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A particle swarm-based algorithm for optimization of multi-layered and graded dental ceramics

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ABSTRACT

The thermal residual stresses (TRSs) generated owing to the cooling down from the processing temperature in layered ceramic systems can lead to crack formation as well as influence the bending stress distribution and the strength of the structure. The purpose of this study is to minimize the thermal residual and bending stresses in dental ceramics to enhance their strength as well as to prevent the structure failure. Analytical parametric models are developed to evaluate thermal residual stresses in zirconia-porcelain multi-layered and graded discs and to simulate the piston-on-ring test. To identify optimal designs of zirconia-based dental restorations, a particle swarm optimizer is also developed. The thickness of each interlayer and compositional distribution are referred to as design variables. The effect of layers number constituting the interlayer between two based materials on the performance of graded prosthetic systems is also investigated. The developed methodology is validated against results available in literature and a finite element model constructed in the present study. Three different cases are considered to determine the optimal design of graded prosthesis based on minimizing (a) TRSs; (b) bending stresses; and (c) both TRS and bending stresses. It is demonstrated that each layer thickness and composition profile have important contributions into the resulting stress field and magnitude.

1. Introduction

Zirconia is material of interest to be used as the framework in dental restorations due to its superior mechanical properties and biocompatibility, enabling the prosthesis to withstand masticating loadings (Zarone et al., 2011; Denry and Kelly, 2008). As veneer, porcelain is also the common material of choice owing to its colour matching the remaining teeth and aesthetic (Fischer et al., 2008). In the production process of ceramic restoration, porcelain is fired onto the framework at high temperature. As constituting materials have different thermal expansion coefficients, the process of cooling temperature down to the room temperature leads to thermal residual stresses within the prosthesis (Baldassarri et al., 2011; Choi et al., 2011). On top of that, the mismatch of elastic characteristics between multi-material prostheses when subjected to occlusion loadings forms undesired stress fields along the corresponding interfaces (Choi et al., 2011; Swain, 2009). These all can lead to crack formation and propagation, veneer chipping and eventually catastrophic feature of the prosthesis (Choi et al., 2011; Swain, 2009; Isgrò et al., 2005; DeHoff and Anusavice, 2009; Tholey et al., 2011; Benetti et al., 2010; Baldassarri et al., 2012).

Making use of functionally graded materials (FGMs) can bypass drawbacks associated with the sharp transition from ceramic to porcelain. A typical FGM is an inhomogeneous composite made of different phases of constituent materials. By gradually varying the material composition involving constituent materials, the thermal and mechanical behavior of such materials vary smoothly and change continuously between different layers. This advantage eliminates interface problems of composite materials and the stress distribution becomes smooth. The influence of gradient variation of material properties in the FGMs on thermal residual stresses has been investigated by previous research studies analytically and numerically (Ravichandran, 1995; Becker et al., 2000; Koohbor et al., 2015; Birman and Byrd, 2007; Kesler et al., 1998; Cannillo et al., 2006). The readers interested in the origin and advancement of functionally graded materials are referred to very comprehensive review papers (Suresh and Mortensen, 1997; Mortensen and Suresh, 1995; Jha et al., 2013; Naebe and Shirvanimoghaddam, 2016). An interlayer with a gradation of properties between two base materials, the framework and the interlay, has therefore been used for dental restorations in order to reduce the mismatches in thermal and mechanical properties (Zhang and Kim, 2009, 2010; Y. Zhang et al., 2012; Chai et al., 2014; Z. Zhang et al., 2012). This solution has resulted in excellent load-bearing capacity, improved damage resistance and bond

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strength resistance, as a consequent of a reduction in resulting stresses associated with graded prostheses (Zhang and Kim, 2009; Y. Zhang et al., 2012; Henriques et al., 2012a, 2012b; Hsueha et al., 2008; Tsukada et al., 2014; Fabris et al., 2016). Moreover, design parameters of functionally graded restorations can significantly influence the resulting stress distribution and magnitude (Paul et al., 2016; Chen and Tong, 2005; Stump et al., 2007; Mohammadiha and Beheshti, 2014; Fereidoon et al., 2012). It is, therefore, of paramount importance to develop an optimization algorithm to optimize the thickness of each layer and the composition profile.

In addition to thermal residual stresses, the flexural strength of ceramic restorations plays very important role in the performance and longevity of dental implants. The biaxial flexure tests are commonly employed to evaluate flexural strengths of dental materials. The associated stresses can also mimic multiaxial loading nature existing due to occlusion forces on restoration (Thompson, 2004; Hsueh et al., 2006a). In biaxial tests, the sample is supported on either three balls or a ring near its periphery and a load is applied on its upper surface through a piston placed at the centre of the specimen (Thompson, 2004). Due to loading and boundary conditions, a multiaxial stress state is generated near the specimen's centre, eliminating undesired edge failures taking place in uniaxial tests (Hsueh et al., 2006b).

