The Preliminary Investigation of the Effect of Caries on the Extension of Dentin Cracks

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Abstract: Dentin is part of the structural composition of the teeth and consists of intertubular dentin (ITD), peritubular dentin (PTD) and the dentinal tubules. The interaction of the three components provides significant strength and durability to the dentin. Caries is a dental disease caused by bacteria, which can damage the microstructure of teeth and lead to teeth damage or even fracture. It is necessary to investigate the mechanism of teeth damage from the perspective of fracture mechanics. In order to study the effect of caries on crack extension, this study uses finite element simulation (FEM) to establish a monophasic dentin model, a bidirectional dentin model, and a dentin model with different caries degrees to compare and analyze the crack extension under the same magnitude of displacement load. The experimental results reveal the influence of different caries degrees on crack extension, which is important for exploring the damage and fracture mechanism of teeth and the design of bionic teeth.

1 INTRODUCTION

Dentin is a highly mineralized tissue with an average mineral volume fraction of 70% (A.T. Weerakoon, 2022). In addition, the mineral content of PTD is even up to 95%. Previous studies have shown that the mineral content of dentin is an important guarantee for the toughening mechanism of dentin, and the higher the mineral content, the stronger the resistance to damage (Goldberg, 2011). Caries is caused by bacteria which decompose the debris leaving on the teeth into acid, resulting in the demineralization of inorganic substances and the decomposition of organic substances in the teeth. Most of the caries starts from the enamel and is divided into three stages: superficial caries, medium caries and deep caries according to the degree of lesion. Among them, deep caries, also called dentin caries, causes the decomposition of dentin organic matter and interferes with the remineralization of dentin (M.M. Jurasic, 2022). Therefore, it is necessary to study the effect of caries on dentin toughening mechanism from dentin microstructure.

The effect of dental caries on the toughening mechanism of dentin was investigated from the perspective of stress distribution. After the occurrence of caries, the stress distribution gradually shifts from the PTD to the ITD, which leads to a significant increase in the risk of ITD destruction (Hu, 2020).

This paper investigates the effect of caries on the microscopic crack extension of dentin from the perspective of fracture mechanics with the help of finite element analysis software. Comparative experiments demonstrated that carious dentin is more prone to crack extension than healthy dentin, thus affecting the toughening mechanism of dentin.

2 METHODS

2.1 Abaqus

ABAQUS is a powerful suite of engineering analysis software based on the finite element method, and its problem-solving capabilities range from relatively simple linear analysis to many complex nonlinear problems. ABAQUS includes a rich library of cells that can simulate arbitrary geometries. It is capable of both simple finite element analysis, as well as simulating very complex models. static and quasi-static analysis, Elastoplastic analysis, fracture analysis, contact analysis, fatigue and durability analysis, thermosolid coupling analysis (J.A. Moreira, 2022). The Extended Finite Element Method (XFEM) has been introduced as a new feature in ABAQUS version 6.9.

2.2 XFEM

The core idea of XFEM cell method is to use the expanded form function basis with discontinuity to represent the discontinuity in the computational domain, which makes the description of the discontinuity field bend independent of the mesh boundary during the computation, and can easily simulate the crack expansion along an arbitrary path.

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In addition, the extended finite element can use known analytic solutions to construct the basis of the form function, which makes it possible to obtain more accurate solutions on coarser meshes, saving computational costs.

The fundamental principle of XFEM is to modify the form function to represent the discontinuity spots in the displacement field, (or any other variable). For instance, to explicitly represent fracture in an element, for each normal degree of freedom, XFEM takes into account an additional degree of freedom (F. Cruz, 2018), which is multiplied by a non-continuous function as shown in Equation (1).

$$u(\mathrm{x,t}) = \sum_{\mathrm{i=0}}^{N} u_i(t) \cdot N_{ui}^{std} + \sum_{i=0}^{N^{dis}} a_j(t). N_{uj}^{enr} \quad (1)$$

This represents a jump to the crack point, which provides a discrete field. The parameter $\mathrm{N_{uj}^{enr}}$represents the additional degree of freedom, obtained by multiplying the type function $\mathrm{N_{ui}^{std}}$ with a rich function θ.

$$\mathrm{N_{uj}^{enr}} = \mathrm{N_{ui}^{std}} \cdot \theta \quad (2)$$

The maximum principal strain failure criterion of XFEM is used to specify that a pure compressive strain rate does not cause damage. Damage begins at a certain value of maximum principal strain. Energy damage evolution defines damage in terms of the energy required for failure after the initiation of damage. The damage evolution criterion is selected as an energy-based, linearly softened, mixed-mode exponential damage evolution law.

