



Journal of Computational and Applied Research in Mechanical Engineering Vol. 6, No. 1, pp. 1- 9, Aut.-Win. 2016-17 http://jcarme.srttu.edu



An investigation into finding the optimum combination for dental restorations

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Article info:

Received: 16/07/2015 Accepted: 03/01/2016 Online: 11/09/2016

Keywords:

Porcelain, Dental, Restorations, Plastic deformation, Radial Cracks, XFEM.

Abstract

The aim of the study was to find the optimum combination of materials and thicknesses to provide a tough, damage resistant multi-layer system with numerical methods to restore the damaged teeth. Extended Finite Element Method (XFEM) was used to assess the critical loads for the onset of damage modes such as radial cracks and plastic deformation in dental prostheses, which consist of a brittle outerlayer (porcelain)/ metal (Au, Pd, Co)-core/ substrate (dentin) trilayer system. XFEM not only has the ability to model crack initiation process, but also could solve crack propagation problems. Generally speaking, porcelain layer shouldn't be thinner than 0.5 mm, as the stresses due to bending become tensile critically in porcelain undersurfaces and radial cracks would occur in low loads. Also, it could be concluded that XFEM in axisymmetric model could properly estimate crack initiation and propagation path. Yielding of metal core makes additional flexural stress at overlaying brittle surface and consequently, facilitates radial cracks. In dental applications, the optimum porcelain thickness would be between 0.75 and 1.25 mm. Furthermore, yield strength and stiffness of metal is better to be high sufficiently to prevent it from plastic deformation and ensuing radial cracks.

1. Introduction

Nowadays, ceramics are used extensively in restorative dentistry; since they are biocompatible, stiff, wear resistance and specifically, their aesthetic property [1-3]. However, they are brittle materials and still suffer high rate of fracture when used as prostheses. It is of significant importance to develop an engineering approach to predict crack initiation and propagation in ceramic structures when exposed to loading. Static indentation on bilayer ceramics structures loaded by a spherical indenter has long been studied in the past [4-8], but quite little research has been done on trilayer systems [9-11]. Ceramic/metal/polymer layer structures are of interest in a wide range of biomechanical applications, since the wear resistance of a brittle coating combines with the toughness of a ductile metal underlayer. A classic example can be found in dentistry, where a restoration composed of a porcelain ceramic veneer fused to a stiff metal core forms an integral crown and then, it is cemented onto a compliant dentin tooth base [12, 13].

Ceramics are attractive dental restoration materials because of their aesthetics, biological acceptance, and chemical durability. Allceramic restorations appear very natural. But the materials used in these restorations are brittle and subject to damage from high tensile In opposite. despite all-metal stresses. restorations are strong and tough, they are not acceptable from an aesthetic viewpoint. Fortunately, the combination of the aesthetic properties of ceramic materials with the strength and toughness of metals has been performed to produce restorations which have both a natural tooth like appearance and very good mechanical properties. As a result, they are more successful restorations than allceramic crowns [14, 15].

Tooth flexure is described as a lateral or axial bending under occlusal loading. Tooth flexure produces high tensile stress gradients in the undersurface ceramic layer which is leading to the formation of cracks at this region and causes eventual failure of the structure [16].

The most frequent failure factors associated with porcelain veneers is fracture. It stands for 67% of total failures after an observational period of 15 years of clinical performance of such restorations [17].

Compared to analytical methods, FEM has fewer limitations in dealing with objects with complex geometries [18]. Increasingly, FEM is also being used as part of the design process to simulate failure of structures and components as a means to reduce the need for making prototypes and performing actual experiments which are usually expensive and timeconsuming [18, 19].

Moreover, fracture mechanics principles are integrated to FEM to analyze the failure process of components. XFEM is commonly used to investigate the fracture evolution in polycrystalline materials. The basic idea of XFEM is to add the enrichment functions to the conventional displacement approximation [19]. XFEM provides flexibility in modeling, as crack doesn't need to be aligned with the element edges. Similar to FEM, it can determine the points which are vulnerable to crack initiation and in addition, it has even the ability to predict crack propagation path in the way of comparing the stress intensity factor with fracture toughness. However, XFEM analysis is much more time consuming in contrast to conventional finite element method. Barani et al. [20] analyzed the enamel of molar and premolar teeth to find the effect of soft and hard indenters on longitudinal cracking. They used XFEM to simulate the growth of embedded cracks in enamel. Barani et al. [21] utilized XFEM to analyze longitudinal cracking from initial propagation to final failure. They simulated crack growth in tooth enamel as a function of biting forces. Lawn et al. [22] analyzed transverse fracture in canine teeth with applying XFEM package in order to visualize crack evolution process.

