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A Study on the Fracture Behavior of Tooth Interfacial Layer, DEJ (Dental Enamel Junction)

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치아 계면 층 DEJ(Dental Enamel Junction)의 파괴 거동에 관한 수치해석적 연구

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Abstract

Numerical experiments on biological interfacial layer, DEJ by finite element software ABAQUS have been conducted to study its fracture behavior including crack bridging / arresting characteristics in the model. Crack growth simulation has been carried out by numerical tool, XFEM, devoted to study cracks and discontinuities. The fracture toughness of DEJ has been estimated before and after crack bridging. The implications of bridging in numerical study of fracture behavior of DEJ-like biological interface have been discussed. It has been observed that the results provided by the numerical studies without proper accommodation of bridging phenomenon can mislead. This study can be helpful for understanding the DEJ-like biological interface in terms of its fracture toughness, an important material characteristics. This property of the material is an important measure that has to be taken care during design and manufacturing processes.

Key Words : Dental Enamel Junction(치아계면층), Graded fracture toughness(계층적 파괴인성), Crack healing/bridging(균열 치유/브리징), Graded microstructure(계층적 미소 구조), Bridging elements(브리징 요소)

1. Introduction

Human-tooth system is one of the most important organs for the mastication process. It consists of a hard and brittle enamel cover and porous dentin. They are separated by very thin interfacial layer, called the Dentin Enamel Junction (DEJ) or crown dentin. DEJ has unique biomechanical properties. It provides crack-arrest barrier for flaws that form in the brittle enamel(1~5). Enamel envelopes the softer dentine, which is a biological composite that is tougher than enamel and similar in terms of the nano-structure to bone.

The DEJ has a hierarchical microstructure with a 3-D scalloped appearance along the interface. It has a different microstructure at the boundaries with enamel and dentin; therefore, DEJ has been represented by a functionally graded structure(1,2,6,7), as shown in Fig. 1. In these works, the authors have discussed profiles of the mechanical properties such as elastic modulus and hardness across the

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DEJ using various experimental techniques. They discussed about amount and orientation of mineral contents in DEJ region near enamel and near dentin region as well. It has been found that elastic modulus and hardness both near the enamel end are higher and decreases sharply within the range of 10-15μ. The region near dentin is reacher in terms of mineral content while amount of mineral decreases while moving towards enamel end. The orientation of these mineral contents is also different at these two ends. The microstructure itself at both the ends is different. These are the factors which heavily influence the mechanical properties along with its special crack arrest behavior. DEJ is very thin functional zone, investigated long ago(3,8,9).

Fracture behavior of DEJ has been investigated by various experimental techniques(1,2,4,5,10~13) and discussed about structure property relations, failure modes and its special crack arresting behavior. Normally in artificial materials, interfaces are more prone to failure and thus more attention is given while designing interfaces. Though DEJ is interface, but due to its microstructure, orientation of its micro-structural constituents, there cannot be catastrophic failure in this region. Rather crack emanated from enamel, when it reaches to this region; it starts bridging/arresting. The crack arrest behavior of tooth at DEJ has been investigated very recently by Bechtle et al.(14). The reason for arresting crack has been attributed to the gradation of elastic modulus of this region. Fracture behavior of dental enamel has been discussed by Bechtle et al.(15) with major focus on changing toughness with location through their investigation on single edge notch beam (SNEB) specimen for enamel layer.

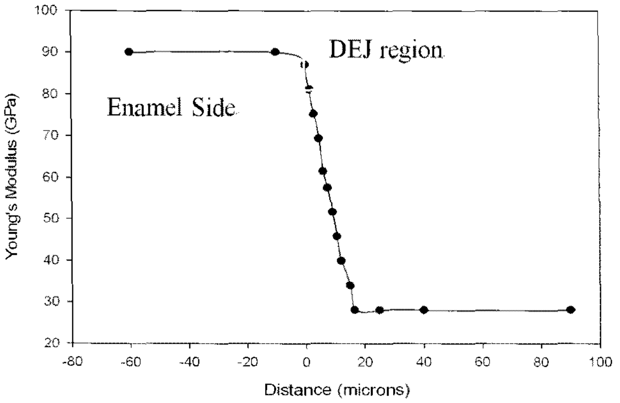

Fig. 1 Young's modulus variation in human tooth from enamel to dentine side

In this paper, we have presented numerical study on fracture behavior of DEJ by extended finite element method (XFEM) taking care of its crack arresting/bridging behavior. This special characteristic of biological interfacial layer DEJ has been numerically simulated. The implications of crack bridging/arresting phenomenon on load carrying capacity and toughness of DEJ have been discussed. Material toughness is an important criterion to decide about manufacturing processes and tools to be used. Thus the importance of including this phenomenon in the numerical model has also been discussed to correctly estimate the fracture toughness of DEJ like biological interface.

