Finite element analysis of the residual thermal stresses on functionally graded dental restorations

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\textbf{A B S T R A C T}

The aim of this work was to study, using the finite element method (FEM), the distribution of thermal residual stresses arising in metal-ceramic dental restorations after cooling from the processing temperature. Three different interface configurations were studied: with conventional sharp transition; one with a 50% metal-50% ceramic interlayer; and one with a compositionally functionally graded material (FGM) interlayer. The FE analysis was performed based on experimental data obtained from Dynamic Mechanical Analysis (DMA) and Dilatometry (DIL) studies of the monolithic materials and metal/ceramic composites.

Results have shown significant benefits of using the 50% metal-50% ceramic interlayer and the FGM interlayer over the conventional sharp transition interface configuration in reduction of the thermal residual stress and improvement of stress profiles. Maximum stresses magnitudes were reduced by 10% for the crowns with 50% metal-50% ceramic interlayer and by 20% with FGM interlayer. The reduction in stress magnitude and smoothness of the stress distribution profile due to the gradated architectures might explain the improved behavior of these novel dental restorative systems relative to the conventional one, demonstrated by in-vitro studies already reported in literature.

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1. Introduction

Dental restorations such as crowns and fixed partial dentures (FPD) are designed to restore functionality and esthetics to failed teeth. They are based on multi-material and multilayered systems, comprising a strong metallic or ceramic substructure veneered and esthetic dental porcelain that mimic the color of the remaining teeth. Failures of the restorative systems are undesired occurrences as they often imply money expenditure and discomfort to patients. Several studies have been conducted...
to understand and determine the failure mechanisms of the metal-ceramic and all-ceramic restorative systems (Yesil et al., 2009; Özcan, 2003; Anusavice, 2012; Swain, 2009, Arman et al., 2009; Zhang et al., 2010, 2012). Failures during the fabrication process related to thermal residual stresses arising from cooling after high temperature processing, and problems due to poor chemical compatibility have been pointed as the main causes for such events (Fischer et al. 2009). The cooling rates, the mismatching thermomechanical properties of materials and the geometry of specimens can greatly impact the transient residual stresses in metal–ceramic and all-ceramic restorations (Zhang et al. 2010; Asaoka and Tesk, 1990; Taskonak et al., 2005, 2008; DeHoff et al., 2008). Moreover, the thermal incompatibility between the materials to join can result in high stresses in regions close to free surface and near the interface, which can lead to either cracking of the ceramic or joints having poor strength (DeHoff et al. 2008; Ravichandran, 1999).

Functionally Graded Materials (FGMs) can be an answer to the thermal stress problems (Gasik, 1998, Gasik et al., 2005) consisting in a gradual change in the volume fractions of constituents from one location to the other in a component. The FGMs were first applied in minimizing thermal stresses and increasing thermal shock resistance of blades in gas turbine engines, with great success (Ravichandran, 1995; Chi and Chung, 2003). The philosophy was rapidly adapted by engineers to other fields of activity such as optics, nuclear energy, engineering, electronics, biomaterials, among others.

The employment of FGM to restorative dentistry is rather novel. Several studies were carried out involving metal–ceramic and all-ceramic dental restorative systems, aiming for the enhancement of the overall clinical performance. Gradated restorations have been shown to display improved properties relative to conventional ones, especially concerning to higher resistance to contact and sliding (Suresh, 2001); higher adhesion of porcelain to the substructure (metal or ceramic) (Henriques et al., 2011, 2012a, 2012b; Zhang and Kim, 2009); improved esthetical properties and improved fatigue performance (Henriques et al. 2012b).

In this study, the finite element analysis (FEA) was used to investigate the influence of the presence of a 50% metal–50% ceramic composite interlayer and a gradated interlayer at interface of a metal–ceramic dental crown on the post processing thermal residual stresses. Therefore, two different classes of gradation were studied, one consisting in a one-step transition only (interlayer with the composition of 50% metal–50% ceramic), and the other consisting in multiple layers of different compositions (each layer with constant composition), both performing a compositional discrete transition between metal and ceramic as a function of distance. The results obtained with these new interface configurations were compared with the conventional sharp transition system. The mechanical and thermal properties of the materials used in this study were experimentally determined through the production and testing of homogeneous specimens of several compositions. The elastic and thermal experimental data were afterwards modeled and uploaded in the materials properties database of the finite element method software.

