Establishment of optimal variable elastic modulus distribution in the design of full-crown restorations by finite element analysis

Jianghai CHEN¹²*, Yutao JIAN²³*, Shumin CHEN¹²*, Xiaodong WANG¹²*, Li DAO¹² and Ke ZHAO¹²

¹ Hospital of Stomatology, Guanghua School of Stomatology, Sun Yat-sen University, 56 Ling-yuan West Street, Guangzhou, 510000, China
² Guangdong Provincial Key Laboratory of Stomatology, Sun Yat-sen University, Zhong-Shan Er Road 74, Guangzhou, 510080, China
³ Institute of Stomatological Research, Sun Yat-sen University, Zhong-Shan Er Road 74, Guangzhou, 510080, China

Corresponding author, Ke ZHAO; E-mail: zhaoke@mail.sysu.edu.cn

To establish optimal elastic modulus distribution throughout the entire all-ceramic crown, aiming at improvement of the mechanical properties of the restoration as well as the adhesive interface, seven 3D models of mandibular first premolars of zirconia monolithic and bilayer crowns and lithium disilicate monolithic and bilayer crowns were constructed. The elastic modulus distribution of 8-layer crown A referred to human enamel, B was calculated by a genetic algorithm (GA) to minimize the principle stresses on the crown, and C minimized the shear stresses at the cementing lines. After applying a static load of 600 N, the maximum principle stresses were calculated and analyzed by finite element analysis (FEA). Group C were found to have the lowest peak shear stress at the cementing line and moderate peak tensile stress in the crown. Introduction of the modified elastic modulus distribution from human enamel into the entire all-ceramic crown reinforces the mechanical properties of the whole restoration as well as the adhesive interface against chipping and debonding.

Keywords: Finite element analysis, Genetic algorithm, Full-crown restorations, Elastic modulus, Stress distribution

INTRODUCTION

Ceramic materials have been widely used in dentistry for their esthetics and biocompatibility. Yet the service life of all-ceramic crown restorations requires improvement, since they still have high failure rates of chipping and fracture, and the 10-year survival/chipping-free rates have been reported as 86.1% and 83.4%, respectively[11]. Another common failure in the clinic has been suggested to be debonding, following the detachment and marginal leakage of the adhesive margins of fixed adhesive prostheses[2,3]. Reducing the failure behavior of all-ceramic crown restorations, such as chipping, fracture, and debonding, and improving the survival rates remain major concerns in the field.

It is well-known that human enamel, although a brittle material, presents less chipping[4-7]. Research has shown that the elastic modulus of enamel ranges from 47 to 120 GPa, decreasing from the surface layer to the dentin-enamel junction[8,9]. In contrast, the elastic modulus of most all-ceramic crown restorations in clinical practice does not vary, being constant from the superficial surface to the inner interface. The divergent arrangement of elastic moduli in both these brittle materials suggested that the resistance of enamel against chipping might be attributable to its gradient change of elastic modulus[7,10-12]. Studies have also suggested that crowns with a graded elastic modulus structure exhibited lower stresses at the cement margins compared with homogeneous crowns[13,14], facilitating bonding strength and reducing crown fracture. The durability of the crown and its resistance to fracture increased bond quality[15].

Traditionally, material characteristics have been improved by adaptations from both animals and plants. The gradient change of the elastic modulus in enamel gave rise to attempts to determine whether the elastic moduli of all-ceramic crowns could be modified to simulate that of enamel. Since the elastic modulus of veneer porcelain can be distinguished from that of core ceramic as well as crown and dentin, an intermediate layer of elastic modulus other than porcelain and core ceramic was first inserted, suggesting that the bonding strength of the porcelain core was increased[15,16] and the stress at the interface was reduced[6,17]. When a modified layer with a change in elastic modulus gradient was introduced on the surface of the ceramic, the maximum principle stress inside the material was decreased, the fracture load increased[18], and the mechanical properties of the entire material were improved[19,20]. Yet when the addition of only an elastic modulus transition layer was attempted in all-ceramic crowns, it did not fully mimic the elastic modulus gradient distribution of the entire enamel layer[21].

