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Effects of Material Modulus on Fracture Toughness of Human Enamel, a Natural Biocomposite

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Abstract The enamel, the upper layer of a tooth has remarkable capability of bearing severe loading on the tooth. The fracture behavior is important to understand the mechanism of load bearing and it could be very useful for developing new materials. Non-destructive evaluation of such materials will also benefit from this knowledge. The graded microstructures of enamel were modeled by finite element analysis software and the J-integrals and the stress intensity factors were evaluated as the fracture parameters. The results show that these parameters are location dependent. Those values increase when measured in the direction of dentine enamel junction. This finding matched well with experiments and implies many useful understanding of biomaterials and applications to new materials.

Keywords: Human Tooth Enamel, XFEM, Biocomposite, Fracture Toughness, J Integral, Stress Intensity Factor, Biomaterial

1. Introduction

Human tooth system is one of the most important organs that plays vital role in mastication process by which food is crushed and ground. It consists of 3 layers, namely an upper hard envelope enamel and inner porous dentine separated by interfacial layer dentine enamel junction (DEJ). The upper cover enamel is most important layer as it has to withstand various types of loads and loading environment at first hand. The enamel is composed of 85%, hydroxypatite crystal, 12%, water and 3% organic matrix by volume[1]. On microstructural level, the enamel is composed of enamel rods of key hole shape of about 5m diameter right from dentine enamel junction towards its upper surface just below 6-12 m from the upper surface of tooth[2]. Each single enamel rod consists of bundles of hydroxyapatite crystals of about 50nm in diameter covered by an approximately 1nm thick organic layer[3,4]. It has been explained in literature that enamel dictates whole tooth deformation[5]. Mechanical properties of enamel are depth dependent[6,7] and represents functionally graded structure. It has highest elastic modulus at upper layer and gradually reduces when it is measured towards dentine enamel junction[6-8] (Fig. 1) and it works as natural coating due to its wear resistant property. There are various experimental techniques employed to study enamel and its behavior against different loading environments. Atomic force microscope study of dental enamel structure and synthesis has been carried out to understand its structure[4]. Fatigue crack growth in human enamel and hydroxyapatite comparison have been presented[9-11]. Nanoindentation technique has been employed to determine elastic/inelastic/plastic transition of human

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enamel and mapping of mechanical properties of molar tooth[12-15]. Micro-indentation fracture behavior of human enamel was carried out to determine crack resistance behavior in relation to its microstructure[16]. The resilience of human tooth and its fracture mode[17-19] have been studied to understand the failure behavior of its layers. The fracture behavior of dental enamel is studied with single edged notched bending specimens(SNEB) in three point bending and thereafter analyzing with optical and environmental scanning electron microscopy[20, 21]. Mixed-mode stress intensity factors for kink cracks with finite kink length loaded in tension and bending have been determined for dentine and enamel[22].

Literature survey shows that there are only few works for investigation on toughening properties of enamel and most of them are experimental techniques. Proper estimation of toughness of enamel by modeling and simulation of crack growth along with its crack bridging capability will help to understand this natural composite much better and can help further development of dental implant materials with toughening behavior.

2. Material and Method

2.1 Extended Finite Element Method (XFEM)

The extended finite element method (XFEM), also known as generalized finite element method (GFEM) or partition of unity method (PUM) is a numerical technique that extends the classical (FEM) approach by enriching the solution space for solutions to differential equations with discontinuous functions. This method was first introduced by Melenk and Babuska[23] by exploiting partition of unity concept in finite element. Thereafter many authors[24-30] have contributed to development of this method and presently it became one of the most powerful techniques to study cracks and discontinuities in materials. Moreover, treating problems with discontinuities with Extended Finite Element Methods suppresses the need to mesh and remesh the discontinuity surfaces, thus alleviating the computational costs and projection errors associated with conventional finite element methods at the cost of restricting the discontinuities to mesh edges.

2.2 Introducing Nodal Enrichment Functions

For the purpose of fracture analysis, the enrichment functions typically consist of the near-tip asymptotic functions that capture the singularity around the crack tip and a discontinuous function that represents the jump in displacement across the crack surfaces. The approximation for a displacement vector function with the partition of unity enrichment is in Fig. 2.

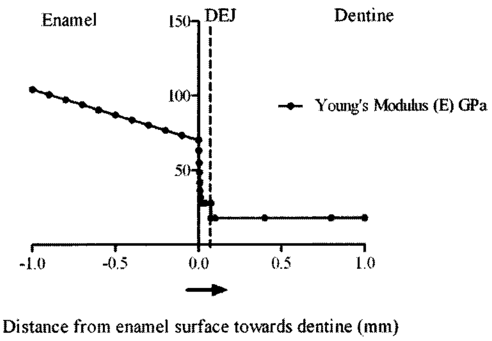


Fig. 1 Young's modulus variation in human tooth from enamel to dentine side

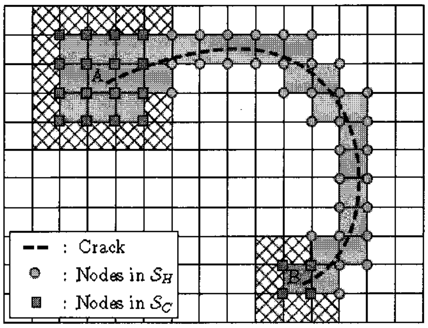


Fig. 2 Enriched nodes around the crack tip in XFEM

$$u=\sum_{I=1}^{N}N_I(x)\left[u_I+H(x)a_I+\sum_{\alpha=1}^{4}F_\alpha(x)b_I\alpha\right].$$