The overall intention of this study was to define the best combination of materials and thicknesses to provide a durable multi-layer system. This research made an XFEM analysis to the work done by Zhao et al. [12], which found the damage caused by two major failure modes; the formation of radial cracks at the bottom surface of the outerlayer, and plastic deformations at the top and bottom surfaces in the metal layer. Other crack type- cone crack which is initiated at the top surface of the outerlayer near the contact point- can occur, but it is not the focus of the present study. The XFEM provided the opportunity to study the stress fields in the coating and substrate which is typical in FEM, in addition to the initiation points and propagation path of cracks, in order to follow and predict the critical conditions under which different modes of failure occur.

2. Materials and Methods

Due to symmetry, the model was analyzed in an axisymmetric simulation with a hemispherical tungsten carbide indenter (3.96 mm radius) in a frictionless contact with multilayer (8 mm radius). The substrate layer was assumed to be constant with 12.5 mm thickness (d_s) for all models. Model of coating/metal/substrate trilavers were simulated according to Fig. 1.



Fig. 1. Model of coating/metal/substrate trilayers.

2. 1. Comparison of models with or without adhesive layer

Due to the existence of experimental results from [12] and in order to compare numerical results with them, two different metal cores (aluminum and steel) under constant thickness of glass coating (1.2 mm) were modeled to investigate the effect of adhesive layer (h)between coating and metal. The metal layer thickness was assumed to change from 0 to 3.5 mm. Polycarbonate was used as substrate. Included in Table 1 are some materials used in the simulation, in addition to their mechanical

properties [12, 23], while those of tungsten carbide have been taken from [24]. XFEM was applied to measure the critical loads in the brittle outerlayer for nucleation of radial cracks, and also calculating the required loads for reaching the plastic zone at the top and bottom surfaces of the metal core. Moreover, XFEM enables crack extension through elements based on linear elastic fracture mechanics without the need for repeated remeshing. In solution of such systems, nonlinear geometry with large deflection is allowed [13]. The ABAQUS (v. 6.12, ABAQUS Inc., Dassault Systems) software was used to model the real geometry, comprising a total of 115000 elements. approximately. Mesh refinement was performed around the crack region to the approximate size of 1 m to ensure the accuracy of the simulated results, while in the bulk it's about 20 m (Fig. 2). A convergence test was used to verify the FEA results and to guarantee that no further mesh refinement was necessary. To avoid numerical differences in the stress values, all axisymmetric models were analyzed with the same mesh pattern.



Fig. 2. A model of 0.5 mm ceramic thickness.

I able 1. Mechanical properties of materials				
Material	Young's Modulus E (GPa)	Poisson's Ratio v	Yield Stress Y (MPa)	Strain-hardening coefficient α
Tungsten-Carbide	626	0.22	3400	0.5
Glass	70	0.22		
Porcelain	66	0.22		
Steel	199	0.35	400	0.006
Aluminum	71	0.35	200	0.005
Au-alloy	92	0.35	370	0.001
Pd-alloy	126	0.35	550	0.01
Co-alloy	231	0.35	700	0.03
Epoxy Adhesive	3.7	0.35	93	0.001
Polycarbonate	2.35	0.35	65	0.05
Dentin	18	0.35		

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For indenter, metal and adhesive layers, a bilinear elastic–plastic stress–strain function $\sigma(\varepsilon)$ was prescribed. Initially, each material has a linear elastic behavior, as defined by modulus of elasticity and Poisson's ratio; once yield occurs, the materials follow a linear strain hardening approach of form $\sigma = Y + \alpha(\varepsilon E - Y)$, with *Y* a uniaxial yield stress and α a dimensionless strain-hardening coefficient (values between 0, fully plastic, and 1, fully elastic) [12].

