van der Meulen et al., 2004). Both porosity and microcrack density in human femoral cortical bone increase with age (Schaffler et al., 1995; Courtney et al., 1996; Norman and Wang, 1997; Zioupos and Currey, 1998; Zioupos et al., 1999; Zioupos, 2001a and b). Correlations of fracture properties of human femoral cortical bone with microcrack density (Zioupos and Currey, 1998; Zioupos et al., 1999) and age (Zioupos and Currey, 1998; Zioupos et al., 1999; Nyman et al., 2006; Wu and Vashishth, 2002; Nalla et al., 2004; Ritchie et al., 2005; Zimmermann et al., 2012) showed

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Corresponding author: Kwai S. Chan, Southwest Research Institute® Tel: 210-522-2053; Fax: 210-522-6965; kchan@swri.edu.

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that decreases in fracture toughness of cortical bone with increasing age may be attributed to, at least partly, the accumulation of submicron- sized microcracks during the aging process (Schaffler et al., 1995; Norman and Wang, 1997; Zioupos and Currey, 1998). The microcrack density in bone tissues appeared to increase more rapidly in elderly women than in elderly men at the same age (Schaffler et al., 1995).

Recent work has shown that cortical bone exhibits a resistance-curve (R-curve) fracture behavior that varies with age (Nalla et al., 2004; Chan et al., 2009). Both the initiation toughness and the initial slope of the R-curve decrease with increasing age (Wu and Vashishth; 2002; Nalla et al., 2004; Chan et al., 2009). The R-curve behaviors in cortical bone originates from crack deflection and bridging of crack surfaces by uncracked ligaments at several length scales (Nalla et al., 2004; Ritchie et al; 2005; Chan et al., 2009), ranging from bridging by osteons, lamella, and a nanoscaled non-fibrous organic glue material found between mineralized collagen fibrils (Fantner et al., 2005). Despite these recent advances, the role of the bone microstructure, which is comprised of Haversian, lamellar and interstitial bone tissue, and the corresponding porosity and in-situ microcrack density accumulated over daily activities in affecting the risk of bone fracture still cannot be fully predicted quantitatively, even though their effects are understood qualitatively. For example, the fracture mechanics parameter commonly utilized for fracture toughness characterization is the stress intensity factor, K , which is strictly applicable for linear-elastic materials with little or no porosity. Human cortical bone can contain greater than 30% porosity (McCalden et al., 1993; Wang and Ni, 2003; Chan et al., 2009; Nicolella et al., 2011) and some microcracks; the applicability of linear-elastic fracture mechanics to treat fracture in bone tissues has not been addressed fully. The presence of in-situ microcracks in aged bone tissues requires consideration of the effects of both distributed pores and microcracks on fracture resistance of cortical bone.

There are at least three approaches that have been proposed for estimating the effective modulus of a cracked solid (Budiansky and O'Connell; 1976; Benveniste, 1987; Kachanov, 1992, 1994; Hu et al., 1993; Huang et al., 1994; Feng, 2001; Feng et al., 2003). The simplest one is the dilute or non-interacting solution (Kachanov, 1992, 1994; Huang et al., 1994; Feng, 2001; Feng et al., 2003), which treats the effect of individual microcracks on the main crack by summing the shielding or antishielding contributions of individual microcracks in a cracked solid without considering the interactions among the microcracks. Crack-tip shielding occurs when a microcrack lowers the local stress intensity factor, while antishielding occurs when a microcrack enhances the local stress intensity factor of the main crack. In the self-consistent method (Budiansky and O'Connell, 1976), the effect of crack interaction is taken into account approximately by embedding each microcrack in an effective medium. The differential method is an incremental form of the self-consistent method (Huang et al., 1994). The effective modulus of a heterogeneous medium with inclusions was treated by Mori and Tanaka (1973). This model can be extended to porous solids by treating the pores as inclusions with a zero modulus. In the generalized self-consistent method (Huang, et al., 1994), for each inclusion the effect of interaction from other inclusion is treated approximately by embedding the inclusions in a finite matrix which, in turn, is embedded in a composite. Recent reviews of the various methods (Kachanov, 1992, 1994; Hu et al. 1993; Huang et al., 1994; Feng, 2001; Feng et al., 2003) indicate that non-interacting (dilute) solution remains valid over a wide range of microcrack density. In addition, the Mori-Tanaka method (1973) yields a solution that is identical to the dilute solution for non-interacting microcracks in a cracked solid (Benveniste, 1987). These reviews also indicate that in general, the elastic properties of a porous or cracked solid subjected to uniform remote loading can be solved by decomposing the problem into two simpler problems: (1) a homogeneous problem in which the matrix subjected to the same remote loading in the absence of any crack, and (2) one or more perturbed problems in

which only the crack or pore surfaces are subjected to pseudo-tractions that satisfy the traction-free boundary conditions on the crack or pore surfaces in the original, more complex problem (Hu et al., 1993; Huang et al., 1994). The final solution to the original problem is then obtained by superposition of the solutions to the two simpler problems. A graphical illustration of this approach is shown in Figure 1(a) and Figure 2 of Hu et al. (1993).

