

# Residual Thermal Stress Simulation in Three-Dimensional Molar Crown Systems: A Finite Element Analysis

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## Keywords

Coefficient of thermal expansion; all-ceramics; zirconia; alumina; metal ceramic; porcelain.

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## Abstract

**Purpose:** To simulate coefficient of thermal expansion (CTE)-generated stress fields in monolithic metal and ceramic crowns, and CTE mismatch stresses between metal, alumina, or zirconia cores and veneer layered crowns when cooled from high temperature processing.

**Materials and Methods:** A 3D computer-aided design model of a mandibular first molar crown was generated. Tooth preparation comprised reduction of proximal walls by 1.5 mm and of occlusal surfaces by 2.0 mm. Crown systems were monolithic (all-porcelain, alumina, metal, or zirconia) or subdivided into a core (metallic, zirconia, or alumina) and a porcelain veneer layer. The model was thermally loaded from 900°C to 25°C. A finite element mesh of three nodes per edge and a first/last node interval ratio of 1 was used, resulting in approximately 60,000 elements for both solids. Regions and values of maximum principal stress at the core and veneer layers were determined through 3D graphs and software output.

**Results:** The metal-porcelain and zirconia-porcelain systems showed compressive fields within the veneer cusp bulk, whereas alumina-porcelain presented tensile fields. At the core/veneer interface, compressive fields were observed for the metal-porcelain system, slightly tensile for the zirconia-porcelain, and higher tensile stress magnitudes for the alumina-porcelain. Increasingly compressive stresses were observed for the metal, alumina, zirconia, and all-porcelain monolithic systems.

**Conclusions:** Variations in residual thermal stress levels were observed between bilayered and single-material systems due to the interaction between crown configuration and material properties.

High-strength ceramics have been successfully used as structural ceramics in posterior regions with esthetic advantages. Remarkably, cohesive failures within the veneering porcelain of zirconia (yttria tetragonal zirconia polycrystals, Y-TZP) restorations, for example, have represented the chief failure mode in a number of studies.<sup>1–5</sup> This finding does not seem to be system-specific, as recently shown in a fatigue study of two zirconia molar crown systems,<sup>6</sup> but is related to several factors that may influence initial and long-term survival, such as laboratory processing steps, during restoration fabrication (prosthesis design, sandblasting, grinding for adjustments).<sup>7,8</sup>

Understanding the possible contribution of coefficient of thermal expansion (CTE) mismatches to the development of residual stresses in the veneering porcelain is crucial to avoid cracking after firing.<sup>8</sup> The concept of applying veneering ceramics with a CTE slightly below (10% or less) that of the framework used for metal ceramic restorations (MCR) and also for all-ceramics is desired to generate compressive stresses.<sup>9,10</sup> If the veneer has a significantly higher CTE than that of the framework, tensile stresses are created, and veneer delamination may occur. Hence, due to thermal behavior differences among core materials, veneering porcelains' microstructure and

chemistry are tailored to expand and match accordingly.<sup>11</sup> The presence of high-expansion leucite reinforcement, for instance, will render the veneer compatible to the metal core, whereas its reduction or absence when layered onto the low thermal conducting zirconia core is important for thermal compatibility.<sup>12,13</sup> However, since the CTE of several ceramic materials has been shown to be nonlinear, mismatch calculations of generated prestresses based on linear equations should be interpreted with caution.<sup>14</sup> In addition, the contribution of cooling rate, differences in thermal conductivity among core materials (which will affect the rate of cooling of the veneer), and complex tooth geometry need to be considered as potential sources of residual stresses within the veneer.<sup>8,15-17</sup>

The positive CTE created in MCR creates beneficial compressive stresses in the veneer layer, whereas it results in tensile stresses in the metal substructure.<sup>14</sup> This approach has been described to increase the strength of the MCR system.<sup>9</sup> However, the effect of tensile stresses in all-ceramic cores is controversial. Unlike ductile metals, ceramics are liable to fail under tensile stresses. Hence, understanding the stresses in the veneer and core/veneer interface is paramount to avoid cohesive and delamination veneer failures of restorations under function. Recently, a minimal difference in CTE between all-ceramic core and veneer has been associated with a reduction in prestresses in the veneer.<sup>15</sup>

A previous study investigated changes in the CTE of the porcelain layer to match that of the underlying core layer,<sup>18</sup> while a more recent study looked into nine types of layering porcelains used for veneering high-strength ceramic core materials<sup>19</sup> to determine their material properties. Finite element analysis (FEA) has also been used to investigate the stress distribution of bilayered discs of Y-TZP and dental porcelain under tensile stresses caused by the thermal mismatch.<sup>20</sup> Although comprehensive, for clinical purposes these studies are limited in that they only showed the material properties of the porcelain layers. Clinicians need a better understanding of how CTE will affect the materials once they are fired.

