International Journal of Solids and Structures 000 (2017) 1–8

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

Crack initiation and propagation in composite microstructure of dentin

Bingbing An[a,b,*], Yuanzhi Xu[c], Dongsheng Zhang[a,b]

[a] Department of Mechanics, Shanghai University, Shanghai 200444, China
[b] Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai, 200072, China
[c] Department of Prosthodontics, School of medicine, Tongji University, Shanghai, 200011, PR China

ARTICLE INFO

Article history:
Received 11 October 2016
Revised 30 January 2017
Available online xxx

Keywords:
Dentin
Composite microstructure
Toughness
Plastic deformation
Microcracking

ABSTRACT

Dentin possesses unique hierarchical structure through long-term natural selection, which imparts exceptional mechanical properties to this hard tissue. In this study, the combined effects of ductile fracture of intertubular dentin (ITD) and brittle cracking of peritubular dentin (PTD) on the crack initiation and propagation in the composite microstructure of dentin are explored. A micromechanical model accounting for the unique two-layer microstructure of dentin is developed and numerical simulations of fracture of microstructured dentin are performed. It is found that microcracking of PTD prior to the penetration of main crack into PTD and crack deflection along the interface between PTD and ITD are two major mechanisms involved in the fracture of microstructured dentin, which is in a good agreement with experimental observations. The competition between the two mechanisms is governed by PTD strength. Furthermore, we reveal that the elastic and fracture properties of PTD and strain hardening of ITD greatly affect the fracture behavior of dentin. The decrease in elastic modulus and increase in tensile strength of PTD elevate the notch tip plasticity, increasing the propensity of crack initiation at notch tip. Whereas such variations in elastic modulus and tensile strength of PTD can lead to the transition of fracture mechanism from multiple void interactions to crack-void interaction, thereby enhancing toughness of dentin. Increasing the strain hardening exponent of ITD can also give rise to the amplified toughness.

1. Introduction

Dentin is a hierarchically structured biocomposite consisting of mineral crystals embedded in soft protein matrix (Gao et al., 2003; Bar-On and Wagner, 2012). At the microscale, dentin exhibits two-layer structure, where the tubules are bounded by the mineral-rich peritubular dentin (PTD) which is further embedded in the protein-rich intertubular dentin (ITD) (Bertassoni et al., 2012; Ryou et al., 2012; An and Zhang, 2015). The variations in diameter and density of tubules in dentin are observed (Garberoglio and Brannstrom, 1976; Mjör and Nordahl, 1996). Compared with the tubules at the dentin enamel junction (DEJ), the tubules in the deep dentin adjacent to pulp cavity display larger diameters and higher density (Pashley, 1989). In addition, the thickness of PTD also varies with location. The coronal dentin has thicker PTD in comparison to the root dentin, and the thickness of PTD in the middle coronal dentin is larger than that in the outer coronal dentin (Chu et al., 2010).

The unique structural design exhibits significant influence on the mechanical properties of dentin. Lertchirakarm et al. (2001) showed experimentally that the ultimate tensile strength of root dentin is dependent on the tubule orientation. The low strength is observed when the applied loads are parallel to tubule axis, while the transverse loading perpendicular to tubule orientation could give rise to high strength (Lertchirakarm et al., 2001; Carvalho et al., 2001). Giannini et al. (2004) identified the region-dependent tensile strength of dentin.

In addition to its influence on strength, dentin microstructure also affects the fracture behavior. Iwamoto and Ruse (2003) revealed anisotropic fracture toughness of dentin; the longitudinal fracture toughness corresponding to crack growth along tubules is much higher than the fracture toughness in the case of fracture plane perpendicular to tubules. Indeed, the tubular structure imparts anisotropic mechanical properties to dentin (Kinney et al., 2004). It was found that the shear strength of dentin depends on tubule orientation in the central area (Watanabe et al., 1996). The study by Zaytsev et al. (2015) revealed that the shear deformation behavior of dentin is affected by the magnitude of shear strain. Dentin exhibits isotropic deformation behavior when the shear strain is less than 17%, beyond which the anisotropic shear deformation is observed. Kruzic et al. (2003) reported that dentin

* Corresponding author.
E-mail address: anbingbing@shu.edu.cn (B. An).

http://dx.doi.org/10.1016/j.ijsolstr.2017.02.005
0020-7683/

exhibits rising resistance to crack growth. Such enhanced resistance is attributed to various microstructure-based toughening mechanisms. It was found that the crack bridging, which is caused by uncracked ligaments at microscopic scale and by organic matrix at nanoscale (Kahler et al., 2003; Nalla et al., 2005; Nazari et al., 2009), develops in the crack wake, suppressing crack opening and thereby promoting fracture resistance. Another important toughening mechanism is microcracking appearing in the crack wake, which leads to the dilation of this zone and the increases in the compliance, thereby shielding the crack tip (Nalla et al., 2004). The degree of the toughening mechanisms is affected by the location and tubule orientation. Nalla et al. (2003a) found that the extensive crack bridging by uncracked ligaments and collagen fibrils emerges in the case of crack growth in the direction parallel to dentin tubules, whereas such toughening mechanism is hardly observed for crack path perpendicular to tubules. This discrepancy is responsible for the anisotropic fracture toughness. Ivancik and Arola (2013) conducted experiment on crack growth in coronal dentin, showing that although the degree of microcracking of PTD is nearly similar in the mid-coronal dentin and outer dentin, larger unbroken ligaments form crack bridging in the outer dentin, which gives rise to amplified fracture toughness in this region.

