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Bioinspired design of dental multilayers

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Abstract This paper considers the use of bioinspired functionally graded structures in the design of dental multi-layers that are more resistant to sub-surface crack nucleation. Unlike existing dental crown restorations that give rise to high stress concentration, the functionally graded layers (between crown materials and the joins that attach them to dentin) are shown to promote significant reductions in stress and improvements in the critical crack size. Special inspiration is drawn from the low stress concentrations associated with the graded distributions in the dentin-enamel-junction (DEJ). The implications of such functionally graded structures are also discussed for the design of dental restorations.

1 Introduction

Dental crown restorations are normally used to replace the damaged tooth structure. However, the failure rate is still high, for example, 20% of dental restorations with resin retained ceramics fail within the first five years of service in the oral cavity [1]. The major clinical failure mode is the sub-surface radial crack in the ceramic, at the interface between the crown (dental ceramic) and cement [2]. This failure is caused largely by the tensile stress concentration in the dental ceramic at that interface [3, 4]. It is, therefore, important to explore efficient methods for the reduction of the stress at this interface.

In dental crown restorations, the Young's modulus of the ceramic crown material is typically 65–300 GPa [5], while that of the cement is 2–13 GPa [7], and the supporting of natural tooth (dentin) is ~20 GPa [9]. Hence, there is a tensile stress concentration in the crown at the interface between the crown and the cement [4]. In contrast, in nature, the dentin-enamel-junction (DEJ) provides a graded interface between enamel and dentin [8, 9]. This is shown to significantly reduce the stress in the enamel or crown layer.

Due to the complex structure of actual dental restorations, flat multi-layered structures (with equivalent elastic properties) are often used to study contact-induced damage in dental multi-layers [3, 4]. Figure 1 shows an example of a tri-layer model. Following Herzian indentation, a sub-surface radial crack is observed in the model structure [3, 4]. This is also the major clinical failure mode as reported by Kelly [2].

In this study, we will add a functionally graded material (FGM) layer between the ceramic and the cement, and investigate the effects of the FGM layer. The initial grading is inspired by measurements of modulus variations across the dentin-enamel junction [8, 9]. Subsequent architectures then explore the possibility of designing FGM layer with lower internal stresses. The stress and critical crack length of the graded and layered structures are then computed.

2 Stress reduction by the bioinspired functionally graded material layer

Natural tooth consists of two distinct materials: enamel with ~65 GPa Young's modulus and dentin with ~20 GPa

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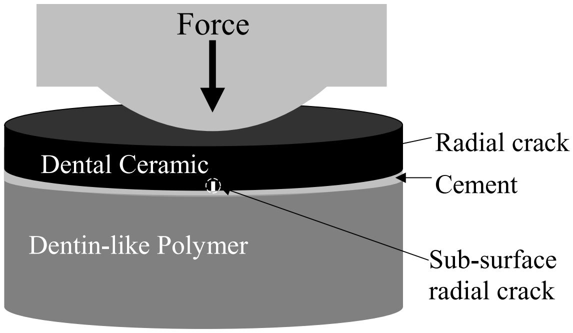


Fig. 1 Dental crown restoration tri-layer model under Herzian indentation

Young's modulus. They are bonded by dentin-enamel-junction (DEJ). Figures 2a and b show the variations in Young's modulus across the DEJ reported by Marshall et al. [9]. These were measured by nano-indentation across the enamel, DEJ and dentin layers [9]. We can see that in DEJ, the Young's modulus changes linearly from that of enamel to that of dentin. This will dramatically reduce the stress in the enamel, as will be shown later.