### 2. Materials and methods

#### 2.1. Experimental determination of the elastic modulus and the coefficient of thermal expansion

In this study a CoCrMo alloy (Nobil 4000, Nobilmetal, Villafranca d’Asti, Italy) and a dental porcelain (Ceramco3, Dentsply, York, USA) (batch number: 08004925) were used. The chemical compositions of the metallic and ceramic particles are presented in Table 1 and Table 2, respectively. The micrographs of CoCrMo and porcelain powders show angular shapes and spherical shapes, respectively (Fig. 1). The CoCrMo powders display a broad size distribution: $D_{10}=4.44 \mu m$; $D_{50}=8.27 \mu m$ and $D_{90}=12.76 \mu m$.

The manufacturing of the metal–ceramic composite specimens comprised the following steps: several powder mixtures with different metal/porcelain volume fractions were produced. After weighting, the powders mixtures were blended in a rotary machine at 40 rpm during 10 min. The following mixtures were produced (vol%): pure porcelain (0% metal) and compositions with 20% metal, 40%, 60%, 80% and 100% metal, marked further as “n%M” where nn stays for the percentage of metal phase. Afterwards, the powder mixtures were hot pressed in a graphite die (Fig. 2). The hot pressing sequence comprised the following steps: first, the cavity of the graphite die was veneered with ZrO2 paint to prevent carbon diffusion to specimens. Then the metal–ceramic powder mixture was inserted into the cavity. The hot pressing was performed under vacuum ($\sim 10^{-2}$ mBar) at a temperature of 970 °C and a constant pressure of $\sim 20$ MPa. The selected heat rate was 70 °C/min and after a 2 min stage at 970 °C the induction heating furnace was shut down. Specimens cooled down to room temperature inside the hot pressing equipment.

Two types of specimens’ geometries were processed, rectangular and cylindrical. The dimensions of the rectangular samples used for flexural tests were $36 \times 6 \times 2.5$ mm, while those of the cylindrical samples used for shear tests were Ø4 × 4 mm.

The measurements of Young’s moduli (YM) of all materials were obtained by the means of Dynamic Mechanical Analysis (DMA 242C, Netzsch Gerätebau GmbH, Germany) using a three-point bending sample holder. The coefficient of thermal expansion (CTE) of composites and the monolithic materials was also assessed using dilatometry (DIL 402C, Netzsch Gerätebau GmbH, Germany). Both properties were measured through a range of temperatures starting in 100 °C up to 500 °C. It was estimated that materials properties at 100 °C did not differ significantly from properties at room temperature. Poisson’s ratio was fixed to be the following for the different materials: metal (0.25); porcelain (0.2); 50M composite interlayer (0.23). For the gradated transition Poisson’s ratio was approximated varying linearly from that of metal to that of porcelain. Data were post-processed with the

| Table 1 – Base alloy composition (wt%) (according to manufacturer). |
|---|---|---|---|---|---|
| Co | Cr | Mo | Si | Impurities |
| 62 | 31 | 4  | 2.2 | Mn, Fe, W |
software TableCurve3D (Systat Software, Inc., San Jose, California, USA) to produce functional equations and the surface plots of Young’s moduli (YM) and the coefficient of thermal expansion, which are shown in Fig. 2A and B, respectively. The YM variation is given by the Eq. (1) and the thermal expansion coefficient is given by the Eq. (2). The values of the constants for both equations are shown in Table 3.

\[
YM = A + Bx + Cy + Dy^2 + Cy^3
\]  
\[
CTE = A + Bx + Cy + Dx^2 + Ey^2 + Fxy
\]

where \( x \) is the temperature (degrees Celsius) and \( y \) is the ceramic content in the composite (vol%).

Table 2 – Porcelain chemical composition (wt%).

<table>
<thead>
<tr>
<th>SiO₂</th>
<th>Al₂O₃</th>
<th>K₂O</th>
<th>SnO₂</th>
<th>ZrO₂</th>
<th>CaO</th>
<th>P₂O₅</th>
<th>Na₂O</th>
<th>Impurities</th>
</tr>
</thead>
<tbody>
<tr>
<td>41.3</td>
<td>14.5</td>
<td>14.0</td>
<td>11.9</td>
<td>5.8</td>
<td>4.1</td>
<td>4.1</td>
<td>3.0</td>
<td>MgO, SO₃, ZnO, Cr₂O₃, Fe₂O₃, CuO, Rb₂O</td>
</tr>
</tbody>
</table>

Table 3 – Constants used in Eqs. (1) and (2).