Glass and porcelain coatings are supposed to be brittle. Based on [12], glass strength is equal to 110 MPa and for porcelain, this value is 130 MPa. It is assumed that crack will nucleate when the first stress component reaches these values.

The fracture criterion is based on power law relation of critical energy release rate (G_{IC}). If the energy release rate (G_I) reaches the critical value in each element, the crack propagates through. The typical value of fracture toughness (K_{IC}) for soda-lime glass and porcelain are nearly 0.75 and 1 MPa \sqrt{m} respectively; consequently, according to Eq. (1), the critical energy release rate for the former is 0.009 mm and for the latter is 0.015 mm [25, 26].

$$G_{IC} = K_{IC}^{2} / E \tag{1}$$

Critical loads to initiate radial cracks at the glass undersurfaces were recorded in each specimen. Monitoring generated stresses due to occlusal loading is interesting, since they can specify the morphology and location of radial cracks.

Load $P=P_R$ for radial cracking in the coating layer was determined by specifying the required load for the first increment of crack initiation. Similarly, loads $P=P_Y$ for yield in the top and bottom surface of metal layers were determined by imposing $\sigma_{von mises}=Y$.

2.2. Dental crown-like structures

For more realistic structure, dental metals (Au-, Pd-, and Co-alloy) were used as core layer, porcelain as veneer, and dentin as substrate which mechanical properties are shown in Table 1. To simulate what happens in practical limitations imposed on dental crowns, total thickness of metal and porcelain is constrained to be 1.5 mm. It is assumed there is no adhesive at the porcelain-metal interface and instead, they are fused to each other and then, this bilayer bonds to dentin substrate with a 15 μ m adhesive layer.

3. Results and discussion

XFEM has the ability to show the tooth mechanical behavior. In fact, stress and strain redistribution due to occlusal loading in each node of the structure can be known. In this way, FEM gives useful mechanical information in detail.

Fracture modes of dental trilayer structures were examined. Totally, radial cracks located in the coating undersurface are the major failure mode in dental systems and it is tried not to reach them. Also, plastic deformation in top surface and bottom surface of metal core are supposed to be other damage modes [27-29]. These damage modes in addition to crack propagation process based on fracture mechanics theory were simulated using XFEM.

3. 1. Adhesive layer effects

Critical loads of radial cracks embedded in coating, and plastic deformation of top surface and undersurface of two different kinds of metal (steel and aluminum) are demonstrated in Fig. 3, which compares the results for models with or without a 15 μ m adhesive thickness in the interface of metal and glass. Experimental results of radial crack critical loads taken from [12] for the model with adhesive layer are shown with triangle points. As the FEA validated well with experimental data, it is assumed that the simulation can be trusted for other thicknesses and materials.

It is clear there is a legitimate compatibility between experimental results of P_R and the curve estimated by XFEM.

Some data points of experimental outcomes are a little smaller than the estimated ones,

where it may result from the fact that natural specimens have somewhat inherent flaws which make radial cracks occur in lower loads than for the perfect model [15, 30].



Fig. 3. Critical loads for (a) steel and (b) aluminum metal cores.

From the comparison of the critical load maps, it is noticeable that with adhesive interlayer, the maximum stress area at top of the metal core decreases. This means that the adhesive layer heightens the elastic release effect: the stress difference is transformed in adhesive layer deformation and thus $P_Y(top)$ occurs in dramatic higher loads in comparison to the lack of adhesive layer models. However, adhesive layer doesn't have any incredible influence on $P_Y(bottom)$.

On the one hand, existence of adhesive layer makes radial cracks occur in lower loads for both metal cores, since it makes glass undersurface suffers higher flexural stresses and leads to lower critical loads for radial cracks initiation. On the other hand, adhesive layer postpones metal top surface entering yield zone by absorption most of energy; even in some metal thicknesses, top surface doesn't reach plastic zone and it can be the positive point of adhesive layer existence. In contrast, for no adhesive models, it is obvious that radial cracks always occur after the top surface of metal layer becomes plastic. In other words, entering to plastic zone makes glass undersurface bends more and radial cracks nucleate; the matter which can't be seen in included adhesive layer models. P_R is approximately 3 and 1.5 times greater than that of the systems with adhesive for steel and aluminum metal cores, respectively. Removing adhesive layer eliminates tensile stress in coating or at least, postpones the stress to reach the critical values. Therefore, it is avoided in dental applications and instead porcelain layer is fused to metal core.

