Optimizing the design of bio-inspired functionally graded material (FGM) layer in all-ceramic dental restorations

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INTRODUCTION

All-ceramic restorations are an attractive choice for dental prostheses because of their excellent esthetics and unsurpassed biocompatibility. However, ceramic materials are brittle and prone to premature failure when deformation exceeds 0.1–0.3%\(^1\). Due to mismatch in elastic moduli between the ceramic core (65–300 GPa), cement (2–13 GPa), and supporting tooth structure (dentin: 20 GPa), high tensile stress concentrates at the interface between the ceramic core and cement, which can give rise to subsurface radial cracks at the bottom of the ceramic core and result in restoration failure\(^3\).\(^5\).

To reduce stress concentration and improve the success rate of all-ceramic restorations, the natural tooth structure was studied. It was found that enamel and dentin were interconnected by a functionally graded dentin-enamel junction (DEJ) layer of approximately 100-μm thickness. Within DEJ, elastic modulus gradually decreased from hard brittle enamel to soft durable dentin, which can give rise to subsurface radial cracks at the bottom of the ceramic core and result in restoration failure\(^6\).\(^8\).

The aim of this study was to explore the optimum design of a bio-inspired functionally graded material (FGM) layer in all-ceramic dental restorations to achieve excellent stress reduction and distribution. Three-dimensional finite element model of a multi-layer structure was developed, which comprised bilayered ceramic, bio-inspired FGM layer, cement, and dentin. Finite element method and first-order optimization technique were used to realize the optimal bio-inspired FGM layer design. The bio-inspired FGM layer significantly reduced stress concentration at the interface between the crown and cement, and stresses were evenly distributed in FGM layer. With the optimal design, an elastic modulus distribution similar to that in DEJ occurred in the FGM layer.

KEYWORDS: All-ceramic dental restoration, Bio-inspired functionally graded material layer, Finite element, Optimization

MATERIALS AND METHODS

Finite element modeling and the experimental groups

Using the ANSYS package, a three-dimensional finite element model of a multi-layer structure was developed, which comprised bilayered ceramic, bio-inspired functionally material graded layer, cement, and dentin. The three-dimensional model was 8 mm long and 2 mm wide.

In the simulation, the thicknesses of the veneering porcelain layer, ceramic core layer, cement layer, functionally graded layer, and dentin layer were 1.4, 0.5, 0.1, 0.09, and 10 mm respectively. Functionally graded layer was divided into 10 layers at 0.01 mm each (layer 1 to layer 10 from ceramic core to cement). Bilayered ceramic/cement/dentin model without FGM layer was constructed to be the control group. Models were exported into ANSYS to reconstruct FE mesh models with a tetrahedral structural solid element. Each FE mesh model was generated with 97405 nodes and 557312 tetrahedral solid elements. For the FGM layer, there were 74497 nodes and 390521 tetrahedral solid elements, constituting 76% and 70% of the whole model.
Table 1 Material properties of experimental Group 1

<table>
<thead>
<tr>
<th>Material</th>
<th>Elastic modulus (GPa)</th>
<th>Poisson’s ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Veneering</td>
<td>60</td>
<td>0.265</td>
</tr>
<tr>
<td>Core</td>
<td>210</td>
<td>0.3</td>
</tr>
<tr>
<td>FGM</td>
<td>210–5.9 change along thickness</td>
<td>0.3–0.27 change along thickness</td>
</tr>
<tr>
<td>Cement</td>
<td>5.9</td>
<td>0.27</td>
</tr>
<tr>
<td>Dentin</td>
<td>18.6</td>
<td>0.31</td>
</tr>
</tbody>
</table>

Table 2 Material properties of experimental Group 2

<table>
<thead>
<tr>
<th>Material</th>
<th>Elastic modulus (GPa)</th>
<th>Poisson’s ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Veneering</td>
<td>68</td>
<td>0.265</td>
</tr>
<tr>
<td>Core</td>
<td>100</td>
<td>0.3</td>
</tr>
<tr>
<td>FGM</td>
<td>100–5.9 (change along thickness)</td>
<td>0.3–0.27 (change along thickness)</td>
</tr>
<tr>
<td>Cement</td>
<td>5.9</td>
<td>0.27</td>
</tr>
<tr>
<td>Dentin</td>
<td>18.6</td>
<td>0.31</td>
</tr>
</tbody>
</table>

Density of the FE meshes varied with parts of the models, which was higher in the FGM layer than in the other parts (Fig. 1). Material properties of experimental Group 1 (zirconia as the core) and experimental Group 2 (Diene acid aluminum as the core) were summarized in Tables 1 and 2.

**Optimization**

The purpose of optimization is to find the minimum value of an objective function. In this study, the design variables were the elastic moduli (En(n=1,2,...,10)) of the basic constituent materials of each FGM layer. Thus, the objective function of the optimization problem was to minimize the maximum stress in FGM layer. Design variables (En) of experimental Group 1 layer ranged from 5.9 GPa to 210 GPa (5.9 GPa≤En≤210 GPa). Design variables (En) of experimental Group 2 ranged from 5.9 GPa to 100 GPa (5.9 GPa≤En≤100 GPa).

A numerical optimization procedure, using the first-order method in ANSYS program, was applied to the FE model. After the design variables were appointed, the computer program was developed to calculate the modulus of elasticity (En) of each FGM layer.

**Loading**

A 600-N static vertical load was applied to the model. A
perfectly bonded interface under the dentin layer was assumed.