Where ‘S’, set of all nodes in the FE mesh, ‘S_c’, set of nodes around the crack tip and ‘S_H’, set of nodes of elements cut by the crack but not in S_c.

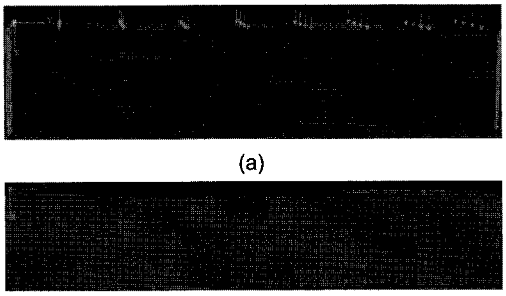
$$u^h(x)=\sum_{\forall I}N_I(x)u_I+\sum_{j\in S_c}N_J(x)[H(f(x))-H(f(x_J))]q_J^0$$
$$+\sum_j\sum_{k\in S_c}N_K(x)[\psi^j(x)-\psi^j(x_j)]q_K^j$$

where H(.) is the Heaviside step function.

Where Ψ^J is set of enrichment functions which approximate the near tip behavior, q_I^J are the enrichment coefficients and X^J is position of node J.

2.3 Finite Element Analysis

The upper cover of tooth, the enamel, has been modeled in ABAQUS 6.9 as three points bending test specimen with 34 layers with a through crack at the outer surface below and moving towards dentine enamel junction upward considering all the layers with homogeneous, elastic and isotropic material property as shown in Fig. 3 The location of the crack is considered at the outer portion of the enamel. Both the ends are fixed and compressive pressure loads are applied at the upper surface of the model. The whole model has been meshed by 100 thousands of 3-D stress elements available in ABAQUS. XFEM is mesh insensitive and cannot be affected by the number of elements considered near the crack. Taking advantage of this phenomenon of XFEM, we have meshed the whole model homogeneously and no extra mesh concentration was adopted near the crack surface. General static analysis is carried out to simulate crack growth and thus estimated the J-integral.


(a)

(b)

Fig. 3 ABAQUS Model with (a) load, boundary condition and (b) mesh

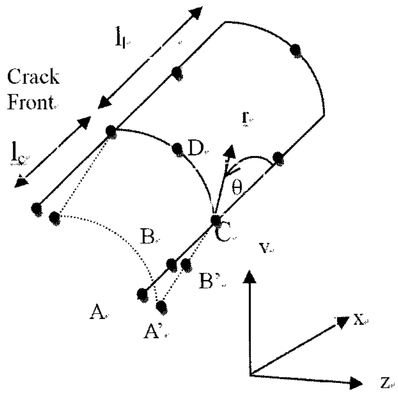


Fig. 4 Extraction of different modes of SIF in functionally graded materials [31]

2.4 Extraction of Mixed Mode Stress Intensity Factors

Luchi and Rizzuti[31] developed a method to extract mixed mode stress intensity factors in terms of displacements at the crack-tip node and at the nodes vicinity of the crack-tip as shown in Fig. 4.

The mode I, II and III stress intensity factors can be evaluated as

$$K_I=\frac{E}{4(1-\nu^2)}\sqrt{\frac{\pi}{2}}\frac{2\sqrt{2}(u_y^B-u_y^{B'})-(u_y^A-u_y^{A'})}{\sqrt{I_c}}$$

$$K_{II}=\frac{E}{4(1-\nu^2)}\sqrt{\frac{\pi}{2}}\frac{2\sqrt{2}(u_x^B-u_x^{B'})-(u_x^A-u_x^{A'})}{\sqrt{I_c}}$$

$$K_{III}=\frac{E}{4(1-\nu^2)}\sqrt{\frac{\pi}{2}}\,\frac{2\sqrt{2}(u_z^B-u_z^{B'})-(u_z^A-u_z^{A'})}{\sqrt{l_c}}$$

Where 'E' is Young's modulus of material, 'v' is Poisson's ratio and u_x, u_y, u_z are displacements at crack-tip node and at the node in the vicinity of the crack-tip as shown in Fig. 4.

We have evaluated the mixed mode stress intensity factors at different locations of enamel by using above relations. Though the enamel acquires functionally graded micro structure, we can use this method as it is modeled as 34 homogeneous, isotropic layers.