The objective of this article is to present the results of an investigation aimed at elucidating the effects of porosity and microcrack density on the R-curve behaviors of human cortical bone. The assumption of non-interacting pores or microcracks provides a simple means for estimating the reduction in the elastic modulus, fracture strength, and fracture toughness of human femur as a function of porosity and microcrack density. Since information on porosity and microcrack density are available as a function of age and sex, the influence of age on ductile to brittle fracture transition in human cortical bone can be elucidated by examining how porosity and microcrack density affect the R-curve behavior for different age levels. In particular, the initiation toughness and the initial slope of the R-curve of bone are assessed by considering the corresponding increase of porosity and microcrack density as a function of age and sex. Since the ductile to brittle fracture transition as determined by the slope of the R-curve is also influenced by crack deflection, the dependence of interface toughness and the relevant elastic properties that dictate crack penetration or crack deflection at an interface is considered on the basis of the crack deflection analysis by He and Hutchinson (1989). The results of this investigation show that the decrease in the fracture resistance with increasing age in female cortical bone may be attributed to an increase in the accumulated number of microcracks, porosity, and changes to relevant material properties such as interface toughness and elastic modulus during aging.

II. Fracture Mechanics of Cracked Porous Materials

Despite the presence of pores in the microstructure, linear elastic fracture mechanics and the stress intensity factor, K , is commonly used to characterize the fracture resistance of cortical bone because of the lack of a methodology to account for the stress concentration effects of the porosity. The semi-brittle nature of bone is another complicating factor since it results in a nonlinear fracture response that is commonly described in the form of a K_R curve (Vashishth et al., 1997) or simply R-curve (Nalla et al., 2004), which is a plot of stress intensity factor as a function of crack extension. A previous analysis has shown that the interaction of a crack with an array of pores or voids can result in shielding or anti-shielding and cause changes to the local stress intensity factor at the crack tip (Ciarletta et al., 2003). To account for the effects of porosity on fracture resistance in a porous material such as cortical bone, we consider a cracked solid with an array of uniformly distributed pores or microcracks subjected to an remotely applied stress, σ , as shown in Figure 1(a). The length of the crack is c , the number of pores is n and the pore radius is r . The same approach is also applicable to a set of n microcracks with length $2a$. By considering the porous solid as a composite with voids embedded in a matrix, the stress intensity factor, K_C , of the composite at fracture is given by

$$K_C = Y \sigma_C \sqrt{\pi c} \quad (1)$$

where Y is the boundary-correction factor, and σ_C is the critical stress in the composite at fracture. For a composite with non-interacting pores, the elastic strain energy in the composite is supported entirely by the matrix and the average elastic strain, ϵ_C , of the composite is essentially identical to that of the matrix (ϵ_M), as demonstrated previously by El-Hadek and Tippur (2002) using a finite-element analysis. The results of this work indicated that for a porous composite,

$$\frac{\sigma_c}{E_c} = \frac{\sigma_m}{E_m} \quad (2)$$

where E_c is the Young's modulus of the composite; E_m and σ_m are the Young's modulus and the critical stress of the matrix, respectively. Substituting Eq. (2) into Eq. (1) gives

$$K_c = \left(\frac{E_c}{E_m} \right) Y \sigma_m \sqrt{\pi c} \quad (3)$$

and a general relation for relating the composite properties to the matrix properties as given by

$$\frac{K_c}{K_m} = \frac{\sigma_c}{\sigma_m} = \frac{E_c}{E_m} \quad (4)$$

where

$$K_m = Y \sigma_m \sqrt{\pi c} \quad (5)$$

represents the critical stress intensity factor at fracture of the matrix in the absence of porosity. Eq. (4) indicates that the reduction of fracture toughness, fracture stress, and Young's modulus due to the presence of pores in the microstructure should be identical when the approximation of non-interaction is satisfied. In general, the non-interaction assumption is satisfied when the pores or microcracks are sufficiently far apart such that they do not interact with each other's stress field (Kachanov, 1992, 1994, 2007).

The elastic modulus of a porous solid has been shown to be identical to that of a solid with microcracks for dilute concentrations of pores or microcracks in the matrix. In this context, dilute concentration means that the pores and microcracks do not interact with each other. Mori and Tanaka (1973) computed the effective modulus of porous solids by treating the voids in a heterogeneous medium as inclusions with a zero modulus. The Mori-Tanaka method (1973) yields the solution that is identical to the dilute solution for non-interacting microcracks in a cracked solid. The effects of non-interacting microcracks on the elastic properties of a solid with randomly oriented microcracks have been analyzed by a number of investigators. For noninteracting microcracks, the effective elastic properties of a cracked solid were obtained first by treating: (1) a single semi-circular microcrack of length $2a$ oriented in an arbitrary angle, α , ahead of a main crack, and (2) summing the contributions of individual microcracks by integrating the orientation distribution function for a group of randomly oriented microcracks over the entire spherical angles. The effective Young's modulus, E , of a cracked or voided solid normalized by that of the uncracked solid, E_m , is a function of the crack or pore density parameter and is given by (Feng, 2001)

$$\frac{E_c}{E_m} = F(\chi_i) = \left[1 + \frac{16(1-\nu^2)\chi_i}{3(2-\nu)\left(1 - \frac{4}{9}\chi_i\right)} \right]^{-1} \quad (6)$$

where $i = c$ for microcracks and $i = p$ for pores. The crack density parameter introduced by Budiansky and O'Connell (1976) is used and it is defined as (Budiansky and O'Connell, 1976)

$$\chi_c = \frac{n}{V} a^3 \text{ for the 3-D case,} \quad (7)$$

and

$$\chi_c = \frac{n}{A} a^2 \text{ for the 2 - D case, } (8)$$

where n is the number of microcracks, V is a representative volume, and A is the representative area.