2. Extended Finite Element Method

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 finite element method (FEM) approach by enriching the solution space for solutions to differential equations with discontinuous functions. This method was first introduced by Melenk and Babushka(16) by exploiting partition of unity concept in finite element. There after many authors(17~23) have contributed to develop this method and presently 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.

2.1 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 (Fig. 2).

$$u^h(x) = \Sigma_{i\in I} N_i(x) u_i + \Sigma_{i\in I} M_i(x) a_i \tag{1}$$

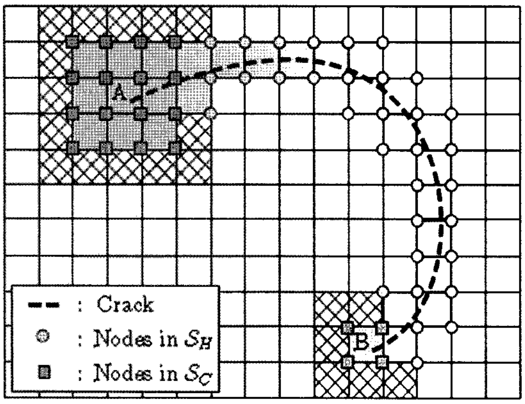

Fig. 2 Enriched nodes around the crack tip in XFEM

The first term of the equation 1 is related to finite element approximation and second term is enrichment of the crack tip nodes in XFEM analysis.

Fig. 2 shows schematic representation of crack in XFEM. Here 'S' is the 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'.

3. Materials and Methods

The tooth interfacial layer DEJ has been modeled in ABAQUS to understand the crack growth and thus to determine the critical loads at which crack starts growing. The fracture toughness of biological interfacial layer DEJ has been estimated in terms of J-integral and stress intensity factors. The modeling strategies have been discussed below.

3.1 Modeling strategy for DEJ

The interfacial layer of tooth, the DEJ has been modeled in ABAQUS 6.9 as three points bending test specimen of size 10mm×0.075mm (Fig. 3). This has been divided into 11 homogeneous, isotropic layers with a through crack at the surface near enamel end and moving towards dentine side (Fig. 4). The elastic modulus of DEJ drops sharply from enamel side to dentine side within a distance of 15 μ (Fig. 1). Thus 10 layers near enamel surface each of 1.5μ have been modeled with decreasing Young's modulus layer by layer from 70GPa to 32.2GPa. The eleventh layer near dentine surface of 60μ thickness has Young's modulus of 28GPa. The location of the crack is considered at the surface near enamel end as shown in Fig. 4. 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 56 thousand 2-D plain strain elements (Fig. 5) available in ABAQUS. XFEM is mesh insensitive and cannot be affected by the number of elements in the vicinity of the crack. Taking advantage of this phenomenon of XFEM, we have meshed the whole model homogeneously and no extra mesh concentrations near the crack surface have been created.

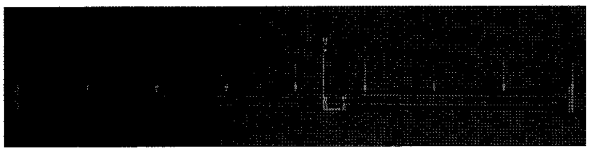

Fig. 3 Geometry, loading and boundary conditions in DEJ model

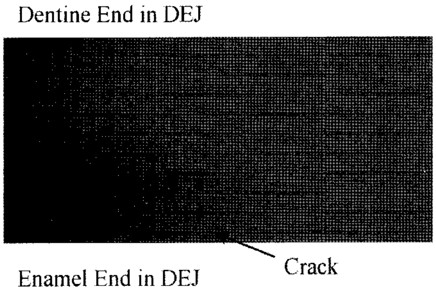

Fig. 4 Layers in DEJ with crack location

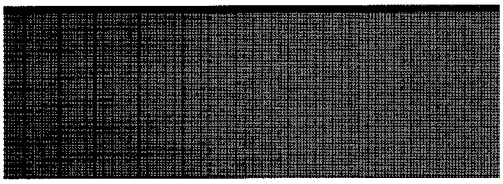

Fig. 5 FE 2D mesh with plain strain elements

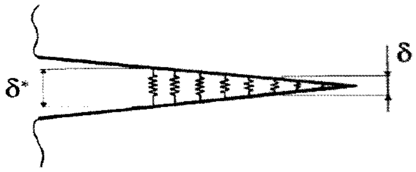

Fig. 6 Schematic representation of crack bridging

The crack arresting/bridging behavior of DEJ has been modeled and simulated by introducing one-D spring elements joining opening nodes by the crack surface (Fig. 6). It is based on the concept that the energy released while growing the crack due to excessive load can be absorbed by the bridging elements and thus crack cannot grow further. Rather the crack arresting/bridging takes place due to the amount of energy absorbed by the bridging elements