Furthermore, it can be inferred that stiffer core with higher yield point results in higher critical loads, specifically in the no adhesive layer models (solid lines).

3. 2. Dental crown-like analysis

Figure 4 demonstrates critical loads of dental trilayers in various porcelain thicknesses by the means of XFEM.

It is noticeable that all 3 critical loads have the same trends for various metal cores, but in different quantities. P_R and $P_Y(top)$ graphs increase till around 1 mm porcelain thickness and then decrease, where their steep are different for each metal core. The trend is gradual for Au-alloy, while the slopes become sharper for Pd- and Co-alloy, respectively. According to the previous section, here also the stiffer metal causes significant rise in P_R and $P_Y(top)$, but it doesn't have any dramatic effect on $P_Y(bottom)$ which is approximately constant for each metal core.

Under occlusal loading, the model predicts that radial cracks start at the porcelain undersurface, where the flexural tensile stress reaches the porcelain strength and then propagates toward each element which meets the porcelain fracture toughness.

Whenever the top surface of metal faces the plastic deformation and hence large strain values along the indenter axis, it facilitates flexure of porcelain layer. Thereby, as a result of creation of high tensile stresses at the porcelain undersurface, radial cracks initiate.



In this way, P_R diagrams are higher than $P_Y(top)$ for all three dental metals.

consequently, there is no data for P_R in too thin thicknesses.

Thick porcelain layer shields the top surface of metal from going to plastic region and results in higher $P_Y(top)$ in comparison to $P_Y(bottom)$. Consequently, $P_Y(top)$ gets dominated.

Declining P_R and $P_Y(top)$ for porcelain thicknesses higher than 1 mm can be relevant to the fact that porcelain undersurface is so close to adhesive layer between metal and dentin. Therefore, it would impose more bending and P_R reduces clear and straight, even below $P_Y(top)$ in minuscule metal thicknesses.

The main purpose is making a trilayer structure not to reach critical load for radial cracking $(P < P_R)$. Generally, high metal stiffness is useful, which postpones flexure of brittle layer and indeed leads to higher P_R . Furthermore, as discussed before, plastic deformation of metal is not desirable, which makes porcelain layer encounters flexure and hence the more conservative design is to ensure $P < P_Y(top)$.

3. 3. Radial crack analysis with XFEM

The most important ability of XFEM is predicting the crack initiation point and also determining crack propagation path, based on the fracture mechanics approach. For instance, the radial crack nucleation and evolution through porcelain layer for co-alloy core with 0.5 mm porcelain thickness is illustrated in Fig. 5.

First figure demonstrates radial crack initiation point at load 1616.13 N and following figures show crack propagation views at elevated contact loads. FEM accompanying with fracture mechanics can determine crack growth path.

By applying XFEM simulation, it can be seen that radial cracks spread over comparatively long distance. However, even the longest radial cracks remain confined to the bottom surface region of porcelain layer. Since in porcelain top regions, bending moments become compressive and no longer crack propagate. XFEM applicability for more complicated geometries could be tested in future works.

Fig. 4. Critical loads versus porcelain thickness for three metal cores: (a) Au-alloy, (b) Pd-alloy, (c) Co-alloy.

In very thin porcelain thicknesses (smaller than 0.1 mm), so much great compressive stresses are created in the porcelain undersurface due to the small distance between the indenter contact point and porcelain undersurface at the early steps of loading. Therefore, it takes a long time for tensile stresses to be created due to bending of porcelain layer undersurfaces, which are required for radial cracks initiations and



Fig. 5. Radial crack initiation and propagation through 0.5 mm porcelain thickness for co-alloy core layer.

4. Conclusions

The minimum thickness of porcelain layer is recommended to be 0.5 mm. Furthermore, the metal layer shouldn't be too thin to be able to protect dentin and inhibit radial cracking. Conservatively, porcelain thickness's range between 0.75 and 1.25 mm is the most desirable design, avoiding the structure from radial cracks. Moreover, the models with stiffer metal cores meet higher resistance to radial cracking in all thickness ranges. Finally, XFEM would be an appropriate method to estimate crack initiation points and also, their evolution path in axisymmetric simulations.

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