3. Results and Discussion

The crack growth simulation for straight crack, slant crack, and fracture toughness estimate in terms of J-integral and mixed mode stress intensity factors at various locations have been presented and discussed below.

3.1 Crack Growth Simulation

Crack growth simulation has been carried out in XFEM environment for slant and straight cracks to see the nature of crack growth and crack growth direction as shown in Fig. 5. It has been observed that the crack grows in different direction than the initially specified direction in both straight and slant crack cases as shown in Fig. 5. This phenomenon has been observed experimentally too[20]. The bottom part shows full crack opening while the upper light part shows partial crack opening in XFEM environment in Fig. 5 (a)[32]. We have recorded amount of load required to achieve particular amount of crack growth (Fig. 6). It has been found that as we move towards dentine side, the load required for crack to grow increases. This phenomenon is in agreement with the amount of brittleness. The outer surface is more brittle in nature and while moving towards dentine side, the amount of brittleness decreases and the load carrying capacity also increases.

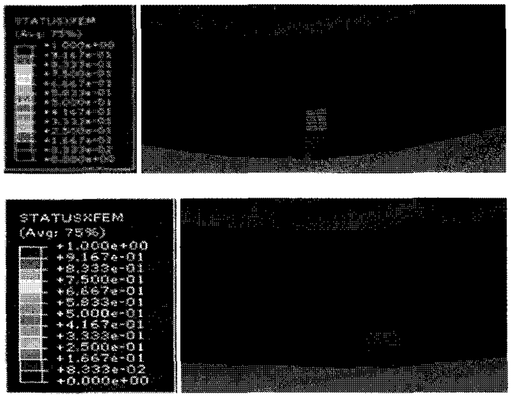


Fig. 5 Crack growth simulation for (a) slant crack (b) straight crack

3.2 J-Integral Estimate

The analysis shows the crack can grow from the initial crack size of 30 microns when we apply pressure load more than 12.5 kPa. The amount of load increases to achieve the crack growth (Fig. 6) and 400 micron growth towards the dentine has been achieved at 37.5 kPa pressure load applied to the upper surface of the model. The J-integral values have been estimated in XFEM directly from ABAQUS. It has been found that the J-integral values are not constant like other artificial materials and rather it is location dependent. At the upper tooth surface, the J-integral value (Fig. 7) is 75 J/m^2, and at a distance of 500 microns, it has been found to be 115J/m^2. This location dependent property of energy release can be attributed to its functionally graded micro structure so that the upper surface is more brittle and crack grows at lesser value of critical energy release rate. While moving towards dentine side, the amount of energy to be released to create another surface i.e. to grow crack is more due

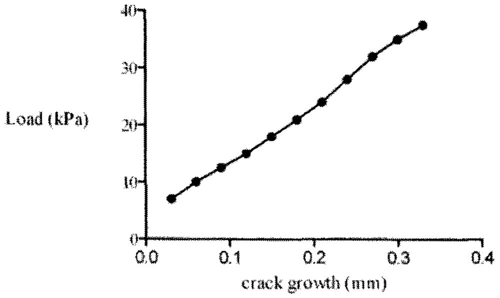


Fig. 6 Crack growth verses load in enamel from upper surface towards dentine side

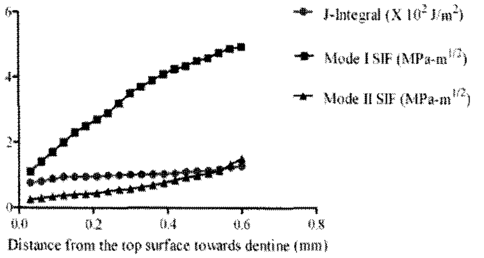


Fig. 7 J-integral, I and II Mode SIF versus distance from the enamel upper surface

to decreased brittleness. It can be attributed to orientation of enamel rods as well. The enamel rods are perpendicular near the dentine side while it is parallel near the upper surface.

3.3 Stress Intensity Factors

The stress intensity factors have been extracted by recording displacements at the crack-tip node and the nodes at the vicinity of the crack-tip as shown in Fig. 4 using the relations expressed above. The stress intensity factors (Fig. 7) also have been found to be location dependent like J-integral values. These results are in agreement with the results provided by Bechtle et al. [20]. These location dependent properties can be again attributed as in case of J-integrals.

4. Conclusions

The present study shows that FE analysis can enable first-hand estimation of the fracture toughness of the human-tooth system, which subsumes its own composite that has very complex material properties. The location dependent fracture toughness of this biological composite, enamel, with hierarchical material property is in agreement with the experimental observation by Bechtle et al. [20]. The crack growth simulation shows that the crack changes its predefined path as observed experiment. The Extended Finite Element Method (XFEM) proves to be very effective tool in such case where we conducted crack growth simulation for model with graded material properties and thus for evaluation of fracture toughness parameter too. The J-integral determined here can be a basis for non-destructive estimation of enamel to investigate overall properties.

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