In bionics, not all natural findings can be directly duplicated without modification or adjustment[22,23]. Thus the questions remain: To what extent can the distribution of elastic moduli in human enamel be introduced into all-ceramic restorations? and How will this distribution affect the mechanical properties of the crown and the adhesive interface?

Here, with the aid of finite element analysis (FEA) and a genetic algorithm (GA), we present the purpose of

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a preliminary study into the establishment of optimal elastic modulus distribution throughout the entire all-ceramic crown, aiming at improvement of the mechanical properties of the restoration and the adhesive interface.

MATERIALS AND METHODS

FEA pre-processing

An axisymmetric 3D model of a mandibular first premolar was constructed based on average anatomical size\(^{24}\). Beginning from the anatomic contour of the crown, the tooth was prepared, as in the clinic, for a full crown. The occlusal surface was reduced by 2 mm. A crown preparation was constructed with 4° of occlusal convergence in the axial walls, and the crown margin was 1 mm wide and 3 mm above the alveolar ridge crest. The external layer of the dental preparation was subsequently duplicated and used as a base for the cementing line with a thickness of 0.1 mm\(^{25}\). This allowed all the contacting faces of the preparation and the cement to be the same in quantity, size, and shape, reducing interference during the subsequent mathematical analysis. The outer surface of the cement was treated as a base for the inner surface of the crown. The bone surrounding the tooth was modeled according to average anatomical dimensions\(^{26,27}\). The periodontal ligament (PDL) and cement layers were included in the models. Since the thickness of the PDL varies from 0.15 to 0.25 mm depending on depth and age, the average thickness of the PDL in the model was set at 0.2 mm.

The crown was constructed with 3 different models. Model A was constructed as a monolithic crown, and Models B and C were comprised of 2 and 8 layers throughout the crown, so that the final geometries represented a monolithic crown, a bilayer crown, and an 8-layer crown, all with cement line, dental preparation, PDL, and bone block (Fig. 1). All bodies were considered volumetric solids. The modeling was performed by means of Solidworks Premium 2013 SP 4.0 (Dassault Systèmes SolidWorks, Waltham, MA, USA) and further imported into Ansys/CAE 17.0 (ANSYS, Canonsburg, PA, USA) for stress analysis.

FEA solution

1. Mesh generation

The geometries were imported into ANSYS in STEP format, and the mesh elements were formed in tetrahedrons after convergence analysis. Models of monolithic, bilayer, and 8-layer crowns contained 221,489 elements and 334,441 nodes, 221,662 elements and 337,151 nodes, and 232,848 elements and 367,161 nodes, respectively.

2. FEA processing

Seven 3D FEA models were studied: a zirconia monolithic crown, a lithium disilicate monolithic crown, a zirconia bilayer crown, a lithium disilicate bilayer crown, an 8-layer crown A with elastic modulus distribution according to human enamel, an 8-layer crown B with elastic modulus distribution calculated by GA to minimize peak tensile stress on the crown, and an 8-layer crown C with elastic modulus distribution calculated by GA to minimize peak shear stress on the cementing line. Materials’ properties were assigned to the components of the models after being imported into the FEA software. All materials were assumed to be homogeneous, isotropic, and linearly elastic\(^{28}\). Mechanical properties (elasticity modulus \([E]\) and Poisson’s ratio \([\nu]\)) of components are listed in Table 1\(^{25-36}\), and all contacts were ideally cast.

Within the thickness of the enamel, from the outer surface toward the dentin–enamel junction, the elastic modulus \(E(x)\) of enamel had an exponential relationship to the normalized thickness \((x)\), as \(E(x)=111.64x^{0.18}\). The elastic modulus of each layer of the biomimetic 8-layer crown was calculated according to this function.

3. Loading and fixations

The load was applied at 600 N\(^{36}\), with consideration of the contact between the food bolus and the tooth surface during the closing phase of the chewing cycle (Fig. 2). The bone block was selected as fixed in the system, ensuring that movement in the Z-axis was restricted only if the deformation generated in all directions could be computed.