Eqs. (6) to (8) are also applicable for porous materials when n is taken to be the number of pores, and the crack length $2a$ is replaced by the pore diameter $2r$, leading to (Kachanov, 1992, 1994)

$$\chi_p = \frac{n}{V} r^3 \text{ for the 3 - D case, } (9)$$

and

$$\chi_p = \frac{n}{A} r^2 \text{ for the 2 - D case. } (10)$$

Eqs. (4), (6), and (7) to (10) provide the relations for predicting the degradation of Young's modulus, fracture strength, and fracture toughness due to the presence of pores or microcracks in a solid when the pores and microcracks do not interact with each other's stress field. It should be noted that Eq. (6) is applicable for solids with a group of randomly distributed pores or microcracks. For non-randomly aligned microcracks, some of the numerical multipliers of the pore or crack density parameter, χ_i , will change and need to be evaluated by integrating the entire range of specific angles for the aligned microcracks (Feng, 2001; Feng et al., 2003).

Initiation Fracture Toughness

The fracture resistance of bone tissue can generally be characterized in terms of the initiation toughness, K_o , which is the stress intensity factor at the onset of crack extension ($\Delta a = 0$) and the initial slope, $C = dK/da$, of the resistance-curve (R-curve), as illustrated in Figure 1(b). In this section, the initiation toughness and slope of the R-curve for cracked and voided materials with a crack density of χ_c and pore density of χ_p are developed by considering a Mode I crack subjected to a remotely applied tensile stress, σ , as shown in Figure 2. It is assumed that the J-field dominates at the crack tip and crack extension occurs when the near-tip J-integral reaches a critical value of J_o . According to an analysis by Rice (1968), the critical J-integral can be related to the fracture stress, σ_c , in the crack-tip process zone and the crack tip opening displacement, δ_c , by the relation given by (Rice, 1968)

$$J_o = \sigma_c \delta_c \quad (11)$$

and the J-integral is related to the stress intensity factor, K_o , at the onset of crack extension,

$$J_o = \frac{(1 - \nu^2) K_o^2}{E_c} \quad (12)$$

for the plane strain condition. Combining Eq. (11) and Eq. (12) leads one to

$$K_o = \left[\frac{E_c \sigma_c \delta_c}{1 - \nu^2} \right]^{1/2} \quad (13)$$

for cracked or voided materials. For cracked and voided materials with a crack density of χ_c and a pore density of χ_p , the combination of Eqs. (4) and (6) gives

$$E_c = E_m F(\chi_c) F(\chi_p) \quad (14)$$

and

$$\sigma_c = \sigma_m F(\chi_c) F(\chi_p) \quad (15)$$

which can be combined with Eq. (13) to obtain the expression for K_O given by

$$K_O = \left[\frac{E_m \sigma_m \delta_c}{1 - \nu^2} \right]^{1/2} F(\chi_c) F(\chi_p) \quad (16)$$

leading to

$$\frac{K_O}{K_m} = F(\chi_c) F(\chi_p) \quad (17)$$

for the fracture toughness reduction as the result of the presence of microcracks and pores. In addition, the fracture strength, σ_m , of the matrix can also be approximated by nanoindentation hardness, H , by (Dieter, 1961)

$$\sigma_m = \frac{H}{3} \quad (18)$$

for the plane strain condition. The critical crack opening displacement can be expressed in terms of the critical fracture strain (ϵ_c), and the critical fracture process zone size (l_c). Substituting these relevant parameters into Eq. (16) leads one to

$$K_O = \left[\frac{E_m H \epsilon_c l_c}{3(1 - \nu^2)} \right]^{1/2} F(\chi_c) F(\chi_p) \quad (19)$$

as the initiation toughness expression for a cracked porous material such as cortical bone.

Initial Slope of the R-Curve

A rising R-curve is the result of the formation of a crack bridging zone and the presence of uncracked ligaments in the wake of a loaded main crack. For small-scale bridging, the bridging size is small compared to the length of the main crack and the fracture resistance is still controlled the K-field. Under this circumstance, the R-curve is given by (Budiansky et al., 1988)

$$K = K_O + 2 \sqrt{\frac{2}{\pi}} \sigma_{br} \sqrt{L_{br}} \quad (20)$$

where σ_{br} is the bridging stress and L_{br} is the length of the bridging zone. The slope of the R-curve can be obtained by taking the derivative of Eq. (20) with respect to the crack increment, da , leading to

$$C = \frac{dK}{da} = \sqrt{\frac{2}{\pi}} \frac{\sigma_{br}}{\sqrt{L_{br}}} \frac{dL_{br}}{da} \quad (21)$$

which can be further simplified by recognizing that $\sigma_{br} = \nu_{br} \sigma_c$, where ν_{br} is the volume fraction of bridging ligaments in the bridging zone and that the value of dL_{br}/da , which ranges from 0 to 1, can be taken as $dL_{br}/da = 1$ at the onset of crack extension. Eq. (21) is then simplified to

$$C = \sqrt{\frac{2}{\pi} \frac{\nu_{br} \sigma_c}{\sqrt{L_{br}}}} \quad (22)$$

leading to

$$C = \sqrt{\frac{2}{\pi} \frac{\nu_{br} H}{3 \sqrt{L_{br}}}} F(\chi_c) F(\chi_p) \quad (23)$$

when Eq. (22) is combined with Eq. (15) and Eq. (18).