Inspired by the DEJ structure, we propose a new dental crown restoration structure, shown in Fig. 2c. A functionally graded layer is fabricated at the bottom of the ceramic. In this layer, the Young's modulus gradually decreases from that of the dental ceramic to a lower value. Then the structure is

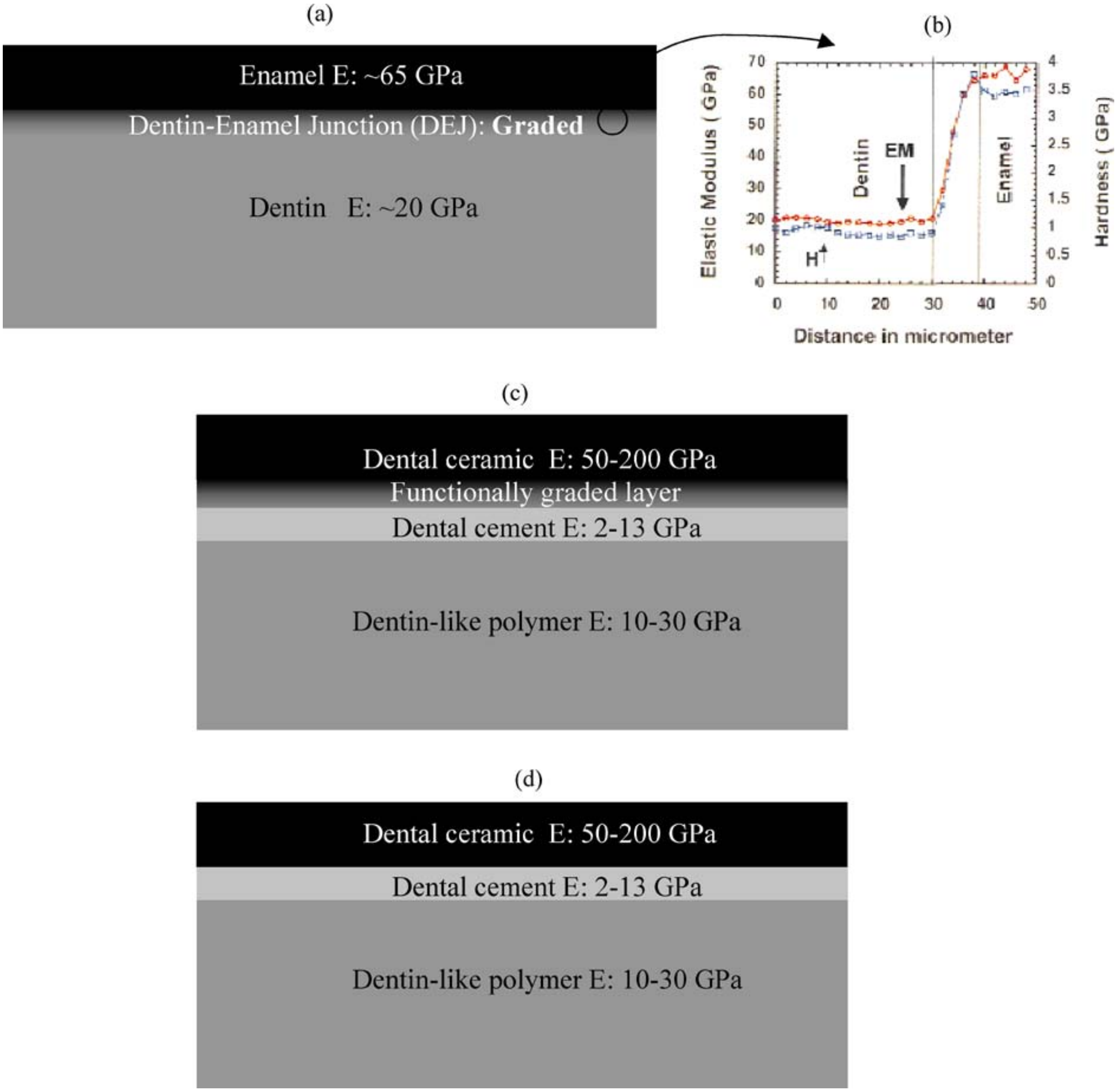


Fig. 2 (a) Natural tooth model; (b) Youngs modulus distribution in DEJ of natural tooth (after Marshall et al., 2001); (c) Dental crown restoration FGM layer model. A functionally graded layer is between the cement and the ceramic; (d) Existing dental crown restoration model;