4. GA processing

Generally, a GA is a method for solving complex problems in the field of engineering. It takes advantage of the feature from FEA that computes precisely and searches for optimal solutions globally and rapidly\(^{37,38}\). We applied a GA in an attempt to calculate the objective elastic modulus distribution of the 8-layer crowns, with which to minimize the maximum tensile stress of the full crown and minimize the maximum shearing stress of the cementing line.

The optimization process was composed of several steps (Fig. 3), including:

1. building a finite element model of an 8-layer crown and setting parameters of mechanical properties

![Fig. 1 3D FEA models of a tooth restored with different crowns. (A) Monolithic crown, (B) Bilayer crown, (C) 8-layer crown](image)
Table 1  Material properties

| Materials                        | $E$ (GPa) | $\nu$ |
|---------------------------------|-----------|-------|
| Dentin$^{28-30}$                | 18.6      | 0.31  |
| Cortical bone$^{26,27,30}$      | 13.7      | 0.30  |
| Spongy bone$^{26,27,30}$        | 1.37      | 0.30  |
| Pulp$^{31}$                     | 0.002     | 0.45  |
| Periodontal ligament$^{30}$     | 0.0689    | 0.45  |
| Zirconia$^{32}$                 | 200       | 0.31  |
| Lithium disilicate$^{33}$       | 95        | 0.25  |
| Zirconia (core)$^{34}$          | 209.3     | 0.32  |
| Porcelain 1 (veneer)$^{34}$     | 66.5      | 0.21  |
| Lithium disilicate (core)$^{35}$| 96        | 0.24  |
| Porcelain 2 (veneer)$^{35}$     | 65        | 0.26  |
| Food block$^{36}$               | 0.00314   | 0.10  |
| Resin cement$^{25}$             | 8.3       | 0.35  |

$E$, Elastic modulus; $\nu$, Poisson’s ratio

Table 2  Parameters used in the GA process

| Parameters                          | Values |
|-------------------------------------|--------|
| Number of initial samples           | 1,000  |
| Number of samples per iteration     | 100    |
| Maximum allowable Pareto percentage| 70     |
| Convergence stability percentage    | 2      |
| Maximum number of iterations        | 20     |

as well as boundary conditions. According to the elastic moduli of natural enamel range from 47 to 120 GPa$^{8,9}$ and 18.6 GPa$^{28-30}$, the parameter of the outer layer of the 8-layer crown was set at 120 GPa, with those for the inner 7 layers between 18.6 and 120 GPa;

(2) setting the GA parameters (Table 2);

(3) initializing the elastic modulus and updating the

Fig. 2  FE model according to the components of geometric models, food bolus, and loading application. (A) Components of geometric models, (B) Food bolus

Fig. 3  A flowchart of the optimization process.
values by finite element calculation;
(4) obtaining the value of the objective function and updating the optimal solution;
(5) calculating the fitness function according to the relevant constraints, and storing the optimal solution in the filter if the maximum number of populations was reached; otherwise, returning to steps (3) and (4);
(6) re-arranging the optimal solution individuals and eliminating the inferior individuals according to the fitness values; and
(7) determining whether the maximum number of iterations was reached, saving the candidates, and exiting the calculation if the number was reached; otherwise, returning to steps (3), (4), (5), and (6).

FEA post-processing
In the literature, FEA has been used to evaluate the stress distribution generated by masticatory loads in restored teeth\(^{36,39}\). In the present study, the maximum

principle stresses in restorations and cementing lines (tensile stress results in MPa) were identified to discriminate among the tensile stress fields, and the maximum shear stress criteria were likewise applied for the cementing lines.

RESULTS

The stress distribution patterns showed that the tensile stress was concentrated in the three regions of the crown, i.e. occlusal face, sagittal cut, and internal surface (Fig. 4). The peak tensile stresses of the monolithic crown, bilayer crown, and 8-layer crown C ranged from 21.21 to 34.45 MPa, while that of 8-layer crown A was 17.72 MPa, which was 16.46% less than that of the lithium disilicate monolithic crown (Table 3). The peak tensile stress of 8-layer crown B decreased to 16.25 MPa, which was also 8.31% and 23.40% less than that of 8-layer crown A and the lithium disilicate monolithic crown, respectively.