III. Model Applications To Porous Materials

The applicability of Eq. (4) to Eq. (8) to porous materials was first evaluated by comparing the predicted dependence of Young's modulus and fracture toughness on pore density against experimental data of porous materials simulated by dispersion of microballoons in epoxy and urethane from the literature (El-Hadek and Tippur, 2002). To simulate the effects of porosity on mechanical properties, El-Hadek and Tippur (2002) introduced microballoon dispersions into epoxy and urethane to form composites with weakly bonded dispersions that debonded readily to form voids under static and dynamic loading. The Young's modulus, fracture strength, and the critical stress intensity factor at fracture (fracture toughness) were measured as function of volume fractions of voids (i.e., microballoons). The mean diameter of the microballoons was 60 μm with a wall thickness of 400 nm, and the volume fraction ranged from 0 to 0.45. The Young's modulus of the microballooned material normalized by that of the unfilled material are compared against the prediction from the model in Figure 3(a), which shows the normalized Young's modulus as a function of volume fraction of pores for microballoon-dispersed epoxy and urethane. The agreement between experimental data and model prediction is excellent. Similar comparisons between measured and predicted normalized fracture toughness for the microballoon dispersed materials are presented in Figure 3(b) for both quasi-static and dynamic loading. The agreement between the experimental data and model prediction is excellent for dynamic loading, but the model under-predicted the fracture toughness under quasi-static loading. It should be noted that independent comparisons are presented in Figures 3(a) and (b) since there are no adjustable parameters in Eqs. (4) and (6).

The applicability of Eqs. (4) and (6) to cortical bone was then evaluated by comparing the predicted modulus reduction against experimental measurements of human cortical bone (Nicolella et al., 2011). In a previous study, Nicolella et al., (2011) utilized a non-destructive nuclear magnetic resonance (NMR) spin-spin (T_2) relaxation technique to quantify the apparent changes in bone porosity as a function of cyclic loading and prior damage accumulation. The technique was first applied to unloaded cortical bone to quantify the initial porosity and subsequently to fatigued cortical bone that was subjected to cyclic loading to various levels of modulus degradation and microdamage in the form of microcracks. The NMR T_2 relaxation time and amplitude data of the fatigued bone were compared against the undamaged state. The difference in the T_2 relaxation time data was taken as a measure of the increase in pore size, bone porosity or microcrack density due to microdamage induced by cyclic loading and a data analysis procedure was developed to deduce the number and size distributions of microcracks formed in cortical bone. In addition, serial sectioning of the fatigued bone showed the formation of microcracks along

the cement lines or within the interstitial tissue. The results on the evolution of microdamage derived from NMR measurements were verified by independent experimental measurements of microcrack density using histological characterization techniques. Both sets of data are compared against the model prediction from Eq. (6) in Figure 4, which shows the normalized modulus as a function of crack density, which is identical to the pore density. There are considerable scatter in the experimental data, but the predicted and observed trends are in fairly good agreement. In particular, both the model prediction and the experimental data show decreasing elastic modulus with increasing crack density.

The applicability of Eq. (19) to the fracture toughness of human femur was evaluated first by assessing the porosity term and ignoring the crack density term and setting $\chi_C = 0$. The fracture toughness of human femur for female donors at an age of 48 and 78 years old were reported previously by Chan et al. (2009). The K_R -curve, the near-tip strain distribution, and porosity of multiple specimens ($n = 4$) were determined for both age groups. These results are presented in Figure 5 as a function of porosity. The K_m values at 0% porosity are 2.8, 1.5, and 0.5 MPa(m)^{1/2} for the three calculated curves shown in Figure 5. These values were estimated on the basis of Eq. (19) and material properties of local measurements of E and H measured using nanoindentation tests. The near-tip strain at the onset of crack extension were measured by a local strain measurement technique, called DIAMAP II (Nicolella et al., 2001), and the results were reported earlier by Chan et al. (2009). In-situ crack-tip observations by Chan et al. (2009) revealed that for 48-year bone tissue, the crack tip often arrested at an osteon, then blunted and opened up or deflected at lamella interface. For the specimens tested, the initiation toughness, the initial slope of the R-curve, the near-tip strains, and the lamella thickness within the osteon all exhibited variations within an age group for both 48- and 78-year-old females. Based on these observations, the fracture strains were determined from the measured near-tip strain fields at a critical distance on the order of the lamella thickness in an osteon located ahead of the crack tip. For 48-year-old females, the critical distance was taken to be 5 μm or 12 μm because the lamella thickness lies between 5 μm to 12 μm . A summary of these local material parameters is presented in Table 1. These material constants were utilized to calculate the K_o value as a function of porosity for both 48- and 78-year-old females. For 48-year-old females, the K_o values varied substantially at a given porosity. This K_o variation was modeled by using two critical strains at fracture, which corresponds to two lamella thickness values and critical distances. The calculated K_o values are compared with the experimental data from Chan et al., (2009) in Figure 5. Experimental porosity values from Chan et al. (2009) were also used. As shown in Figure 5, the calculated K_o values of human femur decrease with increasing porosity for both the 48 and 78 age groups. The good agreement indicates that the reduction in elastic modulus (Figure 4) and fracture toughness (Figure 5) are described by the same function, as predicted by the model (Eq. 4).

To evaluate Eq. (19) and the crack density function, experimental measurements of the number and length of microcracks in human cortical bone from the literature were utilized. Available experimental data of in-situ microcracks, which represent the microcracks that have accumulated in cortical bone during a donor's lifetime, were reported by Schaffler et al. (1995) for both female and male donors, and by Zioupos (2001a and b) for male donors. Limited data were also reported by Courtney et al. (1996), but the sex of this set of data was not identified. These measurements, which included the number of microcracks per area and their average lengths, were converted into crack density values using Eqs. (7) or (8). Norman and Wang (1997) reported microdamage in terms of the number of microcracks per unit field area and microdamage surface density in terms of the sum of crack lengths per unit field area for human tibia and femurs from both male and female donors. Unfortunately, this set of experimental data could not be used because the microdamage parameters could not be converted to the crack density parameter defined by Eq. (7) or Eq. (8). Typical data of the