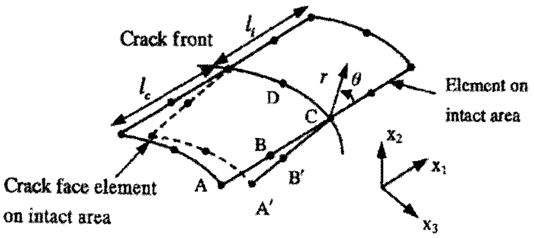

Fig. 7 Extraction of different modes of SIF in Functionally Graded materials(30)

introduced in the numerical model.

3.2 Extraction of Mixed Mode Stress Intensity Factors

Luchi and Rizzuti(30) developed a method to extract mixed mode stress intensity factors for FGMs in terms of displacements at the crack-tip node and at the nodes vicinity of the crack-tip as shown in Fig. 7.

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

$$K_I = \frac{E}{4(1-\nu^2)}\sqrt{\frac{\pi}{2}}\,\frac{2\sqrt{2}\left(u_y^B - u_y^{B'}\right) - \left(u_y^A - u_y^{A'}\right)}{\sqrt{l_c}} \tag{2}$$

$$K_{II} = \frac{E}{4(1-\nu^2)}\sqrt{\frac{\pi}{2}}\,\frac{2\sqrt{2}\left(u_x^B - u_x^{B'}\right) - \left(u_x^A - u_x^{A'}\right)}{\sqrt{l_c}} \tag{3}$$

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

Where 'E' is Young's modulus of material, 'ν' 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. 7.

We have evaluated the mixed mode stress intensity factors at different locations of DEJ by using above relations.

4. Results and Discussions

General static analysis for DEJ has been carried out and crack growth simulation has been done. The critical load at which crack grows has been evaluated based on the crack growth simulation. The fracture toughness of interfacial layer DEJ has been evaluated in terms of J-integral which is measure of energy release rate. The stress intensity factor has been evaluated based on the displacements at the nodes at the crack tip and its vicinity by the relations given in equations(2-4). The crack bridging simulation has been carried out and the actual energy release and the critical load that need to grow the crack have been evaluated.

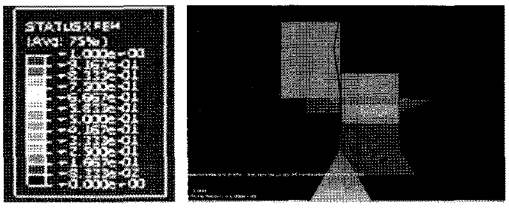

Fig. 8 Crack growth simulation in DEJ

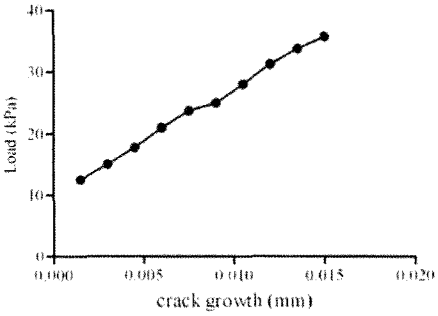

Fig. 9 Load carrying capacity verses crack growth in DEJ

4.1 Crack growth simulation for DEJ

Crack growth simulation has been carried out in XFEM environment, for DEJ to see the nature of crack growth and crack growth direction as shown in Fig. 8. It has been observed that the crack grows more or less in the same direction as initially specified unlike in the case of enamel(15). The red color shows full crack opening while the green color shows partial crack opening in XFEM environment(29). We have recorded amount of load required to achieve particular amount of crack growth (Fig. 9). It has been seen 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. In case of DEJ, the surface near enamel is more brittle in nature and while moving towards dentine side, the amount of brittleness decreases and the load carrying capacity also increases.

