Journal of Biomechanics xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Journal of Biomechanics

journal homepage: www.elsevier.com/locate/jbiomech
www.JBiomech.com

The effect of microcracking in the peritubular dentin on the fracture of dentin

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ARTICLE INFO

Article history:
Accepted 15 October 2017
Available online xxxx

Keywords:
Dentin
Composite structure
Fracture
Microcracking

ABSTRACT

Dentin is a biocomposite possessing elegant hierarchical structure, which allows it to resist fracture effectively. Despite the considerable efforts to unravel the peculiar fracture behavior of dentin, the effect of microstructural features on the fracture process is largely unknown. In this study, we explore the interaction between the primary crack with crack tip located in intertubular dentin (ITD) and microcracking of peritubular dentin (PTD) ahead of the primary crack. A micromechanical model accounting for the unique composite structure of dentin is developed, and computational simulations are performed. It is found that the microcracking of PTD located in the crack plane in front of the primary crack tip can promote the propagation of the primary crack, increasing the propensity of coalescence of primary crack and microcracks nucleating in PTD. We show that the two-layer microstructure of dentin enables reduction in driving force of primary crack, potentially enhancing fracture toughness. The high stiffness of PTD plays a critical role in reducing the driving force of primary crack and activating microcracking of PTD. It is further identified that the microcracking of PTD arranged parallel to the crack plane with an offset could contribute to the shielding of primary crack.

1. Introduction

Dentin is a mineralized hard tissue comprising the bulk of human teeth. The major function of dentin is to carry and transfer stresses from the outer enamel (Eltit et al., 2013; Waters, 1980). To fulfill this function, dentin needs to have the damage tolerance capability to mitigate fracture. Hence, there is increasing interest in unraveling the fracture behavior and underlying mechanisms of dentin. Imbeni et al (2003) conducted fracture toughness testing of dentin based on fracture mechanics, and determined the improved, lower-bound value of fracture toughness. The study by Kruzic et al. (2003) revealed that dentin displays a rising crack growth resistance curve (R-curve), indicating that the fracture toughness increases with crack extension. Such enhanced fracture toughness is attributed to the salient toughening mechanisms. It was found that uncracked ligaments develop in the crack wake, forming crack bridging which reduces the stress intensity at crack tip and leads to the propensity of crack closure (Bajaj et al., 2006; Kruzic et al., 2003; Nalla et al., 2004). In addition, the microcracking surrounding the main crack was observed, which gives rise to the dilation in the region sustaining high stress and increases the compliance, thereby serving as an important toughening mechanism (Nalla et al., 2003a).

These previous studies have identified the unique fracture behavior of dentin, and some important fracture mechanisms have been also revealed. However, a good understanding of how the mechanisms change the driving force necessary for fracture is not achieved. To gain deep insights into the fracture in dentin, it is essential to explore the structure-property relation. Dentin is a nanocomposite consisting of mineral crystals wrapped by soft protein matrix (Ten Cate, 2008). The prominent feature of dentin at the nanoscale is the staggered arrangement of mineral crystals, which is similar to bone and nacre. Such structural feature imparts the fascinating combination of high strength and superior toughness to dentin (Ji and Gao, 2004; Zhang et al., 2010). At the micoscale, dentin is a biocomposite comprised of protein-rich intertubular dentin (ITD) reinforced by mineral-rich peritubular dentin (PTD) containing dentin tubules (Bertassoni et al., 2012; Ryou et al., 2012). The composite microstructure plays a pivotal role in fracture of dentin. Nalla et al (2003b) showed experimentally that there exists a microdamage zone surrounding the main crack, in which the PTDs undergo microcracking, indicating that inelastic deformation takes place in the fracture process of dentin.

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https://doi.org/10.1016/j.jbiomech.2017.10.022
0021-9290/

Such inelastic deformation caused by microcracking of PTD is further investigated by Eltit et al (2013). In their experiments, it was found that the fracture process of dentin involves merging of the microcracks nucleating at dentin tubules. Jainaen et al (2009) experimentally investigated fracture properties of dentin, showing that crack growth in dentin microstructure is accompanied by the fracture of PTD/ITD interface. The study by Ivancik and Arola (2013) reported that the microstructure of dentin exhibits significant influence on the crack growth path, and that microcracking of PTD occurs ahead of the main crack tip. A substantial degree of microcracking in PTD takes place in the region containing high volume fraction of dentin tubules; whereas crack bridging is seldom observed in this region, leading to the low fracture toughness. The dependence of fracture toughness on the tubule density was further elucidated by Montoya et al. (2016). Using an empirical model for porous materials, they showed that the reduction in fracture toughness is associated with the increase in volume fraction of dentin tubules. However, such an empirical model only considers the effect of geometrical feature of tubules and neglects the important deformation mechanisms associated with the microstructure of dentin. The effects of microcracking and elastic modulus ratio between PTD and ITD on the fracture process in dentin are unknown.