average crack half-length are presented as a function of age in Figure 6(a), while the results for the crack density parameter are presented in Figure 6(b). Figure 6(a) shows that the average crack half-length is relatively constant and does not vary significantly with age. The size of in-situ microcracks is limited to a certain size range because larger microcracks would trigger remodeling and the damaged area would be replaced by new, undamaged bone tissue (Doblare et al., 2004). In contrast, the number of microcracks and thus the corresponding crack density parameter increase with increasing age and the increase is more drastic in females than in males, as shown in Figure 6(b). Empirical relations between the number of microcracks per area with age have been reported previously by Schaffler et al. (1995) and Zioupos (2001a and b). The relations were multiplied by the square of the average crack half-length using Eq. (8) to obtain the crack density parameter as a function of age. These relations are given by (Schaffler et al., 1995; Zioupos, 2001a and b)

$$\chi_c = \pi a_o^2 n_o Y^{1.8} \text{ for male} \quad (24)$$

$$\chi_c = \pi a_o^2 n_o Y^{5.6727} \text{ for female} \quad (25)$$

where $n_o = 6.456 \times 10^{-4}$ #/mm for male; $n_o = 4.4392 \times 10^{-10}$ #/mm for female; $a_o = 0.1259$ mm for both male and females; Y is age. Eqs. (24) and (25) are shown as the solid line for female and as dashed line for male in Figure 6(b).

Eqs. (24) and (25) were combined with Eqs. (19) and (23) to compute the dependence of K_o and C of human cortical bone as a function of age of female and male donors. Figure 7 shows a comparison of the measured K_o data from the literature against calculated K_o curves for male and female donors at porosity levels of 10% and 30% and based on their respective crack density curves shown in Figure 6(b). The corresponding comparison for the initial slope, C , of the R-curve is shown in Figure 8. The C curves were computed using Eq. (23) with $H = 700$ MPa $L_{Br} = 12$ μ m, which correspond to the average nanoindentation hardness and the lamellar thickness. The initial volume fraction, V_o , of the bridging ligament was estimated to be 0.0821 or 0.07884 on the basis of the initial crack length and a bridging ligament on the order of one lamellar thickness. The results indicate that the K_o level decrease with increasing porosity for both male and female at all age levels. The K_o value is predicted to decrease rapidly with increasing age in female for ages beyond 60. This rapid decrease in K_o with increasing age corresponds to the exponential increase in the crack density parameter observed in Figure 6(b). Similarly, a rapid decrease in the C value with increasing age in females beyond 60 years of age is observed in Figure 8. Again, the rapid decrease corresponds to the exponential increase in the crack density parameter beyond 60 years of age in Figure 6(b). Rapid decreases in the K_o and C -values are not predicted in males beyond 60 years of age, which are contrary to the experimental data shown in Figures 7 and 8. Since the K_o and C values were predicted on the basis of the microcrack density shown in Figure 6(b), the discrepancies between the computed and measured values may be understood on the basis that the crack density in males beyond 60 years of age may be higher than those shown in Figure 6(b). It is also possible that the extrapolation of the microcrack density from age 60 to age 100 based on Eq. (24) underestimated the actual microcrack density in the bone. Furthermore, it is also possible that the non-interaction approximation utilized to obtain Eq. (6) may become invalid at high microcrack density.

Besides porosity and crack density, other material properties that affect the R-curve behavior of cortical bone are the interface toughness of the cement line and the Young's modulus of the interstitial bone and the osteons as they affect the propensity of a main crack to penetrate or deflect around an osteon. Crack deflection or penetration of an interface is typically determined on the basis of the ratio of the elastic energy release rate, G_I , for interface

deflection to the counterpart, G_p , for penetration. He and Hutchison (1989) have previously established the critical conditions for crack deflection or penetration at an interface in the form of a delamination map, shown in Figure 9, which shows the interface fracture boundary as a solid line in a plot of G_i/G_p versus the Dundurs' parameter (1969). For a crack tip that resides in a region of Young's modulus E_1 and extends into another region of Young's modulus E_2 , the critical G_i/G_p value for crack penetration depends on the Dundurs' elastic mismatch parameter, which is defined as (Dundurs, 1969)

$$\alpha_D = \frac{E_1 - E_2}{E_1 + E_2} \quad (26)$$

as shown in Figure 9. According the theoretical calculation by He and Hutchinson (1989), crack deflection at the interface is favored when G_i/G_p is less than that of the boundary. In contrast, interface penetration of the interface occurs when G_i/G_p exceeds the critical value represented by the solid line. The G_i/G_p ratio associated with a crack tip can be expressed as

$$\frac{G_i}{G_p} = \left[\frac{K_i}{K_p} \right]^2 \left[\frac{E_2}{E_1} \right] \quad (27)$$

where K_i is the interface toughness between region 1 and region 2, and K_p is the fracture toughness for crack penetration into region 2.