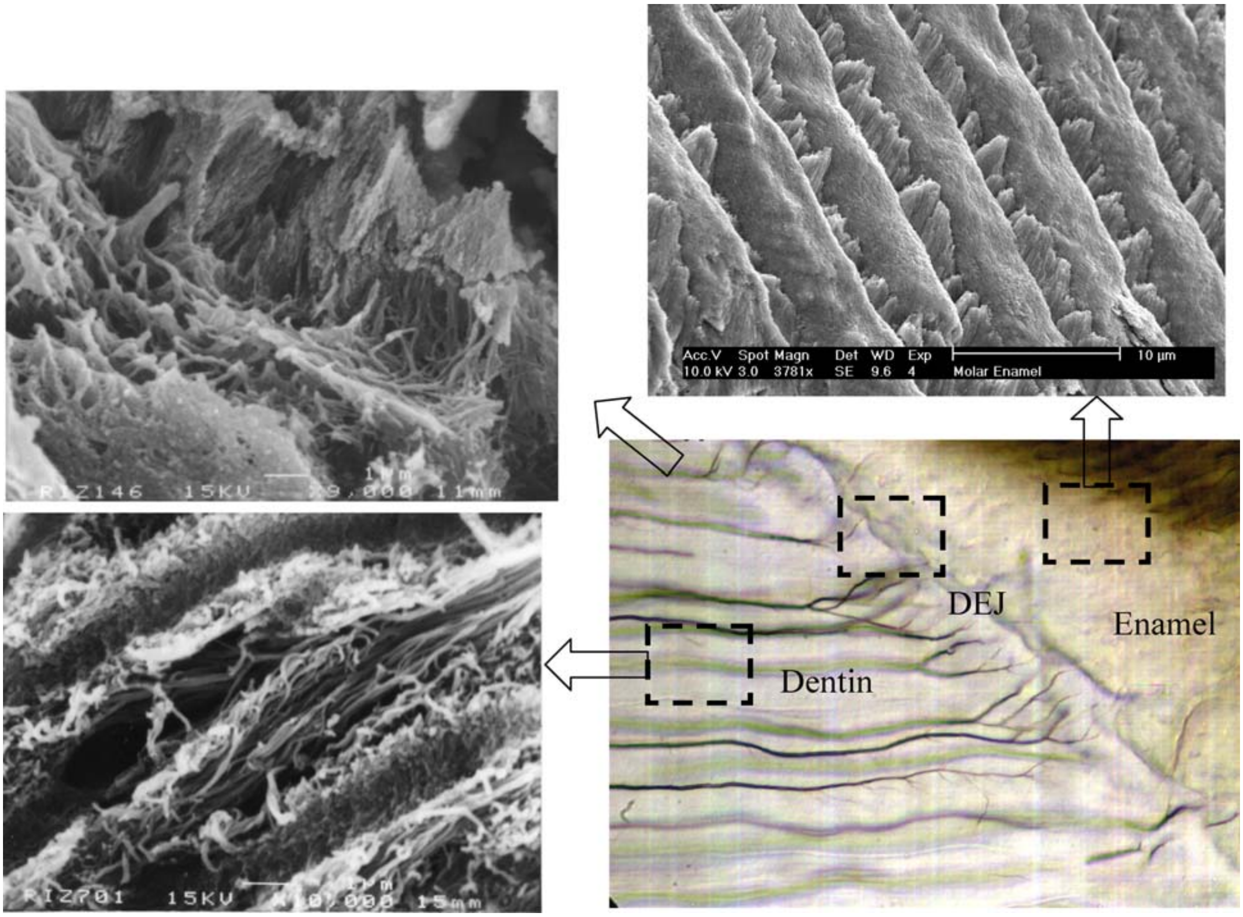


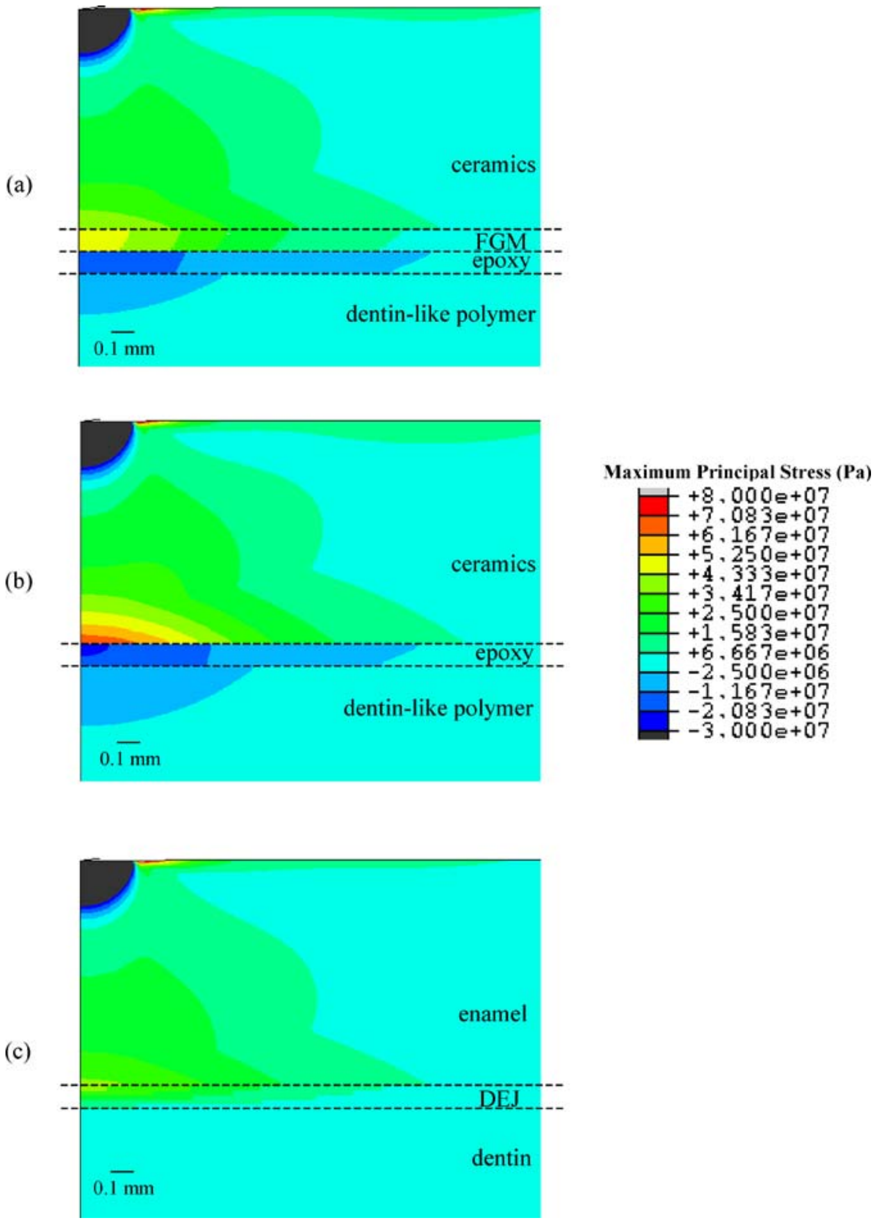
Fig. 3 Microstructure of natural tooth

bonded with the dentin-like polymer by dental cement. The dental cement has lower modulus than the FGM layer, which is analogy to the soft dentin layer beneath DEJ and may help to prevent the crack propagating into bulk dentin [10]. As will be shown later, this FGM layer will dramatically reduce the stress in the ceramic. However, it is important to note that the structure of the natural tooth (Fig. 3) is much more complex than the simple one-dimensional graded structure as suggested in Fig. 2c. Our simple model does not include these complexities, therefore represents a first step in the design of graded architectures that are inspired by the structure of the DEJ.