Despite the relevant information from simplified bilayer systems and 2D finite element models available in the literature, a characterization portraying the thermal-related residual stress states and interplay of the components of the crown system is lacking.<sup>21</sup> Given the significantly higher failure rates of all-ceramic restorations in the molar region<sup>22</sup> and the reported issues of veneer chipping with zirconia crowns,<sup>23</sup> it is desirable to better understand the thermally related underlying residual stresses as a function of CTE mismatches as well as provide insight as to where these stress fields originate. Thus, FEA analysis as a first tool to understanding the effects of CTE on prestresses on a crown system can eliminate the cost and time associated with fabrication and testing a large number of specimens.<sup>24</sup> Also, geometrical resemblance of the model to the true anatomical state is suggested to permit more realistic simulations.<sup>25</sup> The aim of this study was to simulate the stress fields generated in an anatomically correct molar crown due to CTE in monolithic metallic and ceramic systems, as well as due to CTE mismatch between metal, alumina, and zirconia cores and the porcelain veneer layer during its high temperature processing cooling.

## Materials and methods

An anatomically correct mandibular crown was analyzed with 3D FEA in ProEngineer Wildfire (Needham, MA). For this model, the dimensions of an average mandibular first molar crown were imported into CAD software (ProEngineer Wildfire). A tooth preparation was modeled by reducing the lateral wall of the average crown by 1.5 mm and the occlusal surface by 2.0 mm following the anatomy of the occlusal table, cusps, and ridges. Convergence of 12° was created between the buccal and lingual walls as well as between the mesial and distal walls. A chamfer margin was designed. At the center of the mesial and distal faces, the interproximal axial walls were designed to be 1.5 mm shorter than the buccal and lingual axial walls simulating normal crown preparation contours.

The crown was designed using the space between the original tooth form and the prepared tooth design. The crown was subdivided to create a core and a five-cusp veneer layer. The core was designed to be 0.5 mm constant thickness (variable between metallic, zirconia, and alumina cores). The porcelain veneer layer was 1 mm thick on the axial walls and 1.5 mm thick on the occlusal surface. Individual views of the veneer layer along with a complete view of the components and assembly are presented in Figures 1A-C.

The following assumptions were included in the finite element model: (1) all solids are homogeneous, isotropic, and linear elastic; (2) no slip was permitted between components (perfect bonding); and (3) there are no flaws in any component. Each model was run with the constraints placed on the underside of the core below the mesial buccal and distal lingual cusps (Fig 1D). These constraints were chosen in order to avoid artifacts on the occlusal region of the crown, allowing the determination of residual stresses on different cusps, as failures in a clinical setting have been reported to occur through veneer layer chipping.<sup>26,27</sup>

The core-crown model was assembled in ProEngineer Wildfire and constrained as described above, and the model was thermally loaded from a temperature of 900°C to a reference temperature of 25°C. The CTE of each material was assumed to be linear over the temperature range. A finite element mesh of three nodes per edge and a first/last node interval ratio of 1 were used, and following convergence evaluation, the final mesh for the models resulted in approximately 60,000 elements for both solids.

Each simulation had a different combination of materials. The combinations studied were: (1) Porcelain core, porcelain veneer; (2) Y-TZP core, porcelain veneer; (3) Alumina core, porcelain veneer; (4) Metal core (Pd-based), porcelain veneer; (5) Y-TZP core, Y-TZP veneer; (6) Alumina core, alumina veneer; and (7) metal core (Pd-based), metal veneer. The thermal properties used are presented in Table 1.<sup>28-38</sup> Regions and values of maximum principal stress at the core and veneer layers were determined through 3D graphs and software output.

## Results

Overall, the models showed the expected stress states in the core and veneer layers. The abnormally high stress states, observed

**Table 1** Material properties used as software input

Material	Young's modulus (GPa)	Coefficient of thermal expansion ( $10^{-6}/K$ )	Poisson's ratio
Porcelain <sup>28,32,38</sup>	70	10.3	0.22
Y-TZP <sup>29,32,35</sup>	205	11	0.22
Alumina <sup>30,33,36</sup>	370	8	0.22
Metal <sup>31,34,37</sup>	150	13.5	0.33

are artifacts created as a result of the boundary conditions. They did not affect the stress states seen in the occlusal portion of the crown, as such abnormally high stress states rapidly dissipate over a few millimeters from the constrained point from both the lateral and cervical regions toward the occlusal region (especially as failures reported in all-ceramic crowns arise in the veneer layer in the cusp region)<sup>39–42</sup> (Figs 2 and 3).