Recently, An and Wagner (2016) developed a micromechanical model of dentin accounting for the unique composite microstructure and the fracture mechanisms of PTD, ITD and the PTD/ITD interface, and revealed the competing fracture mechanisms in dentin. Subsequently, the interaction between crack and the composite microstructure of dentin was explored and it was revealed that the key factor controlling microcracking of PTD ahead of main crack and crack deflection along PTD/ITD interface is the tensile strength of PTD (An et al., 2017). The low strength of PTD could give rise to microcracking of PTD in front of the main crack. Despite the enormous progress, the role of microcracking of PTD in fracture of the microstructure of dentin is still largely unknown. On the one hand, dentin tubules act as stress concentrations, which could potentially induce microcracking of PTD. On the other hand, the stress intensity at the main crack tip located in ITD is high, which could give rise to crack propagation and fracture of ITD. Why is the microcracking of PTD, rather than fracture of ITD, observed in experiments? How does the microstructure of dentin affect the main crack with crack tip located in ITD? These questions call for a good understanding of the fracture mechanisms of dentin. The present study is motivated by the experiments conducted by Ivancik and Arola (2013) and Koester et al. (2008). The primary goal of this study is to reveal the effects of microcracking of PTD and of the composite microstructure on the fracture of dentin. A computational model is developed accounting for the unique composite microstructure of dentin. The interplay between fracture of ITD and microcracking of PTD ahead of the main crack tip is elucidated, and the role of high stiffness of PTD in reducing the crack driving force of the main crack is identified. In addition, the effect of microcracking of PTD arranged parallel to the crack plane with an offset on the driving force of main crack is also discussed.

2. Computational model

We idealize the microstructure of dentin as a heterogeneous solid consisting of hollow cylindrical reinforcements embedded in soft matrix, as shown in Fig. 1a. Such type of idealized microstructure has been used in previous studies (An et al., 2017; An and Zhang, 2015), and it is demonstrated that the numerical simulations based on such idealization of microstructure can capture the important features of fracture in dentin. A block of dentin having length L and height $2h$ is considered, where three rows of PTD containing tubules with radius r are included. The spacing between neighboring tubules is X_0, and the thickness of PTD is t_p. It is experimentally reported that crack growth in dentin with crack path in-plane with dentin tubules involves the merging of the microcracks nucleating in PTD with the crack located in ITD (Eltit et al., 2013; Ivancik and Arola, 2013). The fracture process in dentin is shown schematically in Fig. 1. Therefore, in this study the main crack is taken to be the crack which propagates through the PTD and the ITD, and the tip of the main crack is located in the ITD, as illustrated in Fig. 2. The plane strain conditions are assumed and the two edges of the dentin block are subjected to tensile strain $\pm\varepsilon$. Owing to the symmetry of dentin block and the loading with respect to crack plane, only half of the block is modeled. To study the influence of microcracking of PTD, we introduce several microcracks in the PTDs ahead of the main crack tip. As shown in Fig. 2, the PTD1, which is nearest to the main crack tip, encompasses one microcrack with length of a_1, and the PTD2, which is arranged parallel to the crack plane with an offset of X_0, contains two microcracks with length of a_2. Similarly, two microcracks of length a_3 are introduced in the PTD3, which is close to the PTD1.

Both the PTD and the ITD are modeled as isotropic and linear elastic solids. The finite element method is employed to obtain the approximate solution of the boundary value problem. The model of dentin block is meshed with eight-node isoparametric elements, and the collapsed quadrilateral elements are used to model the crack tip. A total of approximately 15,000 elements are involved. To assess the fracture resistance of the microstructure of dentin, the crack driving force represented by the energy release rate at crack tip is calculated using the contour integral. Based on dimensional considerations, the driving force for the main crack is given by

$$G_i = E_i^* \varepsilon^2 h f\left(\frac{a_i}{L}, \frac{a_1}{t_p}, \frac{a_2}{t_p}, \frac{a_3}{t_p}, \frac{E_p}{E_i}, \upsilon_i, \upsilon_p, \frac{L}{h}, \frac{t_p}{h}, \frac{r}{h}, \frac{X_0}{r}\right) \quad (1)$$

where $E_i^* = E_i/(1-\upsilon_i^2)$ is the plane strain modulus of the ITD, with E_i and υ_i being the elastic modulus and Poisson ratio of the ITD, respectively. a_i represents the length of the main crack, and E_p and υ_p are elastic modulus and Poisson ratio for the PTD, respectively. In the numerical simulations, we fix $\upsilon_i = 0.3$, $\upsilon_p = 0.3$, $L/h = 2.3$, $t_p/h = 0.125$, $r/h = 0.125$ and $X_0/r = 5$. These values of the parameters are comparable to that observed in experiments (e.g. Ivancik and Arola, 2013; Montoya et al., 2016) and representative of dentin microstructure (An and Wagner, 2016; An et al., 2017). As a consequence, the driving force G_i has the form

$$G_i = E_i^* \varepsilon^2 h F\left(\frac{a_i}{L}, \frac{a_1}{t_p}, \frac{a_2}{t_p}, \frac{a_3}{t_p}, \frac{E_p}{E_i}\right) \quad (2)$$

where F is a dimensionless function. Using the same numerical method, the driving force G_p of the microcrack in the PTD1 can be calculated, which has the form similar to Eq. (2). However, due to the difference in the mechanical properties of PTD and ITD, a distinct dimensionless function for G_p is expected. In the numerical simulations, the range of elastic modulus mismatch, E_p/E_i, is taken to be from 1.2 to 3, which is consistent with the experiments on stiffness of ITD and PTD (Kinney et al., 1996; Ziskind et al., 2011), and the effect of elastic modulus mismatch can be explored by such choice of the values. The numerical simulations are performed based on the fact that PTD exhibits larger elastic modulus than ITD (Kinney et al., 1999).

3. Results and discussion

Fig. 3a shows the normalized driving force for main crack, $G_i/(E_i^* \varepsilon^2 h)$, as a function of crack length a_i/h for three values of modulus mismatch (E_p/E_i). It is found that for large elastic modulus