4.2 Fracture Toughness Estimate for DEJ before Bridging

The fracture toughness of DEJ has been estimated in terms of J-integal, which is measure of energy release and stress intensity factors (Ks). Both of the parameters of measure of fracture toughness have been found to be location dependent (Fig. 10) in place of a single material constant like in most of the artificial materials. Similar property in enamel has been attributed to material gradation(15). So the location dependent fracture toughness of DEJ can also be attributed to its graded micro structure(14). Another reason for the graded toughness of DEJ can be the amount and orientations of mineral contents near enamel and dentine end. It has experimentally found that the dentine end of DEJ is richer in terms of mineral content while at enamel end, amount of mineral is lesser. To validate the result, we have compared our result with the experimental investigation result by Imbeni et al.(5). The critical energy release rate for DEJ, as reported by Imbeni et al.(5) is 115kJ/m^2. The investigation carried out by Imbeni et al.(5) was Vickers indentation method and have not measured the toughness at every location in the thickness direction of the DEJ due to its functional size (75μ). Our result is location dependent as shown in Fig. 10. We found the amount of energy release at a distance 10μ from the enamel surface towards dentine as 116.8 kJ/m^2. This is very close to the result presented by Imbeni et al.(5). The similar location dependent fracture toughness has been presented for enamel(15) for the similar graded micro structure. Thus we can conclude that toughness of the biological interface layer DEJ has graded toughness like graded elastic modulus in place of constant material property in most of the artificial materials. Another interesting finding is, the stress intensity factor found to be pure mode I as moving towards dentine side. Only case of mode mixity has been observed at nearest position from the enamel side. This has been continuation from enamel as in enamel, at the upper surface, mode mixity is higher and it reduces while moving towards DEJ side. Here, the mode mixity ends at very near to the enamel surface and there after it is pure mode I.

4.3 Simulation of Crack Bridging/Arresting behavior of DEJ

It has been experimentally observed that the dentine enamel junction (DEJ) has crack bridging/arresting capability(5). The crack emanated from brittle enamel surface, when reaches to the interfacial DEJ region, it starts arresting/bridging within a distance of 15μ from the enamel surface. There are different types of bridging techniques discussed in literature(24). We have simulated the crack bridging/arresting behavior of DEJ by introducing one dimensional spring elements as shown in Fig.6. The stiffness of spring elements has been found to be 1% of the elastic modulus of the DEJ at that location which can achieve the complete crack closure within a distance of 15μ in DEJ from enamel surface. The crack bridging stress has been evaluated on the basis of the relation $\sigma_b = f(\delta)$. It has been found that the amount of compressive stress in the spring element reduces while moving towards dentine side. Fig. 11 presents crack opening observed due to external pressure load applied at particular location and the subsequent crack closure due to the spring elements introduced at particular locations. Initially the width of crack opening is bigger and the closure is only partial but moving towards dentine side, at 10μ distance, full crack closure has been achieved when we choose the stiffness of spring as 1% of the elastic modulus at that location in the DEJ.

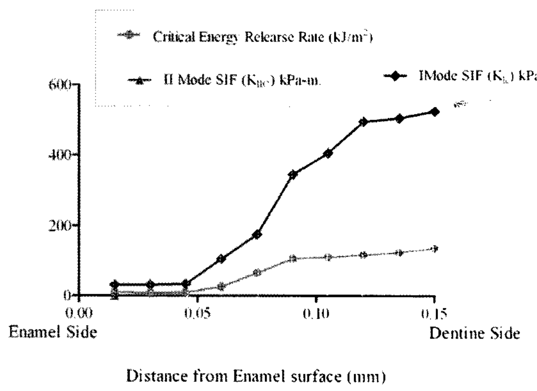

Fig. 10 Fracture toughness of DEJ in terms of J-integral and stress intensity factors

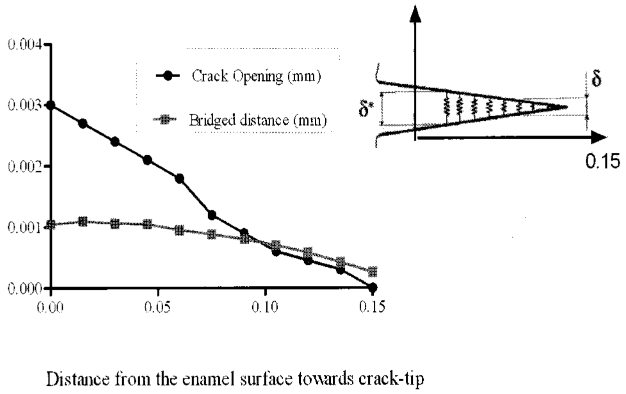

Fig. 11 Crack bridging simulation in DEJ

4.4 Fracture Toughness after Bridging

The DEJ is a biological interfacial layer with special crack bridging capability. Due to this phenomenon of crack bridging in DEJ, it becomes special interface layer and many artificial materials basically the dental implant materials and interfaces have been mimicked. Evaluating fracture toughness of DEJ like materials, crack bridging/arresting property should be taken into consideration which after all increases its load carrying capacity. Here we have estimated fracture toughness of DEJ before and after bridging elements introduced numerically and compared the results.