In the crowns studied, positive CTE mismatches (higher CTE for the core materials relative to the veneer layer) were observed for the metal-porcelain and Y-TZP-porcelain systems (Figs 2A, C). The higher the degree of positive CTE mismatch modeled, the higher the compressive fields observed within the cusp volumes in the veneer layer (Figs 2A, C). On the other hand, the alumina-porcelain crown showed a negative mismatch between the veneer and core material CTEs (Fig 2B). Compared to the metal and Y-TZP core-based systems, the alumina-porcelain crown presented higher amounts of tensile fields throughout the veneer layer (Fig 2B).

At the core/veneer layer interface (Fig 2), compressive fields were observed for the metal-porcelain crown system. Slightly tensile stress fields were observed at the core/veneer interface of the Y-TZP-porcelain system, and higher tensile stress magnitudes were observed in the alumina-porcelain system (Fig 2).

In the single-material crowns (Fig 3), it was apparent that the interplay between crown geometry, material properties such as Young's modulus of elasticity, Poisson's ratio, and CTE results in substantial differences in stress development during cooling. The most compressive stresses throughout the total volume, and specifically the cusp region, were observed in the all-porcelain crown. The all-Y-TZP crown presented less compressive stresses in the volume of the cusp relative to the all-porcelain crown, but more compressive stress compared to the all-alumina crown cusps. The all-alumina crown showed areas of tensile stress on the occlusal surface. In the all-alumina crown, these tensile stress regions decrease and become slightly compressive near the cusp tip. The all-metal crown presented the least amount of compressive stress in the volume of the material.

## Discussion

When above its glass transition temperature ( $T_g$ ), the porcelain veneer has a viscoelastic behavior that allows it to relieve stresses and accommodate to the elastic properties of the core material.<sup>17</sup> As it cools, the porcelain veneer viscosity steadily increases until it turns into an elastic solid.<sup>16</sup> It is common in dental laboratories to cool veneered restorations after the final

firing hold cycle by opening the furnace's door and then allowing the restoration to cool on the bench at room temperature,<sup>11</sup> at unrecorded rates, which could exaggerate the formation of strong thermal stresses. In combination with core materials with different thermal dimensional properties, such as alumina, Y-TZP, and metal, this could lead to the development of stress fields in restorations.

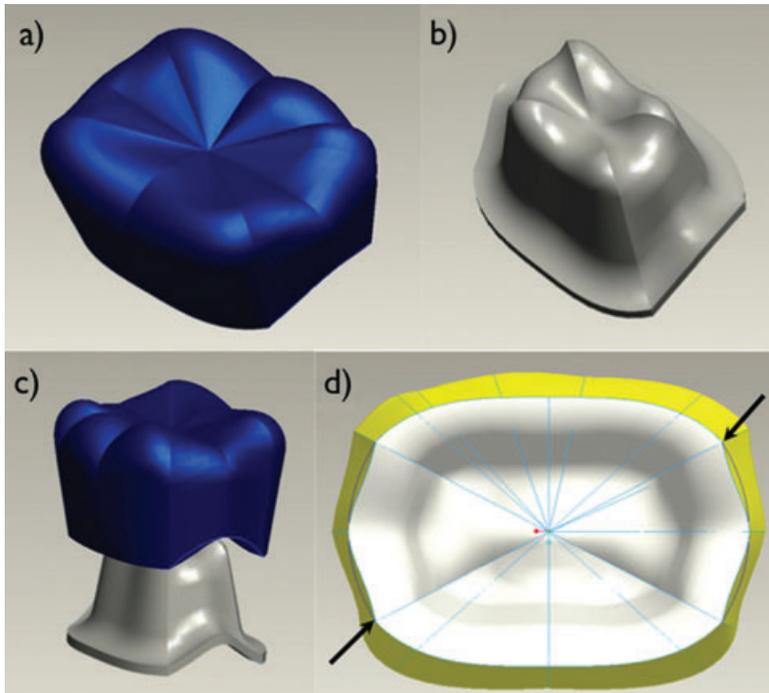
While it is known that several other variables, such as thermal conductivity of materials and surrounding conditions (cooling rate determinants), along with potential nonlinear material CTEs are important, this study aimed to address the effect of the CTE in generating residual stresses in a representative molar crown by variation in its material properties, limited to one cooling rate simulated from high to room temperature. Such an approach, while limited and potentially shifting what more sophisticated simulations including time dependence of variables would show with respect to stress levels, is the first step toward a multivariate analysis to determine single and combined variable contributions to residual stresses for future crown system development.