In an effort to explore the extent to which the stresses can be reduced by functionally graded architectures, finite element models of the bioinspired layers were developed. The layer architectures that were modeled are shown schematically in Fig. 2c. The Young's modulus of dental ceramic has been reported in a wide range from 65 GPa to 300 GPa [5], while that of dentin is in the range from 10 GPa to 30 GPa [11, 12], and that of the cement is 2–13 GPa [7]. The purpose of our simulation is to show the significance of the FGM architecture from the mechanics point of view, so we take Young's modulus of dental ceramic as 65 GPa, that of cement as 5 GPa, and that of dentin as 20 GPa, and the yield strength of the cement as 10 MPa [13] as an example.

The finite element simulations were carried out using the commercial finite element software, ABAQUS (Version 6.3, Hibbitt, Karlsson & Sorensen, Inc., Pawtucket, RI, 2002), adapting four-node axisymmetric elements. This was used to model the axisymmetric geometries shown schematically in Fig. 2. Ten layers were used to model the FGM layer. In the simulations, the thickness of the ceramic layer, FGM layer, cement layer and foundation layer are 1 mm, 0.1 mm, 0.1 mm and 2 mm, respectively. The diameter of the structure is 8 mm. The load applied on the dental multiplayer is 120 N, which is the typical chewing load. Since the measurements of DEJ modulus revealed an almost linear gradation [8, 9], the modulus across the graded interface was assumed to decrease linearly from 65 GPa to 48 GPa in the initial simulations. We will show later that this distribution most efficiently reduces the stress in the ceramic and FGM layer. The Poisson's ratios of each of the layers were assumed to be 0.3. This is clearly a simplification since FGMs are known to exhibit a range of Poisson's ratios. For comparison, simulations were also carried out on a natural tooth model (Fig. 2a) and a dental crown restoration model (Fig. 2d).

Fig. 4 Maximum principal stress distributions in dental multi-layered structures: (a) FGM design; (b) existing dental crown restoration; (c) natural tooth.



The results of the simulations of contact-induced deformation are presented in Fig. 4. As shown in prior studies [4], the existing dental crown restoration model gives rise to high stress concentrations (maximum principal stresses) in the dental ceramic, especially in the interfacial regions near the join layers (Fig. 4b). However, the stress is quite uniform in the FGM layer (Fig. 4a), which reduce the maximum stress in the ceramic and the FGM layer. The maximum principal stresses in the FGM model are reduced by ~30% in the case of the graded systems (Fig. 4a), but is still higher than those in natural tooth model (Fig. 4c).

If the Young's modulus of the FGM layer is high, the stress will be concentrated in the FGM layer at the interface between the FGM layer and the cement; if the Young's modulus of the FGM layer is low, the stress will be concentrated at the interface between the dental ceramic and the FGM layer. The optimal design should ensure the stress uniformly distributed in the FGM layer and continuous at the interface of ceramic and the FGM layer. Based on this design criteria, the Young's modulus in the FGM layer should decrease from that of the ceramic at the interface of ceramic and FGM layer to a lower value at the interface of the FGM layer and the cement layer. The optimal lower value can be obtained by finite element simulation. Figure 5 shows the maximum principal stresses in the ceramic and FGM layer as a function of the Young's modulus at the bottom surface of FGM layer. The Young's modulus of the FGM layer decreases from that of the ceramic, which is 65 GPa, to the

Table 1 Material properties used in analyses [5, 9]

	Enamel	Glass	Dicor-MGC	Dicor	Empress 2	Zirconia	Mark II
E (GPa)	65	72	60.58	74	104	208	56.36
K_c (MPa $\cdot \sqrt{m}$)	0.5–1.3	0.77	1.2	1.2	2.8	4.5	1.8