RESULTS

Stress
For experimental Group 1, maximum principal stress was 27.299 MPa at the top third of the ceramic core. In FGM, maximum principal stress of 23.0186 MPa was found in layer 1. Stress was uniformly distributed in FGM, which gradually reduced from layer 1 to layer 10 and which was smoothly transmitted to the cement layer (Fig. 2). For Control Group 1, stress concentration was found at the interface between ceramic core and cement. Stress value rose from 20.837 to 100.25 MPa at the bottom of ceramic core (0.1 mm thick) (Fig. 3).

For experimental Group 2, maximum principal stress value was 19.547 MPa at the top third of ceramic
core. In FGM, maximum principal stress of 15.9665 MPa was found in layer 1. Stress was uniformly distributed in FGM, which gradually reduced from layer 1 to layer 10 and which was smoothly transmitted to the cement layer (Fig. 4). For Control Group 2, stress concentration was also found at the interface between ceramic core and cement. Stress value rose from 13.352 to 73.884 MPa at the bottom of ceramic core (0.1 mm thick) (Fig. 5).

**Optimization of FGM**

Figure 6 shows the elastic modulus distribution for optimal design in FGM for experimental Group 1. Elastic modulus was gradually reduced from layer 1 to layer 10 (from 210 GPa to 21.71 GPa). Function of elastic modulus curve was $Y=A_1x^3+A_2x^2+A_3x+A_4$ ($A_1=-0.28$, $A_2=23.34$, $A_3=2428.88$, $A_4=11726.53$).

Figure 7 shows the elastic modulus distribution for optimal design in FGM for experimental Group 2.
Elastic modulus was gradually reduced from layer 1 to layer 10 (from 100 GPa to 15.84 GPa). Function of elastic modulus curve was \( Y = A_1x^3 + A_2x^2 + A_3x + A_4 \) (\( A_1 = -0.03, A_2 = -6.33, A_3 = 1811.46, A_4 = 8004.48 \)).

**DISCUSSION**

Researches have shown that the common clinical failure mode of all-ceramic dental restorations is caused by subsurface radial cracks at the interface between ceramic core and dental cement. Although continuous efforts have been made to improve the strength of ceramic core materials, statistics showed that 20% of all-ceramic restorations failed within the first 5 years of service in the oral cavity\(^1\)\(^-\)\(^5\). Therefore, it is imperative that researchers seek to reduce the tensile stress concentration in and improve the durability of all-ceramic restorations.

Dentin-enamel junction (DEJ) is a natural graded structure which interconnects enamel and dentin. Within this functionally graded layer, stress concentration is significantly reduced by virtue of the gradually changing elastic modulus\(^6\)\(^-\)\(^9\). Inspired by DEJ, some researchers introduced the concept of a bio-inspired, functionally graded material layer structure between the ceramic core and cement to reduce stress\(^1\)\(^0\)-\(^1\)\(^5\).

Huang et al.\(^1\)\(^0\) developed a two-dimensional all-ceramic restoration model with a bio-inspired functionally graded material (FGM) layer between the ceramic core and cement. Three kinds of graded distributions were designed for the FGM layer. Finite element simulation showed that maximum principal stresses were reduced by \( \sim 30\% \) and critical crack sizes were improved in the FGM models\(^1\)\(^0\). Niu et al.\(^1\)\(^1\) fabricated a bio-inspired functionally graded structure to bond the ceramic core to dentin-like ceramic-filled polymer substrate. By using a rate-dependent slow crack growth (RDEASCG) model, critical loads were significantly improved and subsurface stresses that might induce cracks in the ceramic layer were reduced\(^1\)\(^1\). Numerous studies have also shown that functionally graded structure fabricated by infiltrating glass into the ceramic core exhibited higher load-bearing capacity through finite element analyses and contact loading experiments\(^1\)\(^2\)-\(^1\)\(^5\). However, few studies focused on the explicit optimal design of bio-inspired functionally graded material layer (variation of gradients in elastic modulus in FGM), which might minimize tensile stress between the ceramic core and cement and uniformly distribute stress in FGM.

In the present study, finite element method and first-order optimization technique were used to obtain the optimal FGM layer design. Compared to the control group, the bio-inspired functionally graded material layer significantly reduced stress concentration at the interface between the crown and cement. The larger the elastic modulus of ceramic core, the larger the decrease in stress would be. Maximum principal stresses were
only about 20% of the control groups, and stresses were evenly distributed in FGM layer. These aspects would certainly contribute toward improving the durability of all-ceramic prostheses. More importantly, the function of elastic modulus curve for optimal design in FGM was obtained by using first-order optimization technique in this study. Elastic modulus distribution for optimal design of FGM was an almost linear gradation, which was nearly consistent with the elastic modulus distribution in DEJ\(^6\) (Fig. 8). In a previous study\(^{10}\), only three predefined kinds of elastic modulus distributions in FGM were simulated and which indicated that optimal design was around linear gradation.

Results of the present study revealed that the optimal design of FGM layer had a beneficial influence on all-ceramic dental restorations. Further researches such as finite element analysis (FEA) and Hertzian contact experiment of the actual dental crown structure should be done to explore the mechanism by which FGM structures give rise to fatigue improvement.

CONCLUSION

A three-dimensional finite element model of a multilayer structure constituted of bilayered ceramic, bio-inspired functionally graded material (FGM) layer, cement, and dentin was developed. First-order optimization technique was used to explore the optimum design of a bio-inspired FGM layer in an all-ceramic dental restoration to achieve excellent stress reduction and distribution. Finite element simulation showed that the bio-inspired FGM layer significantly reduced stress concentration at the interface between the crown and cement. The larger the elastic modulus of ceramic core, the larger the decrease in stress would be. Results of this study revealed that the optimal design of FGM layer had a beneficial influence on all-ceramic dental restorations.

ACKNOWLEDGMENTS

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REFERENCES