2.3 The Theoretical Basis of XFEM

The two theoretical foundations of XFEM are damage mechanics and fracture mechanics. The XFEM analysis of crack generation and extension based on damage mechanics theory requires a loss initiation criterion as well as a damage evolution criterion for the model. The maximum principal strain failure criterion refers to the pure compressive stress rate cannot cause damage. Damage initiation occurs when the maximum principal stress degree reaches a certain value, and the initial strain of the crack for the model is set to 0.1% (D.R. Nolan, 2022). The loss evolution criterion of the model takes the form of energy-based fracture failure, where the stiffness starts to degrade when the starting criterion reaches a critical value. The critical strain energy release rate of the material has the following relationship with the fracture toughness and the elastic modulus the following relationship.

$$K = \sqrt{J \times E'} \quad (3)$$

In Equation (3), K represents the fracture toughness of the material and J represents the strain energy release rate of the material, for the plane strain problem, $E^{`}=E/(1-v^2)$. According to Equation 3.1, the energy fracture of the model damage evolution can be obtained fracture release rate. The strain energy release rate was taken to be 0.285 N/mm for peritubular dentin and 0.762 N/mm for intertubular dentin. The strain energy release rate for peri- and intercanal dentin was taken as 0.285 N/mm and 0.762 N/mm for intercanal dentin.

3 RESULTS AND DISCUSSION

3.1 Crack Sprouting

The fracture of the model at stress concentration is discussed for both cases of single PTD & DT and single DT, respectively, as shown in Fig. 1 The effect of the presence of PTD on crack extension is analyzed. In the finite element model, the components in the lumen of the toothlet, including fluid movement, etc., are neglected and are equated to a circular hole of 3 μm diameter.

In the two RVEs in the Fig. 1, a is used as a control, without considering the case of PTD, the model boundary size is 10 μm × 6 μm, and a circular hole of 3 μm diameter size at the left end of the model is used to represent the cavity of the dentinal tubule. b model considers the effect of PTD, a semicircular ring of 1.5 μm width exists around the cavity, and the rest of the dimensions remain the same as model a. The main difference between PTD and ITD in terms of composition is that ITD contains more minerals, and thus the elastic model of ITD is larger. According to. The modulus of elasticity of ITD is taken as 18GPa, the modulus of elasticity of PTD is taken as 29Gpa, and Poisson's ratio is taken as 0.3. Both models are fixed in the left plane with X and Y direction displacements, and 0.005 micron size displacement load is applied in the right plane. The mesh division is done by using hexahedral cells and ensuring the same number of boundary meshes for both models a and b.

The model is calculated using the XFEM extended finite element method in the commercial software Abaqus. It is necessary to set the loss initiation criterion and damage evolution for the model.

The loss initiation criterion used in the model is the maximum principal strain failure criterion, and the initial strain of the crack is set to 0.1% for both PTD and ITD. The loss evolution criterion of the model takes the form of energy-based fracture failure, and the strain energy release rate is taken as 0.285 N/mm for PTD and 0.762 N/mm for ITD.

The Fig. 2 shows the non-deformation clouds of RVE1 and RVE2 under representative loads. The model dimensions in the Fig. 2 legend are compared using a uniform scale and only the forward view is given for a clearer comparison of the crack extension trajectory. It is observed that both RVEs produce microcracks at the edges of the circumference of the dental tubules and the cracks continue to expand with increasing analysis steps until the crack tip strain value is below the starting strain criterion. It can be clearly seen that the crack of RVE2 is confined to the PTD region and its length is approximately 1/3 of that of RVE1. If the crack is considered to require the same fracture energy per unit length, then it has a crack extension, RVE2 consumes more fracture energy than RVE1 in crack expansion due to the presence of PTD, which undoubtedly increases the resistance of the whole structure to fracture.

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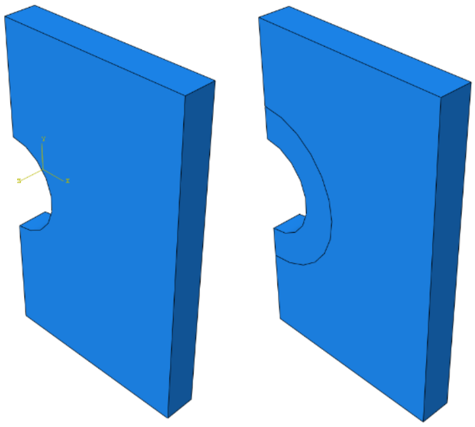
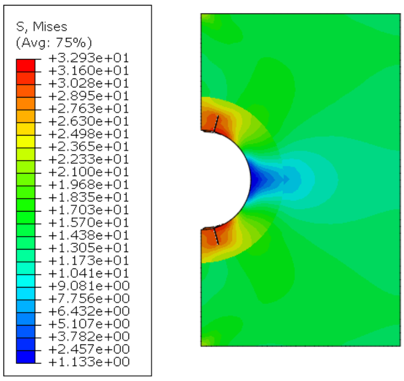
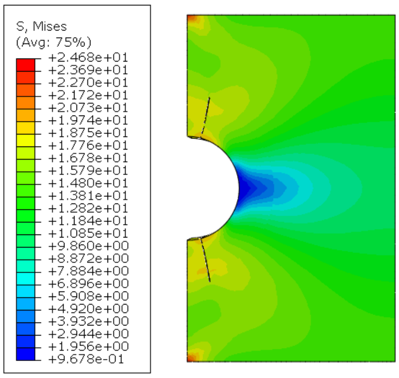


(a) (b)

Figure. 1 A schematic diagram of a collection of monophasic dentin (a) and bidirectional dentin(b).