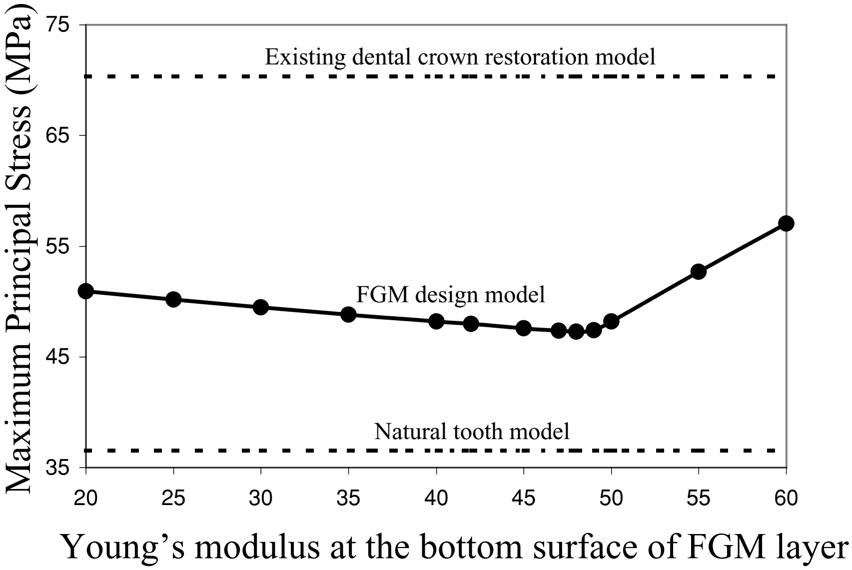


Fig. 5 Maximum principal stress in the ceramic and FGM layer

value indicated as the horizontal axis of Fig. 5. The trend of the curve is consistent with our understanding, and for this case, the Young's modulus distributed from 65 GPa to 48 GPa obtains the minimum stress in the ceramic and the FGM layer.

It is of interest to explore the effects of grading architecture (Fig. 6a) on the maximum principal stresses that were computed for the graded structures. Three kinds of distributions are simulated as shown in Fig. 6a. The results of the finite element simulations are presented in Fig. 6b. We can see that the Young's modulus distributions II and III give the lower stress in FGM layer, and the linear distribution also gives the low stress in the ceramic. This suggests that the optimal design is around linear gradation, which is consistent with the Young's modulus distribution in the DEJ.

We extend our simulations to a range of dental ceramics (Fig. 7) using material properties summarized in Table 1. In all of the cases, the graded architectures reduced the maximum principal stresses by ~30%. Such reductions in stress are likely to improve the durability of dental multi-layers with graded interlayers between the dentin and crown layers.

3 Critical crack length in functionally graded material layer design

It is of interest to examine the possible effects of pre-existing defects on sub-surface crack growth or fracture from its