<table>
<thead>
<tr>
<th></th>
<th>YM</th>
<th>CTE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>234750.25</td>
<td>1.53E-05</td>
</tr>
<tr>
<td>B</td>
<td>-50.80</td>
<td>-1.30E-08</td>
</tr>
<tr>
<td>C</td>
<td>-1865.11</td>
<td>-5.00E-08</td>
</tr>
<tr>
<td>D</td>
<td>-19.68</td>
<td>3.14E-11</td>
</tr>
<tr>
<td>E</td>
<td>0.21</td>
<td>-3.08E-11</td>
</tr>
<tr>
<td>F</td>
<td>1.55E-10</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 1 – Micrograph of the metal and ceramic powders: (A) CoCrMo particles; (B) porcelain powders.

Fig. 2 – Plot of the mechanical (Young’s Modulus) and thermal (CTE) properties of composite materials against temperature variation.

2.2. Finite element analysis

The thermal residual stress analysis after the cooling process was performed for three types of crown designs: sharp
transition; 50M composite interlayer (thickness = 500 μm); and compositionally gradated transition – FGM (total thickness = 500 μm) through 9 discrete intermediate layers (individual thickness = 55 μm). The selection of number of layers in the FGM configuration was arbitrary but chosen to illustrate the relative levels of residual stresses. In this work, a 3D molar tooth model was used (Fig. 3). The FEA was conducted using the commercial finite element software COMSOL Multiphysics 4.3a (Comsol Inc, Los Angeles, USA) adapting triangular elements. In order to simplify the study, the 3D computational model of the crown was sectioned to a 2D-axisymmetric model (Zhang et al., 2010, 2012) (Fig. 3).

The computational procedure consisted in cooling the model from a temperature of 500 °C to 100 °C, during 1000 s in increments of 100 s, i.e. with a constant cooling rate of 0.25 K/s. The thermal residual stresses, in its five components (radial, vertical, shear and hoop), were taken for each model after the cooling time elapsed. The convergence analysis was performed in order to examine the sensitivity of the results to the size of the mesh. Differences in maximum principle stresses were found to be lower than 3% for consecutive mesh refinements. The evolution of the coefficient of thermal expansion and Young’s modulus for the different metal–ceramic interface designs used in this study are schematically shown in Fig. 4. The properties of materials presented are based on experimental data (Fig. 2).

3. Results

The results of the simulations providing information on the thermal residual stresses remaining in the crown after the cooling process are shown in Fig. 5. Stresses were analyzed in terms of their radial (r), vertical (z), shear (rz) and hoop (phi) components due to axial symmetry of the problem. Tensile stresses are mostly developed in the metallic core while the porcelain remains under moderate compressive stresses. Fig. 6 shows a plot of the maximum stresses registered for the three crown configurations. The maximum radial stresses were 280 MPa, for the sharp transition; 253 MPa for the crown with 50M interlayer and 222 MPa for the crown with the gradated interlayer. The highest radial stresses (tensile) were localized in the top part of the metallic core. Regarding the vertical stresses, the highest tensile stresses were registered in the lateral side of the metallic crown. The sharp transition configuration exhibited 179 MPa of maximum tensile stress and the 50M interlayer and gradated interlayer configurations yielded 175 MPa and 163 MPa, respectively.

In terms of hoop stresses, they were also maximum and positive in the metallic core, following the same trend of the radial and vertical stresses analyzed before. Their magnitude was 289 MPa, 259 MPa and 222 MPa, for sharp transition, 50M interlayer and gradated interlayer crown configurations, respectively.

High shear stresses were found within porcelain and they were localized mainly at the vicinities of the convex part of the metallic core. Their highest values were 81 MPa, 66 MPa and 60 MPa for sharp transition, 50M interlayer and gradated interlayer crown configurations, respectively.

Fig. 7 illustrates the spatial variation of the elastic thermal stresses (radial, vertical, shear and hoop), across the metal–ceramic transition zone of a bilayered (sharp transition) and a trilayered (50M interlayer and gradated interlayer) dental crown. The measurements were made through a straight line across the crown profile where maximum stress values for each stress component were observed (Fig. 5).

It can be seen that the FGM structure results in the least residual stresses and the sharp transition in the highest. It was also noticed that the residual stress levels decrease with an increasing number of layers. Regardless of the number of layers, the stresses reverses in sign, alternating tensile and compressive stresses in the different layers.