In comparison with the tensile stresses generated in the cementing lines (Fig. 5), the peak shear stresses at cementing lines of the monolithic crown, bilayer crown, and 8-layer crowns A and B were generally evident,

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Table 3  Stress peaks in crowns, cementing lines, and dentin

| Type of crown                        | Crown (MPa) | Cementing line (MPa) | Dentin (MPa) |
|--------------------------------------|-------------|----------------------|--------------|
|                                      | Tensile     | Tensile              | Shear        | Tensile      |
|                                      | stress      | stress               | stress       | stress       |
| Zirconia monolithic crown            | 27.10       | 5.32                 | 12.24        | 2.04         |
| Lithium disilicate monolithic crown  | 21.21       | 5.63                 | 9.95         | 4.21         |
| Zirconia bilayer crown               | 34.45       | 6.26                 | 10.51        | 3.69         |
| Lithium disilicate bilayer crown     | 26.49       | 6.04                 | 9.22         | 5.39         |
| 8-layer crown A                      | 17.72       | 5.34                 | 11.81        | 4.26         |
| 8-layer crown B                      | 16.25       | 5.47                 | 11.79        | 4.07         |
| 8-layer crown C                      | 25.79       | 4.38                 | 6.14         | 7.28         |
was deemed to be irregular.

lowest in the cementing line, though the distribution underwented less shear stress and the stress remained crown C was adjusted so that the adhesive interface 6). Further, the elastic modulus distribution of 8-layer a modulus more similar to that of human enamel (Fig. 6). The elastic modulus in 8-layer crown B was modified deliberately to be gradient-distributed, and resulted in a modulus more similar to that of human enamel (Fig. 6). The elastic modulus distribution of 8-layer crown C was adjusted so that the adhesive interface underwent less shear stress and the stress remained lowest in the cementing line, though the distribution was deemed to be irregular.

DISCUSSION

A bionic approach has been commonly used to improve material characteristics. The gradient changes of the elastic moduli in enamel gave rise to these attempts, whether the non-varying elastic modulus of an all-ceramic crown could be modified to simulate that of enamel. In the present results, we found that the elastic modulus distribution of a full-crown restoration affected its stress distribution, and the influence relied by far on the specific function of the elastic modulus, which was derived from the modeling of the multi-layer crown.

In the present study, we attempted, by using FEA, to determine an optimal distribution function of the elastic modulus in a multi-layer crown to minimize the tensile stress endured by crown substance, on the one hand, and to minimize the shear stress in the adhesive interface, on the other. A common method for analyzing heterogeneous materials by FEA is to divide the model into multiple thin layers in which the properties of each layer are considered to be uniform and gradually change throughout the layer. Since the crown is formed with irregular geometry, modeling an accurate three-dimensional laminated crown to simulate a functionally graded material (FGM) crown is complicated, the consequence of choosing an 8-layer model based upon the balance of calculation capacity during computation, on the one hand, and the implementation of theoretical distribution into crown fabrication in the reality of clinical applications, on the other.

In the results, the direct mimicking of the elastic modulus distribution from human enamel (8-layer crown A) yielded no minimal stress value, either in the crown or in the cementing line. The distribution of the elastic modulus in another multi-layer model (8-layer crown B) was similar to that of 8-layer crown A, and the lowest tensile stress on the crown has also been achieved, but at the cost of higher shear stress in the cementing line. This clearly suggests that the introduction of elastic modulus distribution in the form of a multi-layer into all-ceramic crowns was a possible way to facilitate its resistance against chipping and debonding, but the distribution function in reference to human enamel could not be directly duplicated in dental ceramic restorations. The question remains: Should tensile stress on the crown or shear stress at the adhesive interface be taken into consideration by implementing the multi-layer model with the ceramic crown?