Despite these efforts devoted to characterization of the structure-property relationship, the role of the unique two-layer microstructure on the fracture behavior of dentin is largely unknown. Using four-point bending tests, Eltit et al. (2013) found that microcracks nucleating at dentin tubules propagate along the direction perpendicular to tensile stress and are prone to merge with the microcracks from neighboring tubules; some microcracks are arrested at the interface between PTD and ITD. To understand the competition between crack penetration into ITD and crack deflection at interface, An and Wagner (2016) developed a micromechanical model and identified the key factors governing the transition between the two mechanisms. However, it is important to note that our previous study is focused on the fracture behavior of the microstructured dentin subjected to uniaxial tensile loading. The interaction between crack and two-layer microstructure of dentin is not taken into account, and the effect of such unique microstructure on crack initiation and propagation is unclear. Recently, Ivancik and Arola (2013) showed experimentally that the main crack propagates from tubule to tubule, and that microcracking of PTD occurs before main crack penetrates into PTD. At some times, the main crack bypasses tubules and deflects into the interface between PTD and ITD (Jainaen et al., 2009). These studies uncovered the novel fracture behavior of microstructured dentin, whereas the underlying mechanisms responsible for such behavior are still unknown. Why does dentin display such two distinct crack growth behaviors? How does the main crack interact with the two-layer microstructure? Since the crack growth in the microstructured dentin is accompanied by ductile fracture of ITD and brittle cracking of PTD (Ivancik and Arola, 2013), how does the interplay of the two mechanisms determine the toughness? These questions call for a good mechanistic understanding of the interaction of crack with two-layer microstructure of dentin, which motivated the present study. In this study we explore the effect of such two-layer structure on the crack initiation and subsequent crack propagation in dentin, focusing on the effects of elastic and fracture properties of PTD and strain hardening of ITD. A micromechanical model accounting for PTD fracture, ITD fracture and plastic deformation of ITD is developed, and numerical simulations of two-layer microstructure of dentin containing a notch subjected to tensile loading are performed. The effects of microstructural features on the toughness and toughening mechanisms of dentin are elucidated, and the key parameters controlling microcracking of PTD and crack deflection are identified.

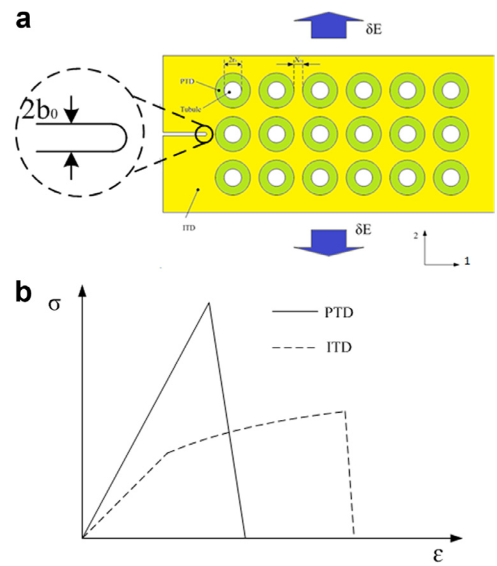

Fig. 1. Micromechanical model of microstructured dentin. (a) The model of notched specimen for dentin with two-layer structure. δ_E represents the increment of applied strain. (b) Schematic illustration of stress-strain responses for PTD and ITD.

2. Method

A notched specimen is used to investigate crack progression in dentin with fracture paths in-plane with dentin tubules, which is consistent with previous experimental studies (e.g. Koester et al., 2008; Ivancik and Arola, 2013). As shown in Fig. 1, the model of dentin specimen with length L, width $2h$ and initial crack length a_0 encompasses 18 tubules, which are idealized as cylindrical voids and arranged in 3 rows. With the help of such arrangement, the effect of multiple void interactions can be assessed. The dentin tubules with radius r are surrounded by PTD with thickness h_p and spacing X_0, which are further embedded in the ITD. A notch with small radius b_0 is introduced in the ITD to model the blunted crack tip (Tvergaard and Hutchinson, 2002), and the spacing of the blunted tip and the nearest tubule is also set to be X_0.

Considering that the PTD is a highly mineralized hard tissue with high elastic modulus and large hardness (Kinney et al., 1996), the mechanical behavior of PTD can be characterized by a brittle fracture model, which is based on the smeared cracking assumption (Weihe and Kröplin, 1998). The additive decomposition of strain rate is adopted,

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{\boldsymbol{e}} + \dot{\boldsymbol{\varepsilon}}^{\boldsymbol{c}} \quad (1)$$

where $\dot{\boldsymbol{\varepsilon}}^{\boldsymbol{e}}$ is the elastic strain rate and $\dot{\boldsymbol{\varepsilon}}^{\boldsymbol{c}}$ denotes cracking strain rate, which delineates additional deformation induced by opening of existing cracks. To facilitate the description of the inelastic deformation of cracked brittle materials, the local Cartesian coordinate system with the coordinate axes aligned with the crack directions is introduced. As such the global strain can be transformed to local strain,

$$\boldsymbol{\varepsilon} = \boldsymbol{T}\epsilon \quad (2)$$

where ε represents local strain tensor and $\boldsymbol{T}$ is transformation matrix. In this study, the cracking model of PTD is based on the assumption of fixed orthogonal cracks, proposed by Rots and Blaauwendraad (1989). For a fixed material point, several cracks can exit. According to this assumption, the subsequent cracks at the considered material point can only emerge in the directions orthogonal to the first crack at the same material point. Due to the assumption of fixed crack, the transformation matrix $\boldsymbol{T}$ is constant. The deformation behavior of PTD involves elastic deformation and