4. Discussion

The results of the simulations providing information on the thermal residual stresses remaining in the specimens after cooling from high temperature processing are shown in Fig. 5 for crowns with three types of interface configurations: sharp transition, 50M composite interlayer and the gradated interlayer. It must be highlighted at this point that all models had identical
nominally dimensions and the only difference between them was the interface design. The crown with sharp interface (abrupt interface between the metal and the ceramic) exhibited the highest stress values while that with a gradated interface exhibited the lowest, for all types of stress components analyzed. The stress distribution in the crown with the 50M interlayer exhibited intermediate stress values. Hence, a reduction of ~21% in maximum radial stresses was observed in the crown with gradated interface relative to that with a sharp interface. The crowns with the 50M interlayer yield a stress reduction of ~10%. Regarding the maximum vertical stresses, the stress reduction relative to the sharp transition configuration was 2% and 8% for the crowns with the 50M interlayer and the gradated interlayer, respectively. The crown with the gradated interlayer also showed significantly lower shear and hoop stresses, 25% and 23% respectively. The 50M interlayer allowed a stress reduction of 19% in shear stresses and 10% of hoop stresses. The stress reduction by using gradated (FGM) architectures was also reported by Huang et al. (2007) for prosthetic systems. They reported ~30% reduction in maximum principal stresses, originated by contact induced deformations, when functionally graded layers (FGM architecture) between the crown materials and the joints that attach them to dentin were applied. Huang et al. (2007) and Niu et al. (2009) have also shown that the functionally gradated architectures, aiming at mimicking the functionally gradated structures of the dentin-enamel-junctions (DEJ) in natural teeth exhibited higher critical loads resistance over a wide range of loading rates.

Fig. 4 – Evolution of the coefficient of thermal expansion (CTE) and Young’s moduli (YM) across the metal–ceramic interfaces for the different configurations studied.

From the technical point of view, the production a crown with a 50M composite interlayer between the metal and ceramic is a simpler process than the production of a gradated interlayer. Results have shown that, despite the gradated interlayer had displayed the best stress distribution profiles among the three models simulated in this study, the crown with the 50M interlayer may also introduce a significant improvement in the clinical performance of the restorations.
Fig. 5 – Radial ($r$), vertical ($z$), shear ($rz$) and hoop ($\phi$) components of the thermal residual stresses [MPa] for different crown designs: (a) sharp transition; (b) 50M composite interlayer; (c) FGM interlayer.
clinical long term success of the restoration (Henriques et al., 2012b). Therefore, the 50M interlayer may be seen as a more immediate solution to be employed in the production of dental restorations. Further, the 50M and gradated configurations, comprising metallic phases embedded in the porcelain, can improve the thermal conductivity, reducing the temperature gradients across the section and hence minimizing the susceptibility to thermal shock-induced fracture.

It should be noted that this study did not account with a hypothetical plastic deformation of the metallic particles from the metal–ceramic composites that compose the crowns with 50M and the gradated interlayers, which can result in some relaxation of accumulated stresses during cooling from the processing temperature. Some practical aspects, related to the fabrication process, must be therefore considered in the analysis. Porosity or incomplete bonding between ceramic and metal can significantly impact the elastic and thermophysical properties (Hasselman and Johnson, 1987; Tummala and Friedberg, 1970; Pawlowski and Fauchais, 1992), and hence affecting the residual stresses.

5. Conclusions

This work includes a study of the thermal residual stresses distributions in dental crowns with different metal–ceramic interface configurations, namely: with a sharp interface (bilayer system); with a 50% metal–50% ceramic (50M–50C)
interlayer and with a gradated interlayer. These stresses are developed during cooling from porcelain firing temperature. The finite element (FE) simulations, using experimentally determined values of the materials properties, showed that the magnitude of thermal residual stresses on the dental crown can be reduced by over 10% using a 50M–50C interlayer and by 20% using a gradated interlayer. The simplified axisymmetric model used in this study has obvious limitations, as it might miss specific components and interactions important in real 3D geometry. Nevertheless, the model indicates the main trends and compares data for different composition profiles and geometries. Improvements in stress distribution profiles were also seen especially in the crown with the gradated interlayer. The benefits of using the 50M–50C interlayer and the gradated interlayer relative to the conventional sharp transition configuration, in terms of thermal residual stresses, shown in this study is expected to positively affect the clinical performance of these restorative systems, especially concerning the fatigue behavior.

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