It has been found that the energy release rate attains critical value at a distance 15μ from enamel surface of the order of $136.5kJ/m^2$ before bridging elements have been introduced, after which it is assumed in most of the materials further crack growth. In case of DEJ, if we assume such phenomenon, our estimates predict misleading results. The bridging elements introduced thereafter absorb the energy released and thus stop the crack growth. In this case, at particular distance of 15μ, the critical energy release has been obtained to be $136.5kJ/m^2$. After the bridging elements, at that particular load, the net energy release reduces to be $6.87kJ/m^2$ (Fig. 12). We can conclude that, it needs more load to further crack growth. Further increase in pressure load, increases the energy release that attains 5 critical value at higher load. This shows, the load bearing capability of the DEJ is far more than it has been estimated before the bridging phenomenon introduced in the numerical model.

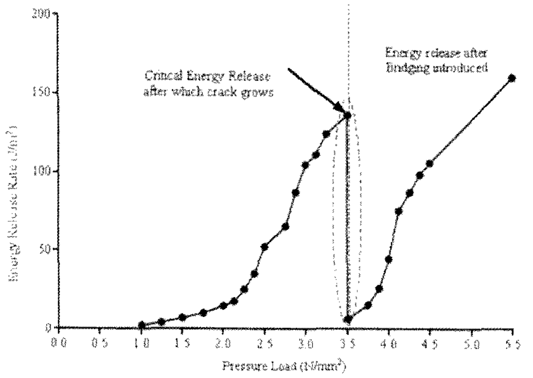

Fig. 12 Energy release before and after bridging elements introduced

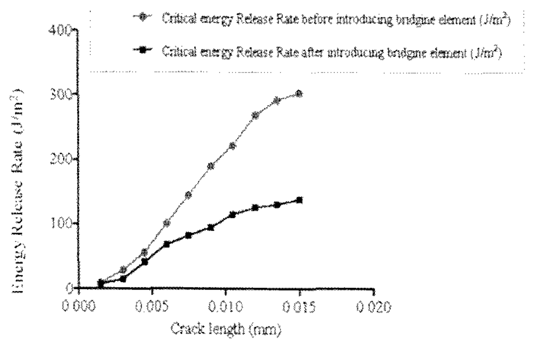

Fig. 13 Critical energy release rate before and after bridging elements introduced

Fig.13. presents critical energy release rate before and after bridging elements introduced. We can see that the critical energy release before and after bridging are different and in the cases of interfaces like DEJ. The fracture toughness estimate without considering the bridging phenomenon provides misleading results. The load carrying capacity increases drastically due to this bridging phenomenon.

4.5 Inspiration of DEJ like interface on Dental implant material Development

The dental implant materials industry is developing newer materials which are biocompatible and can withstand the load and loading environment, the tooth has to undergo inspired from the biological materials and interfaces. In the recent times, these implant materials are being made up of Zirconia, a brittle upper layer and the lower ceramic filled polymer joined by interfacial adhesive layers(25~26). The interfacial adhesive layers are very thin (100μ). Nowadays these adhesive thin layers have been manufactured as functionally graded material modulus in place of isotropic layer(26), inspired from the microstructure of the DEJ. These functionally graded materials for interfacial adhesive layers have improved the load transferring capability as well as prevent the chances of failure. There are many literatures available on this aspect of material development and related investigations(25~28). There are various types of implant materials are being developed. The recent focus of the dental implant industry is to develop composite materials with self healing capabilities.

5. Conclusion

The present study shows that FE analysis can enable first-hand estimation of the fracture toughness of the biological interfaces like DEJ, which subsumes its own composite that has very complex material properties. The

DEJ, which is an interfacial very thin layer but very rich in diversities in its microconstituents and structures inhibit the crack arresting phenomenon. The fracture toughness of DEJ has been found to be location dependent in its thickness direction from enamel side to dentine side. Simulation of crack bridging behavior can be well carried out numerically by introducing one-D spring elements with the stiffness of 1% of the elastic modulus of the DEJ at that location. The implication of bridging on the load carrying capacity and the actual fracture toughness has also been discussed in detail. This type of estimation of the fracture strength of biological interfacial layers, such as the dentine enamel junction (DEJ), helps to better understand the dental layers and thus facilitate the future development of dental implant materials where the focus is on developing new material that is not only friendly to live biological systems and processes but also has the capability of self-healing when damage occurs within. This result can be further improved by considering better modeling techniques and representing the complex material properties of the DEJ as accurately as possible.

Acknowledgement

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