The formation of a bridging ligament in the crack wake often starts with deflection of the main crack tip around an osteon and the nucleation of a microcrack ahead of the deflected crack, as shown in Figure 10. Figure 10(a) shows schematically crack deflection at an osteon and the associated crack tip mechanical parameters, while Figure 10(b) depicts crack deflection at an osteon and ligament formation in the crack wake in cortical bone of a 48-year-old female. Crack deflection by osteons, which becomes less frequent with increasing age, results in the reduction of the initial slope, C , of the R-curve with increasing age observed in Figure 8. To better understand this age-related phenomenon, the K_i/K_p values at crack deflection were deduced from in-situ fracture toughness experiments reported earlier by Chan et al. (2009). The crack deflection at osteons shown in Figures 10(a) and (b) as well as similar crack/osteon interactions in other specimens were analyzed using the results of a finite-element fracture mechanics analysis method (Chan et al., 2007) to obtain the ratio of the stress intensity factor of the deflected crack normalized by that of a straight Mode I crack. The process involved computing an effective stress intensity factor that accounted for the Mode I and II stress intensity factors of a crack deflected around an osteon and normalized the result by the stress intensity factor of a straight Mode I crack at an identical projected crack length without crack deflection. These results, which are summarized in Table 2, show that the average K_i/K_p ratios are 0.51 and 0.68 for 48- and 78-year-old females, respectively. To assess the influence of age and Young's modulus on the relative propensity of crack deflection versus crack penetration, the local hardness and Young's modulus were measured by nanoindentation for osteons and interstitial bone along the fracture path for both 48- and 78-year-old females. The nanoindentation tests were performed on the same human femur specimens previously tested by Chan et al. (2009) to determine the K_R curves for 48- and 78-year-old females, including the specimen shown in Figure 10. Osteons and interstitial bone where the crack deflected or propagated through, including the osteons and interstitial bone shown in Figure 10, were indented along the crack paths of individual fracture specimens. The indents were placed at a small distance away from the fractured osteons and interstitial bone and aligned normal to the crack growth direction. At least ten indentations ($n = 10$) were made for each measurement region (osteon or interstitial bone), and multiple regions along the crack path were tested for both age groups. These results, which have not been published previously, are presented in Figures 11

and 12 for 48- and 78-year-old females, respectively. There are large differences between the Young's moduli of osteons and interstitial bone located along the crack path and the differences increase with increasing age. This set of Young's modulus was utilized to compute the Dundurs' parameter and the G_I/G_P ratio and the results for the 48-year-old female are compared with the delamination map in Figure 9. The same range of G_I/G_P and α_D values were obtained for maximum, average, and minimum values of E_1 and E_2 , as shown in Figure 9. A comparison of the delamination plots for the 48- and 78-year-old female is presented in Figure 13. Figure 13 shows the crack deflection boundary by a singly deflected crack tip as a solid line. All G_I/G_P values that lie above the boundary indicate crack penetration of the interface with crack deflection, while all G_I/G_P values that lie below the solid boundary indicate crack deflection at the cement line (interface between an osteon and interstitial bone). All possible combinations of E_1 and E_2 were used to compute the G_I/G_P values for a given age group. For the 48-year-old female, the Dundurs' α parameter ranges from -0.45 to 0.45 , and the G_I/G_P value ranges from as low as 0.1 to as high as 0.70 . Approximately 38% of the computed G_I/G_P ratios lie above the solid boundary, as shown in Figure 13. For the 78-year-old female group, the Dundurs' α values and the G_I/G_P are increased, shifting the data point and up and to the right. As a result, more of the data points lie in the crack penetration region, as shown in Figure 13, and about 82% of the computed G_I/G_P ratios lie above the solid boundary. A comparison of the theoretical and measured values of crack deflection for the two different age groups is presented in Figure 14. There is a drastic decrease in crack deflection with increasing age. The large decrease appears to originate from: (1) a large decrease in the K_I/K_P ratio, and (2) an increase in the Dundurs' α parameter with increasing age.

IV. Discussion

The findings of this investigation indicate that the increase of microcrack density and porosity with age contributes to the decrease in initiation toughness and the slope of the R-curve of human cortical bone. Since the average crack length remains relatively constant ($a_0 = 0.1259$ mm) over a wide age of ages, the increase in the microcrack density with age originates from an increase in the number of microcracks per unit volume with increasing age. The inability of the remodeling process to reduce the number of small microcracks in microdamaged zones, especially in aging females beyond age 60, appears to be responsible for the exponential increase in microcrack density reported in the literature (Schaffler et al., 1995) and the corresponding decreases in the initiation toughness and the initial slope of the R-curve.

The analysis also demonstrates that reductions in the elastic modulus, fracture strength, and fracture toughness of human cortical depend on the microcrack and pore density and are described by the same function, Eq. (6). Furthermore, both crack density and pore density need to be considered in order to assess the proper role of bone microstructure in the R-curve behavior of cortical bone. In particular, the same function of crack density and pore density describe the reduction of initiation toughness and the initial slope, C , of the R-curves for human cortical bone over the entire range of ages examined for both female and male specimens. This finding explains the observation that a decrease in the crack initiation by age is always accompanied by a reduction in the initial slope, C , of the R-curve. For both K_{I0} and C , their decreases in value with age are intimately related to the corresponding reduction of elastic modulus and fracture strength with age due to the increased influence of crack density and porosity.

Another parameter that has a significant effect on crack deflection and the formation of a bridging zone in bone tissue is the interface toughness, K_I . Crack deflection appears to occur at or near the cement line, which is a thin layer of tissue less than $5\text{ }\mu\text{m}$ in thickness located