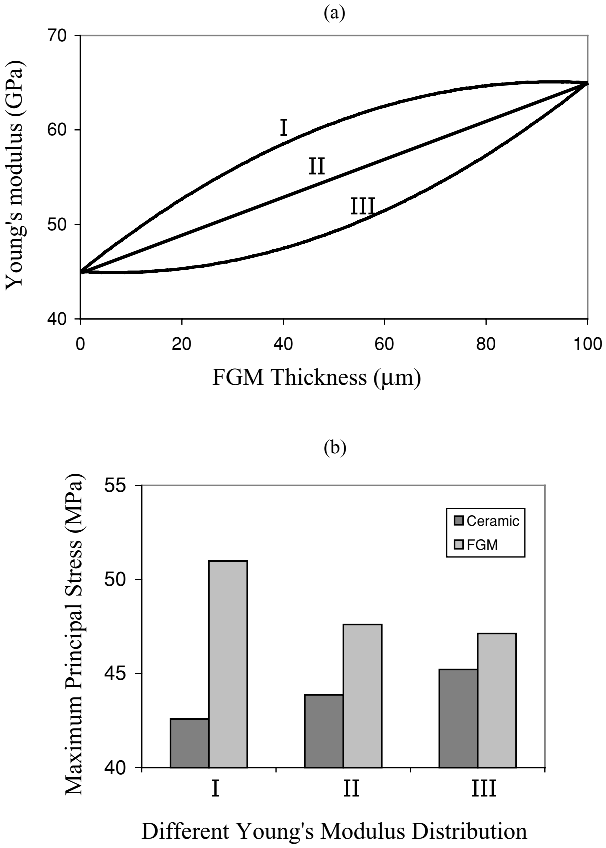
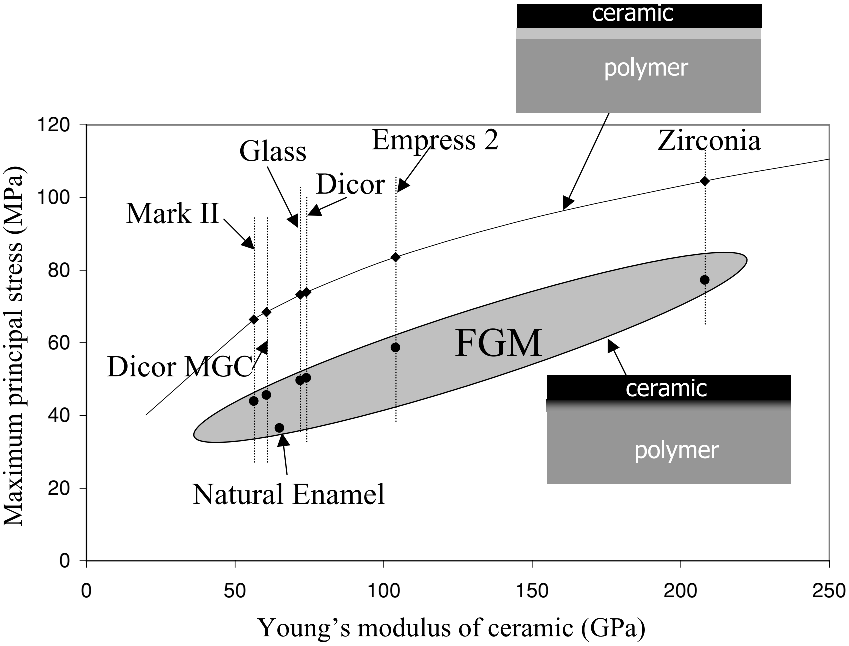


Fig. 6 The effects of Young's modulus distribution on the maximum stresses. (a) Young's modulus distribution in FGM layer; (b) corresponding maximum tensile stress in the top ceramic layer and FGM layer

Fig. 7 Maximum tensile stresses in different dental ceramics and their corresponding FGMs



interfacial regime (Fig. 8). Such cracks can be implicit in the material itself as induced by shaping as laboratory procedures prior to crown placement. New and improved techniques for accurate calculation of fracture parameters using graded finite elements for FGMs have been developed recently [14, 15]. However, in this paper we just use simple fracture mechanics approaches to estimate the critical crack length. Unstable crack growth occurs at a given crack length, a_c, when a critical stress intensity factor, K_c, of the ceramic is reached locally at the crack-tip. Assuming that the critical condition occurred when the crack-tip was located in the ceramic within an FGM structure, the critical crack length is thus given by [16]:

$$a_c = K_c^2 \big/ (\pi \beta^2 \sigma^2), \tag{1}$$

where K_c is the fracture toughness of the ceramic, β is a function of E_2/E_1, ν_1 and ν_2, E and ν are Young's modulus and Poisson's ratio, respectively. It is important to note that Eq. (1) is only valid for edge crack, but here we use it to estimate the critical crack length of radial crack. This approximation should not change the quantitative picture. Using the material properties summarized in Table 1, the critical crack lengths were estimated using Eq. (1). The stress, σ, is estimated by the maximum principal stress, which is plotted in Fig. 7.