The different residual stress fields and magnitudes in the investigated core/veneer combinations were expected in the layered crown systems investigated; however, the interplay between CTE and the complex geometry used in the representative molar crown in this study further reveals the complex nature of dental crown system design, as stress levels comparable or even higher than layered crowns were observed. In our simulation, boundary conditions were chosen at the contralateral cervical regions of the crown to shift abnormal stress states due to geometric constraints to regions other than the cusp's bulk where most crown failures are reported to occur.<sup>39–42</sup>

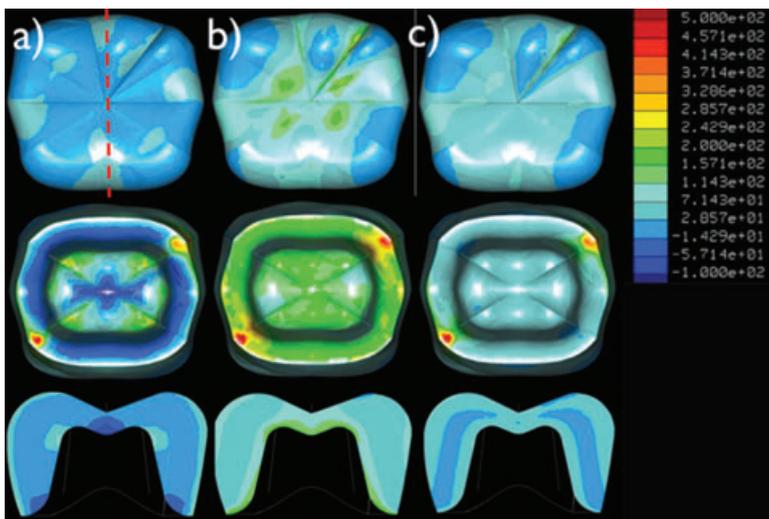
Considering layered systems having cores with higher CTEs compared to the porcelain layer (positive mismatch), the MCR and Y-TZP were the only systems presenting compressive fields at the cusp bulk upon cooling; however, the additional tensile fields observed at the Y-TZP core/veneer interface may account for the higher failure rates of Y-TZP restorations compared to MCR.<sup>43</sup> Once the compressive layer developed at the surface becomes exposed by occlusal adjustments/wear, the propagation of water-assisted cone cracks into the tensile region below the surface observed for all layered models may facilitate porcelain failure.<sup>8</sup>

Although findings from an FEA study evaluating maximum principal stresses in all-ceramic crowns (under mechanical loading), considering several clinical variables, observed that stresses in the porcelain veneer were not affected by core material,<sup>44</sup> a subsequent investigation from the same group has shown significantly higher stress concentration in the alumina relative to zirconia core.<sup>45</sup> In this study, observation of the alumina layered model where the core presented lower CTE compared to the porcelain layer (negative mismatch) revealed highest tensile stresses at the cusp bulk and core/veneer interface. Such an observation may explain clinically observed failure modes of alumina crowns being confined either at the porcelain veneer interface layer or occurring from the cementation surface.<sup>46,47</sup>

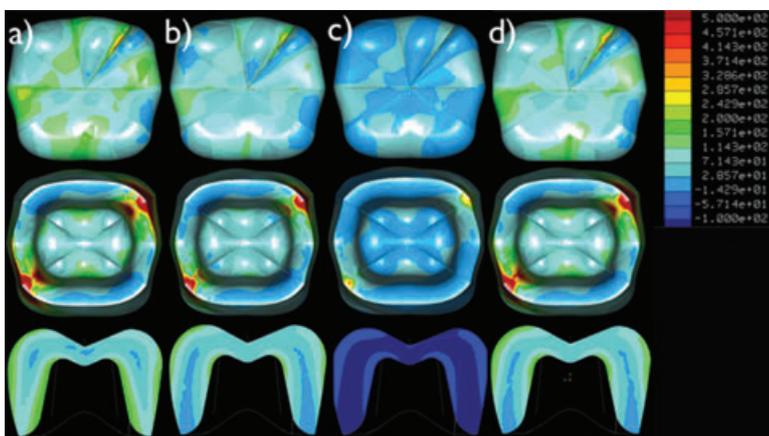
In core/veneer systems, cracks developing from the weak porcelain at the occlusal surface are likely arrested at the core material interface and may result in a porcelain cohesive



**Figure 1** CAD models of the (A) veneer layer, (B) core (metallic, zirconia, or alumina), and (C) exploded view of model assembly. (D) Inner cementation surface view of the crown core (veneered) where the 6 degrees of freedom were constrained in two contralateral points at the bottom part of the core (arrows).