between the interstitial bone and an osteon (Skedros et al., 2005). The cement line is a distinct layer of material with different fracture toughness and elastic properties from those of the osteon and the interstitial bone. Recent studies have shown that the cement line is highly mineralized with a mineral density that is higher than the interstitial bone and the osteons (Skedros et al., 2005; Langer et al., 2012). The high mineral content suggests that the cement line is likely to be more brittle with a lower fracture toughness than either the interstitial bone or the osteons. Two types of interface deflection at a cement line appear to be feasible. One involves crack deflection at the interface between an interstitial bone and a cement line, while the other involves crack deflection at the interface between a cement line and an osteon. Since the cement line is expected to be very brittle, it is also possible that the deflected crack propagates within the cement line. Since the elastic and fracture toughness properties of the cement line were not known, the cement line was assumed to be infinitely thin with a zero thickness so that only the elastic properties of interstitial bone and osteon and an interface toughness, K_i , were considered in the He and Hutchinson analysis (1989). Due to the uncertainties related to the actual crack path (cement line, cement line/interstitial bone interface, and cement line/osteon interface) the interface toughness value is expected to exhibit substantial variability with bone microstructure and the particular interface where deflection occurs. In general, a low value of the interface toughness is desired for instigating crack deflection to promote the formation of uncracked ligaments in the wake of a propagating crack. The results of this investigation reveal that both K_i and K_p decrease with increasing age in female human cortical bone. More importantly, the value of the K_i/K_p ratio increases with increasing age. Coupled with changes of the Dundurs' α_D parameter (Dundurs, 1969) and the Young's modulus of osteons and interstitial bone with age, the G_i/G_p values are increased with increasing age, resulting in increased tendency of crack penetration and reduced crack bridging with increasing age. The decrease in the interface toughness of the cement line can be attributed to increased crosslink density of collagens or EMC materials (Buehler, 2008; Nyman et al., 2006; Zimmermann, 2012), while changes in the Young's modulus of osteons and interstitial bone may be attributed to increased mineralization (Currey, 2004) and the presence of microdamage or submicron-sized microcracks, either at the interface or within the bone tissue.

One of the important implications of the findings of this investigation is that high fracture toughness of bone tissue requires a low porosity (high bone quantity) and a low crack density (high bone quality). A high bone quantity (low porosity) is not sufficient to assure high fracture resistance if there is extensive microdamage in the form of submicron-sized or nano-sized cracks present in the bone tissue. Here, bone quality is taken to be a measure of the quality of collagen and mineral, the crosslink profile, architecture in the ultrastructure, as well as an absence of microdamage zones with submicron- or nano-sized microcracks. Apparently, bone quality can degrade with age by the accumulation of increasing number of microcracks in the bone tissue (Schaffler et al., 1995; Norman and Wang, 1997; Zioupos, 2001a and b). Microdamage in bone can trigger remodeling of bone tissue in a relatively short time (Burr et al., 1985). At the present time, it is not clear why the in-situ microcracks are not removed by remodeling in aged tissue, but it could be caused by high local stresses or strains (Doblare et al., 2004). Using a cell-staining technique, Hazenberg et al. (2006) have shown that microcracks in bone can cause damage to the cellular material through a cell tearing process that is driven by the crack opening and shear displacements. According to Hazenberg et al., the number of broken cell processes may be a mechanism by which bone is able to sense the crack size and initiate mitigation response either by remodeling or bone deposition on the crack surfaces. However, not all cells are torn or ruptured by the crack face opening displacements. The transition point between torn cells and intact cells is poorly understood. The conditions for the onset of remodeling have yet to be established, but it appears that a bioelectromechanical stimulus is required to initiate or trigger bone remodeling. The presence of microcracks in the microstructure may also hinder the

communication between osteocyte lacuna and damage tissue to start the remodeling process. Without appropriate levels of remodeling, microdamage zones with high crack density may be allowed to accumulate over time and lead to low-quality bone that exhibits lower Young's modulus, lower fracture strength, and reduced fracture toughness. To improve bone quality, bone remodeling must be instigated to remove as many submicron-sized microcracks as possible.

The remodeling of a microdamage zone will result in the creation of a temporary pore which must be subsequently filled up with new bone tissue. On a temporary basis, the transition from a microdamage zone to a pore may embrittle (i.e., make brittle) or weaken the bone tissue. To better understand the condition for instigating remodeling, the morphological conditions where remodeling of a microdamaged volume into a porous tissue is computed on the basis that the toughness reduction of a given crack density is equivalent to that of the pore density, as shown in Eq. (17) and (23). Thus,

$$\frac{n_c a^3}{V} = \frac{n_p r^3}{V} \quad (28)$$

when a microdamage zone of n_c microcracks of half-length a , is remodeled into a single pore with $n_p = 1$. The pore radius to crack half-length ratio, r/a , given by

$$\frac{r}{a} = n_c^{1/3} \quad (29)$$

then defines the boundary where remodeling of n_c microcracks into a single pore would not lead to a toughness reduction or enhancement. In contrast, remodeling leads to a toughness reduction when $r/a > n_c^{1/3}$, but results in toughening reduction when $r/a < n_c^{1/3}$. These various effects of remodeling are illustrated in Figure 15, which shows that the r/a ratio must be less than a critical value, which is shown as the solid line in Figure 15 and is defined by Eq. (29), in order to achieve any toughness enhancement by remodeling. This finding provides a possible explanation why remodeling sometimes may not be activated since it would only further weaken and embrittle the bone tissue. The result also indicates that for conditions with $r/a > n_c^{1/3}$, it may be justified to stop remodeling in order not to weaken and embrittle the bone tissue further.

V. Conclusions

A micromechanical modeling approach has been developed to predict the initiation toughness and the initial slope of the R-curve of cortical bone and to examine the influence of increasing porosity and crack density with age on the R-curve response. The conclusions reached in this study are as follows:

1. The reductions of elastic modulus, fracture strength, and fracture toughness observed in human cortical bone with increasing age can be attributed to increases in porosity and microcrack density with increasing age and can be described in terms of the same function of pore density and microcrack density.
2. The reductions of the initiation toughness, K_{I0} , and the initial slope, C , of the R-curve, observed in human cortical bone with increasing age are directly related to the decrease in the Young's modulus and fracture toughness due to the presence of porosity and microcracks in the bone microstructure.
3. Crack deflection at osteons is more difficult with increasing age because the interface toughness of the cement line decreases and the Dundurs' elastic mismatch parameter increases with increasing age.