(a)



(b)

Figure. 2 Finite element simulation stress clouds of RVE1(a) and RVE2(b).

3.2 Occurrence of Caries

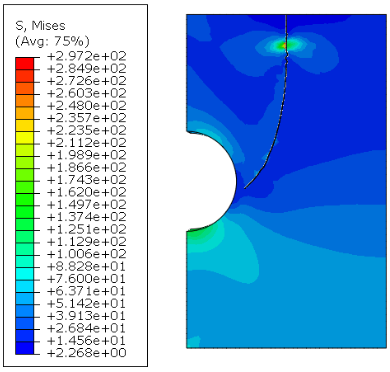
The previous study showed that bi-phase dentin has a limiting effect on crack eruption to some extent. The crack starts to sprout when the maximum principal strain reaches a set value. However, the final crack length is directly related to the presence or absence of PTD. Therefore, it can be assumed that the microstructure of the dentin has a strong influence on the crack extension.

The mechanical properties of dentin are related to its mineral content (F. Lippert,, 2014; N. Gadkari, 2021; J.H. Kinney, 1996). It has been further investigated the toughening mechanism of dentin from two perspectives, PTD and DT. A significant decrease in mineral content and mechanical properties of carious teeth was reported. The decrease in mechanical properties of dental caries is thought to be related to the decrease in demineralization content due to the caries process. The response rate of PTD and ITD to acid dissolution differs due to the different crystal packing density. In the finite element model, the caries is shown as corrosion of PTD.

Rre-add an 1 μm prefabricated crack at the top of RVE1, RVE2 and RVE3, simultaneously fixed X and Y direction displacements in the left plane of the three RVEs, and applied 0.02 μm size displacement load in the right plane.

The Fig. 3 shows the stress clouds of RVE1-3 finite element simulation. In RVE1, the crack extension is relatively smooth, and the crack inflects directly into the periapical dentin region in the junction region of PTD and ITD, almost penetrating into the dentinal tubules. In RVE2, the crack extension path was more tortuous, especially in the junction area of the two phases, the crack was inflected, thus avoiding the dentinal tubules and protecting them from being destroyed. When the caries occurred, the crack completely penetrated the dentinal tubules. The transition section was well protected by PTD before acid dissolution, and the fracture occurred only in the PTD region. After acid dissolution, the protection of the transition section by PTD was weakened, and the fracture penetrated the transition section and extended to the ITD region.

The comparison between RVE1 and RVE2 can show that PTD is able to resist the crack expansion, which makes the crack expand along a longer path, and undoubtedly increases the ability of the whole structure to resist fracture, which certainly explains the existence of PTD. The comparison between RVE2 and RVE3 shows that the latter crack re-expands towards and eventually penetrates the dentinal tubules, which proves that caries causes cracks to tend to expand towards the dentinal tubular cavity, thus destroying the resistance of the tooth to fracture. This is certainly an undesired outcome.



(a)

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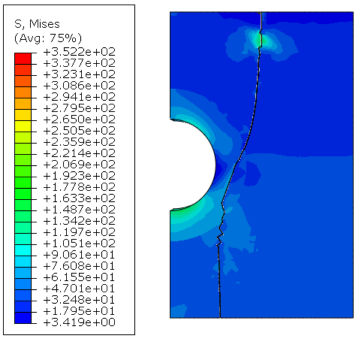
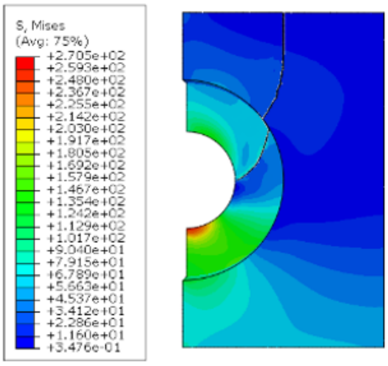


(b)



(c)

Figure. 3 Schematic diagram of finite element simulation of monophasic(a), bidirectional(b) and caries models(c).

4 CONCLUSION

The mechanical properties of the intact as well as the demineralized human dentin were analyzed and studied numerically in three dimensions. The toughening mechanism of dentin was investigated by XFEM extended finite element method. The main conclusions of this study were obtained as follows:

1. RVE1 hinders crack extension. According to the energy-based fracture damage criterion, RVE2 shows longer crack extension compared to RVE1 for the same representative load.

2. The presence of peritubular dentin makes the crack extension more tortuous, with more folding and bending of the crack, which leads to more fracture energy being consumed by the crack during extension and therefore makes the structure able to resist crack extension.

3. Acid etching exacerbates the expansion of microcracks and weaks the shielding effect on cracks. These findings provide support for the study of tooth remineralization and offer the possibility of new biomimetic materials.

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