The particle swarm optimization (PSO) is generally a population-based optimization algorithm based on the hypothesis that social sharing of information among conspecifics offers an evolutionary advantage (Kennedy and Eberhart, 1995). The population of PSO is called a *swarm* and each individual in the population of PSO is called a *particle*, which adjusts its position in the search space regarding its own social experience and the social experience of the community (He et al., 2004a). The PSO algorithm involves in adjusting very few parameters, which makes it easy to implement. The particle swarm optimization has been applied to a broad range of engineering problems in the literature and has shown a faster convergence rate than other evolutionary algorithms (He et al., 2004b; Fourie and Groenwold, 2002; Liu et al., 2016; Mavrovouniotis et al., 2017; Loja, 2014; Kathiravan and Ganguli, 2007; Mashhadban et al., 2016; Li et al., 2007; Chang et al., 2010; Jun et al., 2016).

The present study, therefore, aims to develop a particle swarm optimizer to identify optimal designs of multi-layered and graded dental restorations. The methodology consists of two main parts: (i) simulating thermal residual stresses and the piston-on-ring test analytically; (ii) developing a particle swarm-based algorithm to optimize the design of zirconia-based dental ceramics aiming to minimize resultant stresses. The contribution of the current research work is to develop a procedure to optimize the design of ceramic dental restoration, which can be generalized in order for the optimization of any combinations of multi-layered and graded dental implants. The thickness of each layer and compositional distribution exponent are referred to as design variables. The effect of layer numbers constituting the interlayer between two based materials on graded prosthetic systems is also investigated. A finite element model is constructed to verify the developed methodology, although acquired results are compared to those available in literature. Three different optimization cases are considered to determine the optimal design of graded prosthesis by minimizing (a) TRSs; (b) bending stresses; and (c) both TRS and bending stresses. It is demonstrated that each layer thickness and composition profile have important influences on the stress field and magnitude.

2. Mathematical modelling

For the graded material, a stepwise gradation between the two base materials is considered such that each disc consists of a number of layers each of which is made of a specific homogenous material. The top and bottom layers are monolithic porcelain and zirconia, respectively. The intermediate layers are composed from a mixture of porcelain and zirconia. In order to calculate mechanical properties of each intermediate layer, a continuous change in the volume fraction of porcelain through the thickness is considered. This change is taken into account by a power law function, as follows:

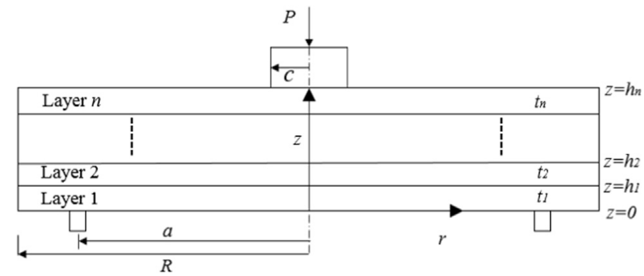

Fig. 1. A schematic representation of the piston-on-ring test with a multi-layered circular disc as the sample.

$$V_p = \left(\frac{z}{t}\right)^p \quad (1)$$

where V_p stands for the volume fraction of porcelain, z is the distance from the bottom, Fig. 1, and t is the overall thickness. For different values of p, the concentration of zirconia and porcelain through the thickness varies. The mechanical properties of intermediate layers, i.e. Young's modulus, Poisson's ratio and thermal expansion coefficient, are determined using the Voigt's rule of mixtures given by (Moshkelgosha et al., 2017; Shafiee et al., 2014)

$$P_i = P_z V_z + P_p V_p \quad (2)$$

where P_i is the property of the ith layer, P_z and P_p are the properties of the zirconia and porcelain, respectively. V_z and V_p are the volume fractions of zirconia and porcelain composition, respectively. The mechanical properties of the base materials are listed in Table 1.

2.1. Thermal residual stress

Considering a disc consisting of several layers, the gradient change of material through the thickness is taken into account. It is assumed that materials remain within the elastic region as well as layers remain bonded over simulation, consequently no slippage between layers takes place. A uniform temperature is considered throughout the plate and no stress relaxation is taken into account during the cooling-down process. The thermal residual stresses through the thickness of the disc can be calculated using laminate theory (Shaw, 1998; Bouchafa et al., 2010):

$$\boldsymbol{\sigma} = \widetilde{\mathbf{Q}}\boldsymbol{\varepsilon} = \widetilde{\mathbf{Q}}(\boldsymbol{\varepsilon}^0 + z\boldsymbol{\kappa} - \boldsymbol{\alpha}\Delta T) \quad (3)$$

$\widetilde{\mathbf{Q}}$ stands for the matrix of the material stiffness and $\boldsymbol{\varepsilon}$ is thermal residual strain vector at location z. while $\boldsymbol{\varepsilon}^0$ is the mid-plane strain, $\boldsymbol{\kappa}$ the vector of the plate curvature, $\boldsymbol{\alpha}$ the coefficient vector of thermal expansion of material as a function of location z, and finally ΔT is the steady-state temperature variation. A polar coordinate system regarding the disc geometry is also considered as (r, θ, z). Considering the plate to be isotropic at each layer, non-zero stress components are σ_r and σ_θ. To compute residual stresses in Eq. (3), the mid-plane strains and curvatures of the circular plate can be determined from

Table 1
Material properties of Zirconia and porcelain (25 °C).

	Zirconia	Porcelain
E (GPa)	210 (200[a])	70
υ	0.3	0.26
α (K^{-1})	10.17e−6 (10.86[a])	9.05e−6 (9.40[a])

[a] The average value obtained within the range of temperature variation during the cooling down process (Becker et al., 2000).