**Figure 2** 3D software output (principal stress, MPa) of the occlusal and internal interface views of the veneer layer (top and middle, respectively), and 2D section (dotted line) of the veneer layer in the buccolingual direction at the center of the mesiodistal length. (A) metal ceramic crown, (B) alumina-porcelain crown, and (C) Y-TZP-porcelain crown. Note the artifact stresses at the bottom view of the crowns at contralateral regions.



**Figure 3** 3D software output for monolithic crowns with occlusal and cementation surface views (top and middle, respectively), and 2D section of the veneer layer in the buccolingual direction at the center of the mesiodistal length. (A) all-metallic crown, (B) all-YTZP crown, (C) all-porcelain crown, and (D) all-alumina crown. Note the artifact stresses at the bottom view of the crowns at contralateral regions.

failure.<sup>48</sup> However, should cracks propagate from the cementation surface through the stiff all-ceramic core and intersect the interface, they extend unimpeded into the porcelain.<sup>49</sup> Thus, not only are Y-TZP cores tougher than alumina cores, they also have a lower modulus, and our results show that residual stresses' nature and magnitude at the interface between core and veneer favors the Y-TZP system configuration. Such observation is supported by previous studies, where compared to alumina cores, Y-TZP core failure is rarely reported.<sup>27,50</sup>

Especially challenging to all-ceramic systems, where an inherent flaw population may decrease the material's ability to withstand crack propagation, is limiting tensile stresses in the veneer and core; however, our results showed that, when thermally loading monolithic crown materials, stress levels comparable to bilayer systems were generated. The low modulus and intermediate CTE value of the all-porcelain crown resulted in the most compressive stresses throughout the total volume and occlusal cusp tip. On the other hand, the all-metal crown intermediate elastic modulus and high CTE resulted in the least compressive stress throughout the crown volume; however, given the fracture toughness of metals (50 MPa<sup>1/2</sup> or higher), this finding is of negligible significance for clinical practice,<sup>13</sup> as metallic yielding is unlikely to result in clinical failures. The monolithic Y-TZP crown had higher compressive stresses in the cusp volumes compared to the monolithic alumina. This finding may be of clinical relevance and preliminary testing of full-contour Y-TZP glazed crowns has shown promising results regarding load-bearing capacity, light transmission, and antagonist dentition wear.<sup>51</sup> Further laboratory cyclic loading experimentation is warranted to determine the reliability of such system configurations.

While our results have shown that the interplay between crown configuration (single or layered) and material properties (modulus, CTE, Poisson's ratio) resulted in variations in residual thermal stress levels between systems, patient-dependent anatomy plays a key role in magnitude of thermally related residual stresses. Thus, although restorations may survive the cooling process, they may either deform, crack, or be more fracture prone due to tensile residual stress fields overlapping with functional occlusal stress fields.<sup>52,53</sup> Thus, high residual stresses may arise from the interrelation between material and anatomic features.<sup>54</sup> Although the establishment of a threshold mismatch for core/veneer combinations such as the previously investigated veneered lithium-disilicate ceramics<sup>53</sup> is valid and must be observed by dental manufacturers, our study identified high stress fields for thermally loaded core/veneer and monolithic material systems regardless of configuration, indicating that the multifaceted cause of restoration failure may be further assisted by patient-dependent anatomy. Thus, multivariable analysis including more sophisticated models including other thermal-related properties such as thermal diffusivity and modification of crown preparation guidelines, and variations in crown layering are warranted for better design of future crown systems.

## Conclusions

Different residual thermal stress levels were observed between systems due to the interaction between crown configuration

and material properties. Compressive (metal-porcelain), tensile (alumina-porcelain), or the combination of compressive within the veneer and tensile stresses at the interface (Y-TZP-porcelain) were observed in the bilayered systems. In single-material crowns, the all-porcelain system presented the highest concentration of compressive stresses followed by the all-Y-TZP, alumina, and metal.

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