4. The fracture resistance (K_{Ic} and C values) of human cortical bone for females decreases rapidly with increasing age and can be directly attributed to the exponential increase in the number of microcracks accumulated in the tissue at ages beyond 60 years.
5. A high fracture toughness of cortical bone requires a low porosity (high bone quantity) and a low crack density (high bone quality). A high bone quantity (low porosity) is not sufficient to assure high fracture resistance if there is extensive microdamage in the form of sub-micron-sized or nano-sized cracks present in the bone tissue.
6. The reduction of Young's modulus, fracture strength and fracture toughness of cracked porous materials such as cortical bone can be predicted on the basis of the assumption of non-interacting microcracks or pores.
7. Bone remodeling of a microdamage zone of n_c microcracks into a single pore of radius r may embrittle or toughen the bone tissue, depending on the r/a ratio.

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(a)

(b)

Figure 1.

Schematics show the superposition method utilized to compute the influence of porosity and microcrack density on the stress intensity factor of a cracked porous solid subjected to a remotely applied stress; modified from Hu et al. (1993), and (b) schematics of the influence of age on the R-curve behaviors of human femur of 48- and 78-year-old females; modified from Chan et al. (2009).

(a)

(b)

Figure 2.

Schematics illustrate the onset of crack extension and the formation of a bridging zone of length, L_{br} , ahead of a main crack in a cortical bone subjected to a remotely applied stress, σ : (a) crack arrest at an osteon and the formation of a microcrack of length, $2a$, and (b) crack deflection around an osteon and the formation of a microcrack ahead of the deflected crack.

Figure 3.

Measured and predicted reductions of Young's modulus and fracture toughness of microballooned epoxy and urethane as a function of volume fraction of microballoon dispersion (pores): (a) Young's modulus reduction, and (b) fracture toughness reduction. Experimental data are from El-Hadek and Tippur (2002).

Figure 4.

Comparison of measured (histological data) and predicted values of modulus reduction as a function of crack density in cortical bone. Modulus prediction (solid line) was obtained using Eq. (9) and the values of the crack density parameter deduced from the NMR measurements. From Nicolella et al. (2011).

Figure 5.

Comparison of measured and predicted initiation toughness, K_o , of human cortical bone as a function of pore density for females at age groups (48- and 78-year-old). Experimental data are from Chan et al. (2009).

(a)

(b)

Figure 6.

Average half-length (a) and crack density (χ_c) of human cortical bone for males and females as a function of age: (a) average half-length of microcracks, and (b) crack density.

Experimental data are from Schaffler et al. (1995), Courtney et al. (1996) and Zioupou (2001a and b).

Figure 7.

Measured and predicted initiation toughness (K_o) of human cortical bone as a function of age for males and females at 10% and 30% porosity. Experimental data are from Vashishth et al. (1997) Wu and Vashishth (2002), Nalla et al. (2004), and Chan et al. (2009).

Figure 8.

Comparison of measured and predicted initial slope, C , and the R-curve of human cortical bone as a function of age for males and females. The pore porosity was taken to be 20%, and the value of the initial uncracked ligament volume fraction (V_o) was taken to be either 0.0784 or 0.0121. Experimental data are from Vashishth et al. (1997), Wu and Vashishth (2002), Nalla et al. (2004), and Chan et al. (2009).

Figure 9.

A plot of G_i/G_p as a function of the Dundurs' elastic parameter shows the boundary for delineating crack deflection and crack penetration of an interface of two elastic solids. Crack deflection along the interface is favored for G_i/G_p values below the boundary and crack penetration is favored for G_i/G_p values above the boundary. Results for a singly deflected crack and a doubly deflected crack, taken from He and Hutchinson, are compared against experimental data for 48-year-old female.

Figure 10.

Crack interaction with osteons in the human cortical bone of a 48-year-old female. (a) crack approaching an osteon, (b) crack deflection at an osteon, (c) crack approaching a second osteon, and (d) crack penetration of a second osteon.

Figure 11. Nanoindentation hardness (a) and Young's modulus (b) of osteon and interstitial bone of 48-year-old female.

Figure 12. Nanoindentation hardness (a) and Young's modulus (b) of osteon and interstitial bone of 78-year-old female.

Figure 13.

Measured G_i/G_p ratios for 48- and 78-year-old female compared to the predicted crack deflection/penetration boundary as a function of Dundurs' elastic mismatch parameter. The crack deflection/penetration boundary is taken from He and Hutchinson (1989).

Figure 14.

Comparison of measured and predicted crack deflection frequency for 48- and 78-year-old female.

Figure 15.

Predicted ratios of pore radius to crack half-length when remodeling of a microdamage zone of n_c microcracks of half-length a into a simple pore of radius r may toughen or embrittle the bone tissue. The solid line defines the boundary where remodeling results in no toughening reduction or enhancement.

Table 1

Summary of material parameters utilized to compute the initiation toughness values (K_{I0}) of 48- and 78-year-old females.

Material Parameter	48 years (thin lamella)	Age (Female) 48 years (thick lamella)	78 years
E (GPa)	19.58	26.0	18.90
H_v (GPa)	0.76	1.0	0.62
ε_p^c	0.05	0.05	0.01
P_c (μm)	5.0	12.0	5.0
Poisson's Ratio (ν)	0.33	0.33	0.33

Table 2

Summary of interface toughness (K_i) and penetration toughness of osteons for 48-year-old and 78-year-old females.

Fracture Toughness	Age (Female)	
	48 years	78 years
K_i (MPa m)	0.89	0.21
K_p (MPa m)	1.74	0.31
K_i/K_p	0.51	0.68