The results are presented in Fig. 9 for selected dental materials. These show clearly that the critical crack lengths can be improved significantly by the use of functionally graded interlayers. For the polymer/ceramic FGMs that were considered in this study, the estimated critical crack lengths were much greater than those estimated for the natural tooth enamel-dentin complex. The estimated critical lengths were also much greater than those obtained for the existing dental crown restoration structures (Fig. 2b), as shown in Fig. 9. In particular, the FGMs consisting of Zirconia or Empress 2 had critical crack lengths (~2 mm) that were much greater than the range estimated for natural tooth structure. This suggests the possibility of engineering bioinspired functionally graded multi-layers that have comparable or better durability than those of natural teeth. Further work is needed to confirm the above speculations.

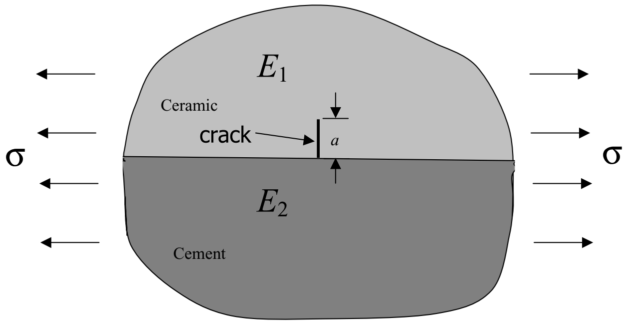


Fig. 8 Schematic of crack in top ceramic layer in dissimilar bi-layer system

Before closing, it is important to note here that Paulino and co-workers [17–19] have recently developed more accurate graded finite elements for the modeling of functionally graded materials (FGMs). Such models could clearly form the basis for future work to compute crack driving forces and better understand fracture processes in FGMs. They could

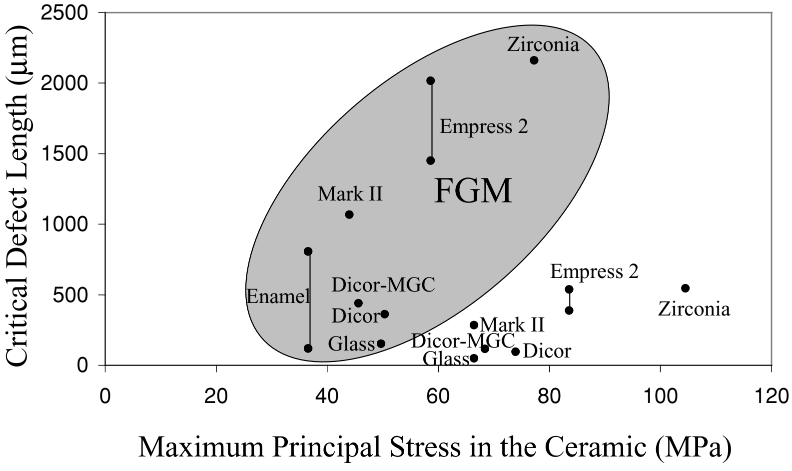


Fig. 9 Critical crack lengths versus maximum principal stresses in graded and tri-layered structures

also be applied to future bioinspired design along with nonlinear material laws that are beyond the scope of this paper.

4 Concluding remarks

This paper proposed to use a bioinspired functionally graded material layer to reduce the stress in the dental crown restoration structures. Finite element simulations show that this method can significantly reduce the stress and increase the critical crack length. This paper considers one-dimensional case, where the Young's modulus is only gradually distributed along thickness direction. This idea needs to be extended to two- and three-dimensional geometries. These include the modulus mapping of the cross-section of natural tooth by using nano-indentation technique and finite element simulation to obtain optimal design for actual dental crown structures. This paper provides new insights in designing the functionally graded crown to increase the durability of dental restorations.

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