In circumstances in which the flexural strength of dental ceramics — e.g., 900–1,200 MPa of zirconia, 350 MPa of lithium disilicate, 77–85 MPa of porcelain, 172.8 MPa of Lava Ultimate, and 148.7 MPa of Vita Enamic — is much higher than the tensile strengths to which a ceramic crown is subjected in the mouth, the shear stress of the adhesive interface should clearly be taken into consideration, and the elastic modulus distribution function should be adjusted so that the shear stress in the cementing line is kept to a minimum. In this context, we found that, in comparison with the shear stress of the cementing line within the 8-layer crown group as well as the other test groups, 8-layer crown C seemed to meet our criteria. Here, in our results, the tensile stress of 8-layer crown C was 25.8 MPa, still less than that of zirconia monolithic and bilayer crowns as well as lithium disilicate bilayer crowns, and also far less than the range of flexural strengths of dental ceramics. This suggested that there could still be an optimal distribution function of the elastic modulus by which the shear stress in the cementing line remained at a minimum, but not at the expense of an unacceptable increase of tensile stress for the crown.

In FEA we found that the stresses of the crowns were concentrated mainly at the cervical margins. Stress-peaking in the lower part of the crown was harmful to retention, since this area, next to the cementing line, could cause the prosthesis to be dislodged. Our finding was in accordance with those of previous clinical studies. Stresses at the cervical margins of crowns and cementing lines were still the major concerns in clinical failure.

In comparison with the peak tensile stresses endured by the crowns, which were far less than the flexural strengths of the materials, the peak shear stresses at the adhesive interface were much closer to the bonding strengths of the corresponding materials, e.g., the mean shear bond strength between zirconia and Variolink II was 14.30 MPa, strength between lithium disilicate
and Variolink II was 31.17 MPa\textsuperscript{46}, strength between Lava Ultimate and Variolink II was 15.21 MPa\textsuperscript{46}, and strength between Vita Enamic and Variolink II was 22.40 MPa\textsuperscript{46}. Since debonding and dislodging of fixed ceramic restorations are common after years of clinical application, minimizing the shear stress between crowns and cementing lines should be the goal of optimization of the elastic modulus distribution. The shear stress at the adhesive interface of 8-layer crown C, calculated by the GA, achieved the lowest value in our results. Higher resistance to shear stress at the adhesive interface has also been known to facilitate the fracture resistance of all-ceramic restorations\textsuperscript{51,52}, suggesting that crown C in the 8-layer arrangement should, in this sense, be optimal with respect to the moderate tensile stress that the crown had to endure at the same time.

Based upon the illustration of the stress map, a tensile zone appeared on the intaglio surfaces of the crowns, which makes the crowns crack easily. However, it was not evident that, in the zone, the stress was concentrated with respect to the sagittal sections of the crowns. A previous study has suggested that the propagation of cracks in brittle materials begins in this zone\textsuperscript{53}. Uniform stress was distributed on the layer-to-layer interfaces in 8-layer crowns A and B, while in the bilayer crowns and 8-layer crown C, uneven stress was found between two distinguished material layers. This suggested that the smoother the elastic moduli of two adjacent materials in transition, the less stress would form at the interface. Since the tensile stress that the dental ceramic crown endured was far less than the flexural strength of the ceramics themselves, stress between adjacent layers or shear stress at the adhesive interface should be taken into consideration in the design of full crowns and adjusted with respect to the fact that dislodging of the crown in clinical applications is largely, if not entirely, attributable to the failure of the detachment and marginal leakage of the adhesive margins\textsuperscript{54,55}.

In the present results, stresses distributed in the cementing lines were found to be closely related to the monolithic crown with non-varying elastic modulus distribution: the higher the elastic modulus of the crown, the more stress reached the cementing line, and the less was concentrated inside the resin cement. Our finding was consistent with that of a previous study\textsuperscript{56}, suggesting that the tough material itself absorbs the applied magnitude of load before it is transmitted to the surrounding dental tissues\textsuperscript{57}. Yet, in crowns with variable elastic moduli, such a relationship was not evident. It was apparently sufficient that the variably distributed elastic modulus was able to alter the stress distribution at the cementing lines.

CONCLUSION

The introduction of elastic modulus distribution in the form of a multi-layer into all-ceramic crowns is a possible way to facilitate crown resistance against chipping and debonding, but the distribution function referring to human enamel could not be directly duplicated in dental ceramic restorations.

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